The geometrical structure of quantum theory as a natural generalization of information geometry

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Abstract. Quantum mechanics has a rich geometrical structure which allows for a geometrical formulation of the theory. This formalism was introduced by Kibble and later developed by a number of other authors. The usual approach has been to start from the standard description of quantum mechanics and identify the relevant geometrical features that can be used for the reformulation of the theory. Here this procedure is inverted: the geometrical structure of quantum theory is derived from information geometry, a geometrical structure that may be considered more fundamental, and the Hilbert space of the standard formulation of quantum mechanics is constructed using geometrical quantities. This suggests that quantum theory has its roots in information geometry.

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INTRODUCTION

In the Schrödinger picture of non-relativistic quantum mechanics, the state of a particle is represented by a wave functions $\psi(x,t)$, where x are the coordinates of the configurations space and t is the time. The probability of finding the particle at position x and time t is given by the probability density $P = \psi^* \psi$. The evolution of the wave function is determined by the Schrödinger equation, $i\hbar\psi = -(\hbar^2/2m)\nabla^2\psi + V\psi$, where m is the mass of the particle and V a potential term. In the Hilbert space formulation of the theory, physical observables are represented by linear operators acting on wave functions and the Schrödinger equation takes the form of an operator equation, $i\hbar\psi = \hat{H}\psi$, where $\hat{H} = -(\hbar^2/2m)\nabla^2 + V$ is the Hamiltonian operator.

The Hilbert space formulation of quantum mechanics [1] is the standard one, but other alternative approaches are possible. The theory has a rich geometrical structure which allows for a geometrical formulation, introduced by Kibble [2] and later developed by a number of other authors. A review of the various geometrical formulations is beyond the scope of this paper. For a detailed but accessible description, see Ref. [3].

The usual approach has been to start from the standard description of quantum mechanics and identify the relevant geometrical features that can be used for the reformulation of the theory. Here this procedure is inverted: the geometrical structure of quantum theory is *derived* from information geometry, a geometrical structure that may be considered more fundamental, and the Hilbert space of the standard formulation of quantum mechanics is constructed using geometrical quantities.

The starting point of the analysis is very basic: A space of probabilities and the information metric, which defines a geometry known as information geometry. The next step is to take dynamics into consideration, via an action principle. Once this

is done, new geometrical structures which go beyond information geometry appear in a natural way. The description of dynamics in terms of an action principle in the Hamiltonian formalism introduces a doubling of the dimensionality of the space and a symplectic structure, and requirements of consistency between metric and symplectic structures lead to a complex structure and to a Kähler geometry. In this way, all the geometrical structure that is needed for the geometrical formulation of quantum theory is derived from information geometry. The procedure, which can be carried out for both continuous [4] and discrete [5, 6] systems, has a number of remarkable features: the complex structure appears by requiring consistency between metric and symplectic structures, wave functions arise as the natural complex coordinates of the Kähler space, and time evolution is described by a one-parameter group of unitary transformations. This suggests that quantum theory has its roots in information geometry.

The work presented here relies heavily on, and extends, work done in collaboration with M. J. W. Hall [4, 5].

INFORMATION GEOMETRY

Consider an *n*-dimensional configuration space, with coordinates $x \equiv \{x^1, ..., x^n\}$, and probability densities P(x) satisfying $P(x) \ge 0$ and $\int d^n x P(x) = 1$. Let the translation group *T* act on the probability densities, $T : P(x) \to P(x+\theta)$. There is a natural metric on the space of parameters, the Fisher-Rao metric [7], given in this case by

$$\gamma_{jk} = \frac{\alpha}{2} \int d^n x \frac{1}{P(x+\theta)} \frac{\partial P(x+\theta)}{\partial \theta^j} \frac{\partial P(x+\theta)}{\partial \theta^k},\tag{1}$$

where α is a constant. The line element $d\sigma^2 = \gamma_{jk}\Delta^j\Delta^k$ (where $|\Delta^k| \ll 1$) defines an infinitesimal distance between two probability distributions $P(x + \theta)$ and $P(x + \theta + \Delta)$.

The metric of Eq. (1) can also be written as a metric on configuration space. To do this, make the change of variables $x + \theta \rightarrow x$ and use $\frac{\partial P(x+\theta)}{\partial \theta^j} = \frac{\partial P(x+\theta)}{\partial x^j}$. The transformation puts the metric in the equivalent form

$$\gamma_{jk} = \frac{\alpha}{2} \int d^n x \frac{1}{P(x)} \frac{\partial P(x)}{\partial x^j} \frac{\partial P(x)}{\partial x^k}$$

The metric is now proportional to the Fisher information matrix. It will be convenient to use this form in what follows.

Finally, the line element $d\sigma^2 = \gamma_{jk} \Delta^j \Delta^k$ induces a line element in the space of probability densities,

$$ds^{2} = \frac{\alpha}{2} \int d^{n}x \frac{1}{P_{x}} \delta P_{x} \delta P_{x} = \int d^{n}x d^{n}x' g_{PP}(x,x') \delta P_{x} \delta P_{x'} , \qquad (2)$$

where I introduced the notation $P_x = P(x)$, $\delta P_x \equiv \frac{\partial P(x)}{\partial x^j} \Delta^j$. The line element of Eq. (2) was introduced by Jeffreys [8]. The induced metric g_{PP} , which is diagonal, is given by

$$g_{PP}(x,x') = \frac{\alpha}{2P_x} \delta(x-x').$$
(3)

DYNAMICS AND SYMPLECTIC GEOMETRY

Consider now probabilities P(x,t) that evolve in time. There are two constraints that must be satisfied at all times *t*: *P* must satisfy $\int d^n x P(x,t) = 1$, which means that the functional $I[P] = \int d^n x P(x,t)$ must be a constant of the motion, and $P(x,t) \ge 0$.

The problem of time evolution under these constraints is solved by deriving the equations of motion from an action principle. This is a reasonable *ansatz*: Constants of the motion like the functional *I* are often associated with invariance of a Lagrangian or Hamiltonian under particular types of transformations.

It will be convenient to write the equations of motion using a Hamiltonian formalism. To do this, introduce an auxiliary field *S* which is canonically conjugate to *P* and a corresponding Poisson bracket for any two functionals F[P,S] and G[P,S] given by

$$\{F_x, G_{x'}\} = \int d^n x'' \left(\frac{\delta F_x}{\delta P_{x''}} \frac{\delta G_{x'}}{\delta S_{x''}} - \frac{\delta F_x}{\delta S_{x''}} \frac{\delta G_{x'}}{\delta P_{x''}}\right),$$

where I introduced the compact notation $F_x = F[P_x, S_x]$ for functionals of *P* and *S*. The equations of motion of the fundamental variables is given by

$$\dot{P} = \{P, \mathscr{H}\} = rac{\delta \mathscr{H}}{\delta S}, \quad \dot{S} = \{S, \mathscr{H}\} = -rac{\delta \mathscr{H}}{\delta P},$$

where $\mathscr{H}[P,S]$ is the *ensemble Hamiltonian* that generates time translations.

The condition that I[P] is a constant of the motion takes the form $\{I, \mathcal{H}\} = 0$ or

$$\int dx \frac{\delta \mathscr{H}}{\delta S} = 0. \tag{4}$$

Consider the most general case in which the ensemble Hamiltonian can depend on P and S and their higher derivatives. Then [9]

$$\frac{\delta \mathscr{H}}{\delta S} = \frac{\partial \mathscr{H}}{\partial S} - \frac{\partial}{\partial x^{\mu}} \left[\frac{\partial \mathscr{H}}{\partial (\partial S / \partial x^{\mu})} \right] + \frac{\partial^2}{\partial x^{\mu} x^{\nu}} \left[\frac{\partial \mathscr{H}}{\partial (\partial^2 S / \partial x^{\mu} \partial x^{\nu})} \right] - \dots$$

After an integration by parts, Eq. (4) reduces to $\int dx \frac{\partial \mathscr{H}}{\partial S} = 0$. This must be satisfied regardless of the choice of *P* and *S*, thus $\frac{\partial \mathscr{H}}{\partial S} = 0$; i.e., \mathscr{H} can not be a function of *S*, it can only be a function of the derivatives of *S*. This implies the invariance of \mathscr{H} under the *gauge transformation*

$$S \to s + c,$$
 (5)

where c is a constant.

One can show that the condition $P(x,t) \ge 0$ is also satisfied at all times provided it is satisfied initially and *P* and the vector field that is associated with its time evolution satisfy some mild smoothness conditions (see the Appendix). Thus Hamiltonian evolution satisfies the necessary requirements provided \mathcal{H} is invariant under the gauge transformation of Eq. (5).

The main advantage of introducing a Hamiltonian formulation of dynamics rather that a Lagrangian formulation comes from the additional geometrical structure that is characteristic of the Hamiltonian formalism. As is well known, the Poisson bracket can be rewritten geometrically as

$$\{F,G\} = \int d^n x d^n x' \left(\delta P_x \ \delta S_x\right) \Omega(x,x') \left(\begin{array}{c} \delta P_{x'} \\ \delta S_{x'} \end{array}\right),$$

where Ω is the corresponding symplectic form, given in this case by

$$\Omega(x,x') = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \delta(x-x') .$$
(6)

A Hamiltonian description therefore leads to a symplectic structure and a corresponding *symplectic geometry* [10]. This has far reaching consequences.

KÄHLER GEOMETRY

The symplectic structure is defined over the whole phase space. The metric, however, is only defined over the subspace of probabilities *P*. This is unsatisfactory. Is it possible to extend the metric of Eq. (3) to define a metric over the complete space?

It can be done provided certain conditions which ensure the compatibility of metric and symplectic structures are satisfied (see the Appendix of Ref. [4] for a discussion). These conditions amount to requiring that the phase space have a Kähler structure. Thus the natural geometry of the space of probabilities in motion is a Kähler geometry.

A Kähler structure brings together metric, symplectic and complex structures in a harmonious way. To define such a space, introduce a complex structure J_b^a and impose the following conditions [11],

$$\Omega_{ab} = g_{ac}J^c_{\ b} , \qquad (7)$$

$$J^a_c g_{ab} J^b_d = g_{cd} , \qquad (8)$$

$$J^a_{\ b}J^b_{\ c} = -\delta^a_{\ c}. \tag{9}$$

Eq. (7) ensures compatibility between Ω_{ab} and g_{ab} , Eq. (8) is the condition that the metric should be Hermitian, and Eq. (9) ensures that J_b^a is a complex structure.

The metric over the subspace of probabilities is diagonal and given by $g_{PP}(x,x') = \frac{\alpha}{2P_x}\delta(x-x')$. Assume that the full metric g_{ab} is also diagonal; that is, of the form $g_{ab}(x,x') = g_{ab}(x)\delta(x-x')$ (this assumption corresponds to a *locality* assumption). Then g_{ab} is real and symmetric, of the form

$$g_{ab} = \begin{pmatrix} \frac{\alpha}{2P_x} & g_{PS} \\ g_{SP} & g_{SS} \end{pmatrix} \delta(x - x').$$

The elements $g_{PS} = g_{SP}$ and g_{SS} need to be determined using the Kähler conditions. The solution is given by [4]

$$g_{ab} = \begin{pmatrix} \frac{\alpha}{2P_x} & A_x \\ A_x & \frac{2P_x}{\alpha}(1+A_x^2) \end{pmatrix} \delta(x-x'), \quad J^a_b = \begin{pmatrix} A_x & \frac{2P_x}{\alpha}(1+A_x^2) \\ -\frac{\alpha}{2P_x} & -A_x \end{pmatrix} \delta(x-x'), \quad (10)$$

with Ω_{ab} as in Eq. (6). The functional A_x is not fixed by the Kähler conditions.

To determine A_x , it is convenient to look at the analogous but simpler formulation for the discrete case [5, 6]. Then, the functionals that define the Kähler conditions are replaced by finite dimensional matrices; in particular, the functional A_x is replaced by a matrix **A**.

In the case of a discrete configuration space, Čencov has shown that the information metric is the only metric that is invariant under a family of probabilistically natural mappings known as *congruent embeddings by a Markov mapping* [12]; see also Refs. [13, 14]. The Markov mappings introduced by Čencov play a crucial role in the proof of uniqueness of the information metric. A similar approach can be applied to the discrete version of the metric of Eq. (10). It turns out that the form of **A** can be determined by requiring invariance of the Kähler metric under a particular type of canonical transformation which extends the notion of a Markov mapping to the full phase space: The result is that **A** must be independent of the coordinates of the phase space and proportional to the the unit matrix [6].

Based on the analogy of the discrete case, I set $A_x = A$, where A is a constant. Whether mappings analogous to the Markov mappings introduced by Čencov in the discrete case can be formulated in the continuous case remains an open question.

COMPLEX COORDINATES AND WAVE FUNCTIONS

Up to now, I have made use of real coordinates P, S. Kähler geometry, however, is best expressed in terms of complex coordinates. I carry out a complex transformation that shows that the metric of Eq. (10) describes in fact a flat Kähler space.

Set $A_x = A$, where A is a constant, in Eqs. (10) and consider first the particular case A = 0. The tensors that define the Kähler geometry take the form

$$\Omega_{ab} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \delta(x - x'), \quad g_{ab} = \begin{pmatrix} \frac{\alpha}{2P_x} & 0 \\ 0 & \frac{2P_x}{\alpha} \end{pmatrix} \delta(x - x'), \quad J^a_{\ b} = \begin{pmatrix} 0 & \frac{2P_x}{\alpha} \\ -\frac{\alpha}{2P_x} & 0 \end{pmatrix} \delta(x - x').$$

Introduce now the Madelung transformation

$$\psi = \sqrt{P} \exp(iS/\alpha), \qquad \psi^* = \sqrt{P} \exp(-iS/\alpha),$$
(11)

which is a canonical transformation. A simple calculation shows that the tensors that define the Kähler geometry, expressed in terms of ψ , ψ^* , take the standard form which is characteristic of flat-space [11],

$$\Omega_{ab} = \begin{pmatrix} 0 & i\alpha \\ -i\alpha & 0 \end{pmatrix} \delta(x - x'), \quad g_{ab} = \begin{pmatrix} 0 & \alpha \\ \alpha & 0 \end{pmatrix} \delta(x - x'), \quad J^a_{\ b} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \delta(x - x').$$

Thus, when A = 0, there is a natural set of fundamental variables given by ψ and ψ^* . In terms of these variables, the tensors that define the Kähler geometry take their simplest form. If α is set equal to \hbar , these fundamental variables are precisely the *wave functions* of quantum mechanics. This is a remarkable result because it is based on geometrical arguments only. The derivation does not use any assumptions from quantum theory.

Consider now the more general case $A \neq 0$. The tensors that define the Kähler structure take the form

$$\Omega_{ab} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \delta(x - x'), g_{ab} = \begin{pmatrix} \frac{\alpha}{2P_x} & A_x \\ A_x & \frac{2P_x(1 + A_x^2)}{\alpha} \end{pmatrix} \delta(x - x'), J^a_b = \begin{pmatrix} A_x & \frac{2P_x(1 + A_x^2)}{\alpha} \\ -\frac{\alpha}{2P_x} & -A_x \end{pmatrix} \delta(x - x').$$

In this case, define the modified Madelung transformation

$$\phi = \sqrt{P} \exp\left[i\left(\Lambda S/\alpha - \gamma \ln \sqrt{P}\right)\right], \quad \phi^* = \sqrt{P} \exp\left[-i\left(\Lambda S/\alpha - \gamma \ln \sqrt{P}\right)\right], \quad (12)$$

where $\Lambda = 1/(1+A^2)$ and $\gamma = -A/(1+A^2)$. Once more, the tensors that define the Kähler geometry, expressed now in terms of ϕ , ϕ^* , take the standard form which is characteristic of flat-space,

$$\Omega_{ab} = \begin{pmatrix} 0 & i\frac{\alpha}{\Lambda} \\ -i\frac{\alpha}{\Lambda} & 0 \end{pmatrix} \delta(x-x'), \quad g_{ab} = \begin{pmatrix} 0 & \frac{\alpha}{\Lambda} \\ \frac{\alpha}{\Lambda} & 0 \end{pmatrix} \delta(x-x'), \quad J^a_{\ b} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \delta(x-x').$$

This shows that the geometry of the Kähler space is the same whether A = 0 or $A \neq 0$. In fact, it is possible to map one case to the other using an A-dependent canonical transformation. It is clear then that both cases lead to the same theory (provided one sets $\alpha = \hbar$ when A = 0 or $\frac{\alpha}{\Lambda} = \hbar$ when $A \neq 0$), and in the following sections I will set A = 0 and use the complex coordinates (wave functions) ψ and ψ^* .

The transformation that takes you from the coordinates of Eq. (11) to the coordinates of Eq. (12) is a particular case of a family of nonlinear gauge transformations introduced by Doebner and Goldin [15] (compare to their Eq. (2.2)). As pointed out by Doebner and Goldin, the theory that results from this particular family of nonlinear gauge transformations is physically equivalent to standard quantum mechanics. Here we arrive at the same conclusion, but now on the basis of the equivalence of the two cases A = 0 and $A \neq 0$ via a canonical transformation. One may therefore view the present derivation of the geometrical formulation of quantum mechanics as providing a new route to this family of Doebner-Goldin nonlinear gauge transformations.

HILBERT SPACE

One can now introduce a Hilbert space formulation. There is a standard construction which associates a complex Hilbert space with any Kähler space. Given two complex functions $\psi(x)$ and $\varphi(x)$, define the Dirac product by [2]

$$\begin{aligned} \langle \phi | \varphi \rangle &= \frac{1}{2} \int d^n x \left\{ (\phi, \phi^*) \cdot [g + i\Omega] \cdot \begin{pmatrix} \varphi \\ \varphi^* \end{pmatrix} \right\} \\ &= \frac{1}{2} \int d^n x \left\{ (\phi, \phi^*) \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + i \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \right] \begin{pmatrix} \varphi \\ \varphi^* \end{pmatrix} \right\} \\ &= \int d^n x \, \phi^* \varphi \end{aligned}$$

In this way, the Hilbert space structure of quantum mechanics follows from the Kähler geometry. This suggests that the Hilbert space structure of quantum mechanics is perhaps not as fundamental as its geometrical structure.

As is well known, the group of unitary transformations plays a fundamental role in quantum theory. To understand the role of the unitary group in the geometrical formulation presented here, it is convenient once more to look at the analogous but simpler formulation for the discrete case of an n-dimensional complex space [5, 6]. Since the

Kähler structure includes a symplectic structure, the group of symplectic transformations, Sp(2*n*,*R*), will play an important role in the theory. But the group of transformations of the theory can not be the full symplectic group due to the additional requirements that they have to satisfy. The first requirement is that they preserve the normalization of the probability. The second requirement is that the metric of the Kähler space be form invariant under the transformations. Requiring normalization of the probability and metric invariance leads to the group of rotations on the 2*n*-dimensional sphere, O(2*n*,*R*). Unitary transformations are the only symplectic transformations which are also rotations; i.e., Sp(2*n*,*R*) \cap O(2*n*,*R*)=*U*(*n*) [10]. Therefore, in the discrete case the group of unitary transformations *U*(*n*) is singled out, with time evolution being described by a one-parameter group of unitary transformations [5, 6]. An analogous results applies to the continuous case.

DISCUSSION

The geometry of quantum theory can be derived from information geometry, the natural geometry on the space of probabilities, using only a few assumptions. The derivation, which can be carried out for both the discrete and continuous cases, has a number of interesting features:

- Doubling of the dimensionality of the space (i.e., $\{P\} \rightarrow \{P,S\}$) from dynamical considerations,
- Complex structure from consistency between metric and symplectic structures,
- Wave functions as the natural complex coordinates of the Kähler space,
- Representation in terms of canonical transformations of a particular case of a family of Doebner-Goldin nonlinear gauge transformations,
- Time evolution described by a one-parameter group of unitary transformations,
- Hilbert space formulation expressed in terms of geometrical quantities associated with the Kähler space.

The derivation presented here relies heavily on, and extends, a geometrical reconstruction of quantum theory by Reginatto and Hall which takes information geometry as its starting point [4, 5]. Mehrafarin [16] and Goyal [17, 18] have also developed reconstructions of quantum theory using information-geometrical approaches. A detailed comparison to their approaches has not been carried out yet; however, one of the main differences is in the handling of *dynamics*, which plays a crucial role here. In particular, the use of an action principle to describe the dynamics of probabilities leads in a natural way to geometrical structure that goes beyond information geometry.

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APPENDIX

I look at the conditions that lead to $P(x,t) \ge 0$ when initially $P(x,0) \ge 0$.

Write the conservation of probability, $\int dx P(x,t) = 1$, as the continuity equation $\dot{P} + \nabla \cdot (P\vec{v}) = 0$, where $\vec{v}(x,t)$ is the vector field associated with the time evolution of *P*. For simplicity, consider the one-dimensional case,

$$\dot{P} = -\frac{\partial P}{\partial x}v - P\frac{\partial v}{\partial x}.$$
(13)

The case of interest is when $v \neq 0$, otherwise *P* is time independent. Taking the time derivative of Eq. (13) and replacing \dot{P} using once more Eq. (13), $\ddot{P}(x)$ can be expressed as

$$\ddot{P} = P\left[\left(\frac{\partial v}{\partial x}\right)^2 + v\frac{\partial^2 v}{\partial x^2} - \left(\frac{\partial v}{\partial x}\right)^2\right] + \frac{\partial P}{\partial x}\left[3v\frac{\partial v}{\partial x} - \dot{v}\right] + \frac{\partial^2 P}{\partial x^2}v^2.$$

I consider the case where $P|_{x=x_0} = 0$ at time t = 0 with $\frac{\partial P}{\partial x}|_{x=x_0} = 0$ and $\frac{\partial^2 P}{\partial x^2}|_{x=x_0} > 0$ (i.e., the point x_0 is a minimum of P). If the vector field v is sufficiently smooth so that $\frac{\partial v}{\partial x}$, \dot{v} and $\left(\frac{\partial v}{\partial x}\right)^{-1}$ remain finite, then $\dot{P}|_{x=x_0} = 0$ and $\ddot{P}|_{x=x_0} = \frac{\partial^2 P}{\partial x^2 v^2}|_{x=x_0} > 0$. Since $P|_{x=x_0} = 0$ at time t = 0, these relations imply that P does not become negative at a later time.

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