Geometric uncertainty relation for quantum ensembles

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Abstract
Geometrical structures of quantum mechanics provide us with new insightful results about the nature of quantum theory. In this work we consider mixed quantum states represented by finite rank density operators. We review our geometrical framework that provide the space of density operators with Riemannian and symplectic structures, and we derive a geometric uncertainty relation for observables acting on mixed quantum states. We also give an example that visualizes the geometric uncertainty relation for spin-$\frac{1}{2}$ particles.

Keywords: uncertainty relation, mixed quantum states, geometry of quantum mechanics

Some figures may appear in colour only in the online journal

1. Introduction
The phase spaces of classical and quantum mechanical systems are symplectic manifolds, and in both cases observables give rise to symplectic flows [1–3]. However, quantum systems exhibit characteristics that have no classical counterparts. One is the impossibility to fully predict results of measurements. In classical mechanics, the results of the measurements are completely predictable. But in quantum mechanics the actual value of an observable cannot be known prior to measurement, and there is a lower bound to the precision with which values of pairs of observables can be known simultaneously which is called uncertainty principles or relations. Pioneering works on the uncertainty relation includes [4–8]. Recently, several other versions of the uncertainty relation were considered in [9–16]. The uncertainty relation not only is one of the most importance and central topic in foundations of quantum mechanics, but also it has many applications in quantum information [17–21]. In particular, the Robertson–Schrödinger uncertainty relation [7, 8] has been used to discriminate between entangled and separable states [22] and in the domain of discrete variables to distinguish pure states from mixed states [23].

The space of a pure quantum state is projective Hilbert space equipped with the Fubini–Study metric. The real and imaginary parts of the Fubini–Study metric equips the projective Hilbert space with Riemannian and symplectic structures. Ashtekar and Schilling [2] have shown that for observables acting on a system in a pure state, the Robertson–Schrödinger uncertainty relation [7, 8] can be expressed entirely in terms of the Riemann and Poisson brackets of the observable’s expectation value functions.

Recently, we introduced a geometric framework for density operators which have resulted in many interesting topics such as geometric phases, uncertainty relations, quantum speed limits, distance measure and a characterization of optimal Hamiltonians [24–28].

In this paper we discuss an uncertainty relation for mixed quantum states based on geometrical structures of the space of density operators which is a generalization of Ashtekar and Schilling [2]. Our geometric framework is a natural generalization of general Hopf bundle for pure quantum states, but it is somewhat more complicated than for the pure states. There are some recent works on geometric formulation of the uncertainty relation which are different from our approach which is based on deep intrinsic geometric structures of quantum phase space of density operators [29–31]. In section 2 we give an short introduction to our geometric framework for mixed quantum states, in section 3 we derive a geometric uncertainty relation, and in section 4 we apply the geometric uncertainty relation to a mixture of spin-$\frac{1}{2}$ particles.
2. Geometry of orbits of isospectral density operators

In this paper we consider finite dimensional quantum systems that evolve unitarily. The systems will be modeled on a Hilbert space $\mathcal{H}$ of unspecified dimension $n$, and their states will be represented by density operators. Now, the orbits of the left conjugation action of the unitary group $U(\mathcal{H})$ on the space of density operators on $\mathcal{H}$ are in one-to-one correspondence with the possible spectra for density operators on $\mathcal{H}$, whereby the spectrum of a density operator of rank $k$ we mean the decreasing sequence

$$
\sigma = (p_1, p_2, \ldots, p_k)
$$

of its, not necessarily distinct, positive eigenvalues. We fix $\sigma$, and write $D(\sigma)$ for the corresponding orbit of density operators.

To furnish $D(\sigma)$ with a geometry, let $\mathcal{L}(\mathbb{C}^k, \mathcal{H})$ be the space of linear maps from $\mathbb{C}^k$ to $\mathcal{H}$, and $P(\sigma)$ be the diagonal $k \times k$ matrix that has $\sigma$ as its diagonal. Now, we let

$$
S(\sigma) = \left\{ \Psi \in \mathcal{L}(\mathbb{C}^k, \mathcal{H}) : \Psi^* \Psi = P(\sigma) \right\},
$$

and define

$$
\pi: S(\sigma) \to D(\sigma), \quad \Psi \mapsto \Psi^* \Psi.
$$

Then $\pi$ is a principal fiber bundle with right acting gauge group

$$
U(\sigma) = \{ U \in U(k) : UP(\sigma)U^* = P(\sigma) \},
$$

whose Lie algebra is

$$
\mathfrak{u}(\sigma) = \{ \xi \in \mathfrak{u}(k) : \xi P(\sigma) = P(\sigma) \xi \}.
$$

We equip $\mathcal{L}(\mathbb{C}^k, \mathcal{H})$ with the Hilbert–Schmidt Hermitian product, and the Riemannian metric $G$ and the symplectic form $\Omega$ given by $2\hbar$ times the real and imaginary parts, respectively, of this product:

$$
G(X, Y) = \hbar \text{Tr} \left( X^* Y + Y^* X \right),
$$

$$
\Omega(X, Y) = -i\hbar \text{Tr} \left( X^* Y - Y^* X \right).
$$

We also equip $D(\sigma)$ with the unique metric $g$ that makes $\pi$ a Riemannian submersion.

The tangent bundle of $S(\sigma)$ can be decomposed as

$$
TS(\sigma) = VS(\sigma) \oplus HS(\sigma),
$$

where $VS(\sigma) = \text{Ker} d\pi$ is the vertical and $HS(\sigma) = TS(\sigma)^{\perp}$ is horizontal bundles of $TS(\sigma)$. Here $\perp$ denotes an orthogonal complement with respect to $G$. Vectors in $VS(\sigma)$ and $HS(\sigma)$ are called vertical and horizontal, respectively, and a curve in $S(\sigma)$ is called horizontal if its velocity vectors are horizontal.

The infinitesimal generators of the gauge group action yield canonical isomorphisms between $\mathfrak{u}(\sigma)$ and the fibers in $VS(\sigma)$:

$$
\mathfrak{u}(\sigma) \ni \xi \mapsto \Psi^* \in \text{ker} S(\sigma).
$$

Furthermore, $HS(\sigma)$ is the kernel bundle of the gauge invariant mechanical connection form $A_\Psi = I_\Psi J_\Psi$, where $I_\Psi: \mathfrak{u}(\sigma) \to \mathfrak{u}(\sigma)^*$ and $J_\Psi: T_\Psi S(\sigma) \to \mathfrak{u}(\sigma)^*$ are the moment of inertia and moment map, respectively

$$
I_\Psi \xi \cdot \eta = G(\Psi^* \xi, \Psi^* \eta), \quad J_\Psi(X) \cdot \xi = G(X, \Psi^* \xi).
$$

The moment of inertia is an adjoint-invariant form on $\mathfrak{u}(\sigma)$ which is independent of $\Psi$ in $S(\sigma)$. Thus it defines a metric on $\mathfrak{u}(\sigma)$:

$$
\xi \cdot \eta = \text{Tr} \left( (\xi^* \eta + \eta^* \xi) P(\sigma) \right).
$$

Using equation (10) we can derive an explicit formula for the connection form.

3. A geometrical uncertainty relation

The form $\Omega$ given by equation (6) is a symplectic form on $\mathcal{L}(\mathbb{C}^k, \mathcal{H})$. It follows from a result by Marsden and Weinstein [32, theorem 1], see [25], that there is a unique symplectic structure $\omega$ on $D(\sigma)$ such that $\pi^* \omega$ equals the restriction of $\Omega$ to $S(\sigma)$. For each observable $\hat{A}$ on $\mathcal{H}$, define the expected value function $A$ and associated Hamiltonian vector field $X_A$ on $D(\sigma)$ by

$$
A(\rho) = \text{Tr} \left( \hat{A} \rho \right), \quad dA = i_{X_A} \omega.
$$

Also, let $X_{A\hat{A}}$ be the gauge invariant vector field on $S(\sigma)$ defined by

$$
X_{A\hat{A}}(\Psi) = \frac{d}{d\epsilon} \left[ \exp \left( \frac{\epsilon}{i\hbar} A \right) \Psi \right]_{\epsilon=0}.
$$

Then $i_{X_{A\hat{A}}} \omega = dA$, which means that $X_{A\hat{A}}$ projects onto $X_A$.

Now, let $\hat{A}$ and $\hat{B}$ be two observables. The Poisson and Riemannian brackets of their expected value functions are $[A, B]_\omega = \omega(X_A, X_B)$ and $[A, B]_g = g(X_A, X_B)$. Let $\chi = 1/k \sqrt{2\hbar}$. Then

$$
A = \sqrt{\frac{\hbar}{2}} \chi \cdot \xi_A, \quad B = \sqrt{\frac{\hbar}{2}} \chi \cdot \xi_B.
$$

2
The estimate together with equation (15) implies

\[ \Delta A = \frac{\hbar}{2} \left( \{ A, B \}_{\hat{g}} + \xi_A \cdot \xi_B \right), \]

where \( \xi_A \) and \( \xi_B \) are the \( u(\sigma) \)-valued fields on \( D(\sigma) \) defined by \( \pi^B x_A = A = X_B \) and \( \pi^B x_B = A = X_B \). Thus we arrive at the following relation

\[ \Delta A = \frac{\hbar}{2} \left( \{ A, B \}_{\hat{g}} + \xi_A \cdot \xi_B \right), \]

where \( \xi_A \) and \( \xi_B \) are the projections of \( \xi_A \) and \( \xi_B \), respectively, on the orthogonal complement of \( \hat{g} \); see figure 1.

In the special case when \( B = A \)

\[ \Delta A^2 = \left( A, A \right) - AA \geq \frac{\hbar}{2} \{ A, A \}_{\hat{g}} (\rho). \]

Now, let \( X_A \) and \( X_B \) be the horizontal lifts of \( A \) and \( B \), respectively. Then the Cauchy–Schwarz inequality applied to the Hilbert–Schmidt Hermitian product gives

\[ G(X_A, X_B)G(X_A, X_B) \geq G(X_A, X_A)^2 + \Omega(X_A, X_B)^2. \]

It follows that

\[ \{ A, A \}_{\hat{g}} \{ B, B \}_{\hat{g}} \geq \{ A, B \}_{\hat{g}}^2 + \{ A, B \}_{\hat{g}}^2 \geq 0. \]

This estimate together with equation (15) implies

\[ \Delta A B \geq \frac{\hbar}{2} \left( \{ A, B \}_{\hat{g}}^2 + \{ A, B \}_{\hat{g}}^2 \right). \]

We have discussed and compared our geometric uncertainty relation with the Robertson–Schrödinger uncertainty relation in detail [25]. The advantages of our geometric uncertainty relation for mixed quantum states are the following. Our geometric uncertainty relation is based on solid and intrinsic geometrical structures of the underlying space of density operators. Moreover, for some class of observables our geometric uncertainty relation performs better than the Robertson–Schrödinger uncertainty relation. Since our geometric uncertainty relation depends on \( \xi_A \) and \( \xi_B \) which are intrinsic to the structures of the quantum phase space \( D(\sigma) \). Thus the application of our geometric uncertainty relation could give rise to some interesting results, e.g., in the field of quantum information processing. However, for a pure quantum state this geometric uncertainty relation coincides with one derived by Kibble [1].

4. Example

Consider an ensemble of electrons, so prepared that the proportion of electrons with spin up polarization is \( p_1 \) and the proportion with spin down polarization is \( p_2 \), and let \( S \) be the spin-\( \frac{1}{2} \) operator. If we model the spin part of the system on \( \mathbb{C}^2 \) in such a way that \( e_1 \) and \( e_2 \) represent the spin up and spin down states, respectively, then the state of the spin part of the ensemble’s wave function can be represented by the density operator \( \rho = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix} \) and the components of \( S \) are:

\[ \hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]

A lift of \( \rho \) to \( S(p_1, p_2) \) is \( \psi = \begin{pmatrix} \sqrt{p_1} & 0 \\ 0 & \sqrt{p_2} \end{pmatrix} \) and the infinitesimal generators of the first two components of \( S \), evaluated at \( \psi \), are

\[ X_{\psi}(\varphi) = \frac{1}{2\sqrt{p_1}} \begin{pmatrix} 0 & \sqrt{p_2} \\ \sqrt{p_1} & 0 \end{pmatrix}, \quad X_{\psi}(\varphi) = \frac{1}{2\sqrt{p_1}} \begin{pmatrix} 0 & -\sqrt{p_2} \\ \sqrt{p_1} & 0 \end{pmatrix}. \]

These vectors are horizontal if \( p_1 \neq p_2 \), and vertical if \( p_1 = p_2 \). Regardless, their projections to vectors at \( \rho \) are orthogonal. E.g., if \( p_1 \neq p_2 \) we have that

\[ \left\{ S_x, S_y \right\}_{\hat{g}} (\rho) = 2\hbar \Re \text{tr} \left( \frac{ip_1}{4} 0 0 -ip_2/4 \right) = 0. \]

Moreover, we have

\[ \left\{ S_x, S_y \right\}_{\hat{g}} (\rho) = 2\hbar \text{tr} \left( \frac{ip_1/4}{0 0 -ip_2/4} \right) = \frac{\hbar}{2} (p_1 - p_2). \]

Consequently

\[ \Delta S_{\psi}(\varphi) \Delta S_{\psi}(\varphi) \geq \frac{\hbar^2}{4} (p_1 - p_2). \]

This example visualizes our geometric uncertainty relation in its simplest form. However, it is a straightforward task to determine the relation for arbitrary density operators of rank \( k \) defined on a finite dimensional Hilbert space.

5. Conclusion

In this paper we have equipped the phase spaces of unitarily evolving quantum systems in mixed states, with Riemannian and symplectic structures, and we have derived a geometric uncertainty principle for observables acting on quantum systems in mixed states. We have briefly discussed and compared our geometric uncertainty relation with other approaches. We have also applied our geometric uncertainty relation to simple physical systems. Uncertainty relations have found many applications in the field of quantum information processing. The
rich geometric structure of our uncertainty relation indicates that it could have many applications in quantum information. However, these issues need further investigations.

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