A geometric framework for mixed quantum states based on a Kähler structure

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Abstract
In this paper we introduce a geometric framework for mixed quantum states based on a Kähler structure. The geometric framework includes a symplectic form, an almost complex structure, and a Riemannian metric that characterize the space of mixed quantum states. We argue that the almost complex structure is integrable. We also in detail discuss a visualizing application of this geometric framework by deriving a geometric uncertainty relation for mixed quantum states. The framework is computationally effective and it provides us with a better understanding of general quantum mechanical systems.

Keywords: geometric quantum mechanics, symplectic geometry, Kähler manifold, mixed quantum states, quantum information

1. Introduction

Geometric quantum mechanics describes quantum mechanical systems based on their underlying geometrical structures [1–4]. Recently, it has been shown that such geometrical structures of quantum theory have profound information about foundations and the nature of the theory with many applications in quantum science and technology [5–9].

In geometric quantum mechanics the projective Hilbert space is constructed by general Hopf fibration of hypersphere and usually is called the quantum phase space of a pure quantum state. However, a pure state is a very limited class of quantum states, namely mixed quantum states. We know a lot about the geometry of pure quantum states but our knowledge are very limited when we consider mixed quantum states.

Recently, we have introduced a geometric framework for density operators based on fiber bundles which has lead to many interesting results such as a geometric phases, an uncertainty relations, quantum speed limits, a distance measure, and an optimal Hamiltonian [10–15]. Note the geometric framework that we introduce in this paper is different from the fiber bundles one.
In this paper we introduce a geometric framework for mixed quantum states based on a specific Kähler structure. The mathematical structure are well-known in the mathematical literature, but is almost unknown to physicists. In section 2 we introduce the geometric framework for mixed quantum states. We will in detail discuss Kirillov–Kostant–Souriau Kähler structure and the existence of an almost complex structure on quantum phase space of mixed states. We will also briefly discuss integrability of the almost complex structure. In section 3 we will apply our geometric framework to quantum systems by deriving a geometric uncertainty relation for mixed quantum states which is one of the most important topics that distinguish quantum physics from classical physics [14].

2. Geometric framework

There are three important geometries. The most well-known one is called Riemannian geometry which is defined to be the geometry of a positive-definite symmetric bilinear form. The Riemannian geometry is a well-developed subject and we will not further discuss it here in this text. Moreover, the geometry of a closed non-degenerate skew-symmetric bilinear form is called symplectic geometry. Finally, the geometry of a linear bundle map with square −1 is called almost complex geometry. A Kähler manifold is symplectic manifold which is equipped with an integrable almost complex structure.

In this section we introduce a new geometric framework for general finite dimensional quantum systems based on a specific Kähler structure which is called Kirillov–Kostant–Souriau Kähler structure. In the following text we will denote the identity map by 1 and we let $\mathbf{1}_n$ be the $n \times n$ identity matrix, and $\mathbf{0}_n$ is the $n \times n$ zero matrix.

2.1. The Kirillov–Kostant–Souriau Kähler structure

In the first step we will define Kirillov–Kostant–Souriau Kähler structure for the space of density operators. To do so we let $\mathcal{H}$ be an $n$-dimensional Hilbert space, $\text{Her}(\mathcal{H})$ be the space of Hermitian operators on $\mathcal{H}$, and the adjoint action of $U(\mathcal{H})$ on $\text{Her}(\mathcal{H})$

$$U(\mathcal{H}) \times \text{Her}(\mathcal{H}) \rightarrow \text{Her}(\mathcal{H}),$$

defined by

$$(U, \hat{A}) \mapsto \text{Ad}_U(\hat{A}) = U\hat{A}U^\dagger. \quad (2)$$

The manifold $\text{Her}(\mathcal{H})$ is diffeomorphic to the homogeneous space $U(n_1)/U(n_1) \times U(n_2) \times \cdots \times U(n_k)$. It is easy to show that $\text{Her}(\mathcal{H})$ is a flag manifold. A density operator on $\mathcal{H}$ is a member of $\text{Her}(\mathcal{H})$ whose eigenvalues are non-negative and sum up to 1. We write $D(\mathcal{H})$ for the space of density operators on $\mathcal{H}$. Note that, the adjoint action preserves $D(\mathcal{H})$, and the orbits of the action in $D(\mathcal{H})$ are in one-to-one correspondence with the possible spectra for density operators on $\mathcal{H}$. To be precise, two density operators belong to the same orbit if and only if they have the same spectrum. Given such a spectrum $\sigma$, we write $D(\sigma)$ for the corresponding orbit. In this section we introduce an $\text{Ad}$-equivariant Kähler structure on $D(\sigma)$ called the Kirillov–Kostant–Souriau Kähler structure [16]. We remind the reader that a Kähler structure is pair $(\omega, J)$ consisting of a symplectic structure $\omega$ and a complex structure $J$, and that associated to such a structure is a Hermitian inner product

$$h(X, Y) = \omega(X, JY) = i\omega(X, Y).$$

Note also that $(X, Y) \mapsto \omega(X, JY)$ is a Riemannian metric on $D(\mathcal{H})$. 

2
2.2. Representation of tangent vectors

Next we want to define representations of tangent vectors on the orbit of the adjoint action. Note that the adjoint action (2) is transitive, therefore for each density operator \( \rho \) we have a surjective linear map \( A_\rho : \text{Her}(\mathcal{H}) \rightarrow T_\rho D(\sigma) \) defined by

\[
A_\rho(\hat{H}) = \frac{1}{i\hbar} \left[ \hat{H}, \rho \right].
\]  

(4)

Note that, since the map \((X, Y) \mapsto \text{Tr}(XY)\) defines a bilinear form on \( u(n) \) which is non-degenerated and invariant under conjugation, the kernel of \( A_\rho(\hat{H}) \) is a subspace of \( u(n) \) which is the Lie algebra of the stabilizer of \( \rho \) for the group action \( U(n) \). We can also identify the Lie algebra \( u(n) \) with its dual \( u^*(n) \) which implies that the \( U(n) \) action on \( u(n) \) or \( H \) is adjoint or co-adjoint action. Thus \( \text{Her}(H) \) can be described by co-adjoint of \( u(n) \). The kernel of \( A_\rho \) consists of all Hermitian operators on \( H \) that commutes with \( \rho \), and we define a complementary space to \( \text{Ker} A_\rho \) as follows.

Let \( p_1 > p_2 > \cdots > p_k \) be the different eigenvalues in the spectrum of the density operator, \( \sigma \), and \( n_j \) be the multiplicity of \( p_j \). We can always find a basis in \( H \) relative which

\[
\rho = \text{diag}(p_1, p_2, \ldots, p_k).
\]

(5)

Moreover, the kernel of \( A_\rho \) consists of all those Hermitian operators \( \hat{A} \) which are represented by block diagonal matrices

\[
\hat{A} = \text{diag}(A_{11}, A_{22}, \ldots, A_{kk}),
\]

(6)

relative to this basis where each \( A_{jj} \) is an \( n_j \times n_j \) Hermitian matrix. We define the complementary space \( \text{Ker} A_\rho^\perp \) to consist of all the Hermitian operators that are represented by off-diagonal matrices

\[
\hat{B} = \begin{bmatrix}
0_{n_1} & B_{12} & B_{13} & \cdots & B_{1k} \\
B_{21} & 0_{n_2} & B_{23} & \cdots & B_{2k} \\
B_{31} & B_{32} & 0_{n_3} & \cdots & B_{3k} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
B_{k1} & B_{k2} & B_{k3} & \cdots & 0_{n_k}
\end{bmatrix}.
\]

(7)

Obviously, \( \text{Her}(H) = \text{Ker} A_\rho \oplus \text{Ker} A_\rho^\perp \), and \( A_\rho \) maps \( \text{Ker} A_\rho^\perp \) isomorphically onto \( T_\rho D(\sigma) \). Now we are in right position to define an almost complex structure on quantum phase space.

2.3. Almost complex structure

An almost complex structure on a manifold is an automorphism of its tangent bundle whose square equals \(-1\). Moreover, the almost complex structure is a complex structure if it is integrable, meaning that a rank two tensor, usually called the Nijenhuis tensor vanishes. We will discuss integrability of almost complex structure in the following text. Note also that manifolds that admit complex structures can be equipped with holomorphic atlases. That is, they are complex manifolds.

The orbit \( D(\sigma) \) does admit an \( \text{Ad} \)-invariant complex structure \( J \); we define an operator \( \hat{B} \mapsto j(\hat{B}) \) on \( \text{Ker} A_\rho \), where, if \( \hat{B} \) is given by (7), the operator \( j(\hat{B}) \) is given by
Now, the bundle map $J: \mathcal{T}D(\sigma) \to \mathcal{T}D(\sigma)$, defined by

$$j(\hat{B}) = \begin{bmatrix} 0_{n_1} & iB_{12} & iB_{13} & \ldots & iB_{1k} \\ -iB_{12}^\dagger & 0_{n_2} & iB_{23} & \ldots & iB_{2k} \\ -iB_{13}^\dagger & -iB_{23}^\dagger & 0_{n_3} & \ldots & iB_{3k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -iB_{1k}^\dagger & -iB_{2k}^\dagger & -iB_{3k}^\dagger & \ldots & 0_{n_k} \end{bmatrix}. \quad (8)$$

where $J$ satisfies $J^2 = -1$, as follows

$$J\left(\frac{1}{\hbar}[\hat{B}, \rho]\right) = \frac{1}{\hbar}[j(\hat{B}), \rho], \text{ e.g., for the matrix } \hat{B} = (B_{ij}) \text{ we have } j(\hat{B}) = (iB_{ij}).$$

and thus is an almost complex structure. Next we show that $J$ is integrable, and hence is a complex structure.

### 2.4. Integrability of $J$ on quantum phase space

We have derived an almost complex structure for the quantum phase space of mixed states. One important question concerning this almost complex structure is the integrability of $J$ which we will investigate in this section. An integrable almost complex structure has the structure of a complex analytic manifold. Let $J$ be an almost complex structure on our quantum phase space. A condition for integrability of $J$ is the following. We can associate a $(2, 1)$-tensor $N_J$ defined by

$$N_J[X, Y] = \frac{1}{\hbar}[j(\hat{B}), \rho], \quad J = \frac{1}{\hbar}[-\hat{B}, \rho] \Rightarrow J^2 = -1, \quad (10)$$

and thus is an almost complex structure. Next we show that $J$ is integrable, and hence is a complex structure.

#### Proposition 2.1.

Let $J$ be an almost complex structure on our quantum phase space $\mathcal{D}(\sigma)$. Then these two statements are equivalent

1. $J$ be an almost complex structure
2. $N_J = 0.$

For the proof and more information see [17–19]. In the next section we define the most important structure of the geometric framework.

### 2.5. Kähler structure

In this section we define Kirillov–Kostant–Souriau symplectic form and derive an explicit expression for Hermitian inner product on the quantum phase space $\mathcal{D}(\sigma)$. The Kirillov–Kostant–Souriau symplectic form on $\mathcal{D}(\sigma)$ is defined by
Theorem 2.2. The symplectic form $\omega$ (12) is non-degenerated and closed.

Proof. The symplectic form $\omega$ is non-degenerated since if we chose $\hat{A} = [\hat{B}, \rho]$ in equation (12) then $\text{Tr} \left( \hat{A} [\hat{B}, \rho] \right) \neq 0$ which implies that $\omega \left( \frac{1}{i\hbar} \left[ \hat{A}, \rho \right], \frac{1}{i\hbar} [\hat{B}, \rho] \right) \neq 0$. Next we will prove that the symplectic form $\omega \left( \frac{1}{i\hbar} \left[ \hat{A}, \rho \right], \frac{1}{i\hbar} [\hat{B}, \rho] \right)$ is closed, that is

$$d\omega \left( \frac{1}{i\hbar} \left[ \hat{A}, \rho \right], \frac{1}{i\hbar} [\hat{B}, \rho], \frac{1}{i\hbar} \left[ \hat{C}, \rho \right] \right) = 0,$$

for all $\hat{A}, \hat{B}, \hat{C} \in u(n)$ as follows. Let $\hat{A}, \hat{B}, \hat{C}$ be the fundamental vector fields representing $\frac{1}{i\hbar} \left[ \hat{A}, \rho \right], \frac{1}{i\hbar} [\hat{B}, \rho], \frac{1}{i\hbar} \left[ \hat{C}, \rho \right]$ respectively. Then we have

$$d\omega \left( \hat{A}, \hat{B}, \hat{C} \right) = \frac{1}{2} \left( \hat{A} \cdot \omega \left( \hat{B}, \hat{C} \right) - \hat{B} \cdot \omega \left( \hat{A}, \hat{C} \right) + \hat{C} \cdot \omega \left( \hat{A}, \hat{B} \right) \right) + \omega \left( \left[ \hat{A}, \hat{B} \right], \hat{C} \right) + \omega \left( \left[ \hat{B}, \hat{C} \right], \hat{A} \right) + \omega \left( \left[ \hat{C}, \hat{A} \right], \hat{B} \right) = 0,$$

since the last three terms vanish by the Jacobi identity and the first three terms also vanish by invariance of the symplectic form $\omega$. \hfill \Box

The importance of this form stems from the fact that if $A$ is the expectation value function of a Hermitian operator $\hat{A}$, that is $A(\rho) = \text{Tr}(\rho \hat{A})$, and $X_A$ is the Hamiltonian vector field associated with $A$, which is implicitly defined by the identity $dA(X) = \omega(X_A, X)$, then

$$X_A(\rho) = \frac{1}{i\hbar} \left[ \hat{A}, \rho \right].$$

(14)

Now, $(\omega, J)$ is a Kähler structure, and we define $h$ to be the associated Hermitian inner product,

$$h(X, Y) = \omega(X, JY) + i\omega(X, Y)$$

(15)

Theorem 2.3. Let $\hat{A}$ and $\hat{B}$ be two observables on the Hilbert space which are off-diagonal at $\rho$. Then we have

$$h(X_A(\rho), X_B(\rho)) = \frac{2}{\hbar} \sum_{i,j} (p_i - p_j) \text{Tr} \left( A^\dagger_{ij} B_{ij} \right),$$

where $A_{ij}$ and $B_{ij}$ are elements of $\hat{A}$ and $\hat{B}$ respectively.

Proof. To prove this theorem we note that $h(X_A(\rho), X_B(\rho))$ can be written as

$$h(X_A(\rho), X_B(\rho)) = \frac{1}{i\hbar} \text{Tr} \left( \left[ \hat{A}, j(\hat{B}) \right] \rho \right) + \frac{1}{\hbar} \text{Tr} \left( \left[ \hat{A}, \hat{B} \right] \rho \right)$$

$$= \frac{1}{i\hbar} \text{Tr} \left( \left[ \hat{A}, \left( \hat{B} - ij(\hat{B}) \right) \right] \rho \right)$$
Now, $\hat{B} - ij(\hat{B})$ is represented by the upper diagonal matrix

$$
\hat{B} - ij(\hat{B}) = 2 \begin{bmatrix}
0_{n_1} & B_{12} & B_{13} & \cdots & B_{1k} \\
0_{n_2} & 0_{n_2} & B_{23} & \cdots & B_{2k} \\
0_{n_3} & 0_{n_3} & 0_{n_3} & \cdots & B_{3k} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0_{n_k} & \cdots & \cdots & \cdots & 0_{n_k}
\end{bmatrix}
$$

which after some straightforward calculation give the following expression for the commutation between $\hat{A}$ and $\hat{B} - ij(\hat{B})$

$$
\left[ \hat{A}, \hat{B} - ij(\hat{B}) \right] = 2 \begin{bmatrix}
-\sum_{j=1} B_{ji}A_{ij} & * & * & \cdots & * \\
* & A_{i2}^+B_{i2} - \sum_{j=2} B_{i2}A_{ij}^+ & * & \cdots & * \\
* & * & \sum_{j=3} A_{i3}^+B_{i3} - \sum_{j=3} B_{i3}A_{ij}^+ & \cdots & * \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
* & * & * & \cdots & \sum_{j=k} A_{ik}^+B_{jk}
\end{bmatrix}
$$

Note that the stars represent expressions whose explicit forms need not be known. Thus we have

$$
h(X_A(\rho), X_B(\rho)) = \frac{2}{\hbar} \sum_{i<j} (p_i - p_j) \text{Tr}(A_{ij}^+B_{ij}).
$$

This end up the prove of our theorem.

The above result is very important in proof of a geometric uncertainty relation for mixed quantum states which we will consider in the following section.

### 3. Geometric uncertainty relation based on Kähler structure

In this section we derive a geometric uncertainty relation for mixed quantum states based on the geometric framework we have introduced in the pervious section. Let $\hat{A}$ be an observable on $\mathcal{H}$, and consider the uncertainty function

$$
\Delta A(\rho) = \sqrt{\text{Tr} \left( \rho \hat{A}^2 \right) - \text{Tr} \left( \rho \hat{A} \right)^2}.
$$

(16)

Now we will state the main result of this section in form of the following theorem.

**Theorem 3.1.** Let $\hat{A}$ and $\hat{B}$ be two observables on $\mathcal{H}$. Then we have

$$
\Delta A \Delta B \geq \frac{\hbar}{2} |h(X_A, X_B)|.
$$

(17)

**Proof.** To prove the theorem we first pick a $\rho$ and fix a basis, so that $\rho = \text{diag}(\rho_1, \rho_2, \ldots, \rho_k)$. Then the observable $\hat{A}$ has the following representation
\[
\hat{A} = \begin{bmatrix}
A_{11} & X_{12} & \cdots & X_{1k} \\
X_{12} & A_{22} & \cdots & X_{2k} \\
\vdots & \vdots & \ddots & \vdots \\
X_{1k} & X_{2k} & \cdots & A_{kk}
\end{bmatrix}.
\]

(18)

Then it is not difficult to derive the following expression for our density operator and observable

\[
\text{Tr}\left(\rho \hat{A}^2\right) = \sum_{i=1}^{k} p_i \text{Tr}\left(A_{ii}^2\right) + \sum_{i<j} \left(p_i + p_j\right) \text{Tr}\left(X_{ij}^\dagger X_{ij}\right),
\]

(19)

\[
\text{Tr}\left(\rho \hat{A}\right) = \sum_{i=1}^{k} p_i \text{Tr}\left(A_{ii}\right).
\]

(20)

Now by inserting these relations into the equation (16) we get

\[
\Delta A(\rho)^2 = \sum_{i=1}^{k} p_i \text{Tr}\left(A_{ii}^2\right) - \left(\sum_{i=1}^{k} p_i \text{Tr}\left(A_{ii}\right)\right)^2 + \sum_{i<j} \left(p_i + p_j\right) \text{Tr}\left(X_{ij}^\dagger X_{ij}\right)
\]

\[
= \left(\Delta \hat{A}^\perp\right)^2 + \sum_{i<j} \left(p_i + p_j\right) \text{Tr}\left(X_{ij}^\dagger X_{ij}\right)
\]

\[
\geq \sum_{i<j} \left(p_i - p_j\right) \text{Tr}\left(X_{ij}^\dagger X_{ij}\right)
\]

\[
= \frac{\hbar}{2} \left( X_A(\rho), X_A(\rho) \right),
\]

(21)

where we have decomposed \(\hat{A}\) as \(\hat{A} = \hat{A}^\parallel + \hat{A}^\perp\) and \(\Delta \hat{A}^\perp = \text{Tr}(\hat{A}^\perp \rho)\). Similarly we get \(\Delta B(\rho)^2 \geq \frac{\hbar}{2} \left( X_B(\rho), X_B(\rho) \right)\). Thus

\[
\Delta A(\rho)^2 \Delta B(\rho)^2 \geq \frac{\hbar^2}{4} \left( X_A(\rho), X_A(\rho) \right) \left( X_B(\rho), X_B(\rho) \right)
\]

\[
\geq \frac{\hbar^2}{4} \left[ h(\rho) \right]^2,
\]

(22)

where in the last step we have used the Schwarz inequality. By taking the square root of both sides of this equation we get (17). This end the proof of our geometric uncertainty relation for mixed quantum states.

□

Our geometric uncertainty relation are related to Robertson–Schrödinger uncertainty relation [20].

4. Conclusion

In this paper we have introduced a geometric framework for mixed quantum states based on a Kähler structure. We have explicitly defined the compatible triplet for our quantum phase space, namely a symplectic form, a Riemannian metric, and an almost complex structure. We have argued that our almost complex structure is integrable since the Nijenhuis tensor vanishes which also implies that our quantum phase space is a Kähler manifold. Finally we have
applied our geometric framework to a quantum system with two observables in order to derive a geometric uncertainty relation for quantum assembles. Our framework can be extended to the infinite dimensional case but this issue needs further investigation. The advantages of the geometric framework is its simplicity and effectiveness. We also believe that the geometric framework can be applied and tested for different quantum systems which also could give rise to very insightful results about quantum mechanics with many applications in the fields of quantum information, quantum computing, and quantum control.

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