Geometry of quantum evolution for mixed quantum states

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Abstract
The geometric formulation of quantum mechanics is a very interesting field of research which has many applications in the emerging field of quantum computation and quantum information, such as schemes for optimal quantum computers. In this work we discuss a geometric formulation of mixed quantum states represented by density operators. Our formulation is based on principal fiber bundles and purifications of quantum states. In our construction, the Riemannian metric and symplectic form on the total space are induced from the real and imaginary parts of the Hilbert–Schmidt Hermitian inner product, and we define a mechanical connection in terms of a locked inertia tensor and moment map. We also discuss some applications of our geometric framework.

Keywords: quantum dynamics, mixed quantum states, geometric quantum mechanics

1. Introduction
Ever since the advent of general relativity, scientists have been looking for geometrical principles underlying physical laws. Nowadays it is well known that geometry affects the physics on all length scales, and physical theory building consists to a large extent of geometrical considerations. This paper concerns geometric quantum mechanics, a branch of quantum physics that has received much attention lately—largely due to the crucial role geometry plays in quantum information and quantum computing. Here we equip the phase spaces for unitarily evolving finite level quantum systems with natural Riemannian and symplectic structures, and establish remarkable but fundamental relations between these and quantum theory. Important previous works on the geometrical formulation of quantum mechanics that should be mentioned in this context are the book by Bengtsson and Życzkowski [1] and the papers by Grabowski et al [2] and by Ashtekar and Schilling [3].

A quantum system prepared in a pure state is usually modeled on a projective Hilbert space, and if the system is closed its state will evolve unitarily in this space. The state of an experimentally prepared quantum system generally exhibits classical uncertainty, and is most appropriately described as a probabilistic mixture of pure states. It is common to represent mixed states by density operators, and many metrics on spaces of density operators have been developed to capture various physical, mathematical or information theoretical aspects of quantum mechanics [1, 4].

In this paper we discuss a geometrical framework for general quantum states represented by density operators on finite dimensional quantum systems. We show that our geometrical framework enable us to establish very important relations between abstract geometrical structures and general quantum systems which gives breakthrough insight in our understanding of the foundations of quantum mechanics and quantum information with many applications. In section 2 we give an introduction to our geometric framework for mixed quantum states, and in section 3 we discuss some recent applications of the framework such as operational geometric phases [5], a geometric uncertainty relation [6] and a dynamic distance measure [7]. This paper is based on [5–9].

2. Geometry of orbits of isospectral density operators
In this paper we will only be interested in finite dimensional quantum systems that evolve unitarily. They will be modeled on a Hilbert space $\mathcal{H}$ of unspecified dimension $n$, and their states will be represented by density operators. Recall that a density operator is a Hermitian, non-negative operator with unit trace. We write $\mathcal{D}(\mathcal{H})$ for the space of density operators on $\mathcal{H}$.

2.1. Riemannian structure on orbits of density operators
A density operator whose evolution is governed by a von Neumann equation remains in a single orbit of the left
conjugation action of the unitary group of \( \mathcal{H} \) on \( \mathcal{D}(\mathcal{H}) \). The orbits of this action are in one-to-one correspondence with the possible spectra for density operators on \( \mathcal{H} \), where by 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. Throughout this paper we fix \( \sigma \), and write \( \mathcal{D}(\sigma) \) for the corresponding orbit.

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

\[
\mathcal{S}(\sigma) = \{ \Psi \in \mathcal{L}(\mathbb{C}^k, \mathcal{H}) : \Psi^\dagger \Psi = P(\sigma) \}
\]

and define

\[
\pi : \mathcal{S}(\sigma) \to \mathcal{D}(\sigma), \quad \Psi \mapsto \Psi \Psi^\dagger.
\]

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

\[
\mathcal{U}(\sigma) = \{ U \in \mathcal{U}(k) : UP(\sigma) = P(\sigma)U \},
\]

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 \( \mathcal{S}(\sigma) \) with the Riemannian metric \( G \) and the symplectic form \( \Omega \) given by \( 2\pi \) times the real and imaginary parts, respectively, of this product

\[
G(X, Y) = \frac{1}{2} \text{Tr}(X^\dagger Y + Y^\dagger X),
\]

\[
\Omega(X, Y) = -\frac{1}{2i} \text{Tr}(X^\dagger Y - Y^\dagger X).
\]

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

### 2.2. Mechanical connection

The vertical and horizontal bundles over \( \mathcal{S}(\sigma) \) are the subbundles \( \mathcal{V}\mathcal{S}(\sigma) = \text{Ker} \pi_* \) and \( \mathcal{H}\mathcal{S}(\sigma) = \mathcal{V}\mathcal{S}(\sigma)^\perp \) of the tangent bundle of \( \mathcal{S}(\sigma) \). Here \( \pi_* \) is the differential of \( \pi \) and \( \perp \) denotes orthogonal complement with respect to \( G \). Vectors in \( \mathcal{V}\mathcal{S}(\sigma) \) and \( \mathcal{H}\mathcal{S}(\sigma) \) are called vertical and horizontal, respectively, and a curve in \( \mathcal{S}(\sigma) \) is called horizontal if its velocity vectors are horizontal. Recall that for every curve \( \rho \) in \( \mathcal{D}(\sigma) \) and every \( \Psi_0 \) in the fiber over \( \rho(0) \) there is a unique horizontal lift of \( \rho \) to \( \mathcal{S}(\sigma) \) that extends from \( \Psi_0 \). This lift and \( \rho \) have the same lengths because \( \pi \) is a Riemannian submersion.

The infinitesimal generators of the gauge group action yield canonical isomorphisms between \( \mathfrak{u}(\sigma) \) and the fibers in \( \mathcal{V}\mathcal{S}(\sigma) \)

\[
\mathfrak{u}(\sigma) \ni \xi \mapsto \Psi \xi \in \mathcal{V}\mathcal{S}(\sigma).
\]

Furthermore, \( \mathcal{H}\mathcal{S}(\sigma) \) is the kernel bundle of the gauge invariant mechanical connection form \( \mathcal{A}_\Psi = \mathcal{I}_\Psi^{-1} J_\Psi \), where \( \mathcal{I}_\Psi : \mathfrak{u}(\sigma) \to \mathfrak{u}(\sigma)^\ast \) and \( J_\Psi : T\Psi \mathcal{S}(\sigma) \to \mathfrak{u}(\sigma)^\ast \) are the moment of inertia and moment map, respectively,

\[
\mathcal{I}_\Psi \xi = G(\Psi \xi, \Psi \eta), \quad J_\Psi (X) \xi = G(X, \Psi \xi).
\]

The moment of inertia is of constant bi-invariant type since it is an adjoint-invariant form on \( \mathfrak{u}(\sigma) \) which is independent of \( \Psi \) in \( \mathcal{S}(\sigma) \). To be exact,

\[
\mathcal{I}_\Psi \xi \eta = \frac{1}{2} \text{Tr}((\xi^\ast \eta + \eta^\ast \xi) P(\sigma)).
\]

Using equation (4) we can derive an explicit formula for the connection form. Indeed, if \( m_1, m_2, \ldots, m_l \) are the multiplicities of the different eigenvalues in \( \sigma \), with \( m_1 \) being the multiplicity of the greatest eigenvalue, \( m_2 \) the multiplicity of the second greatest eigenvalue, etc and if for \( j = 1, 2, \ldots, l \),

\[
E_j = \text{diag}(0, \ldots, 0, m_{j-1}, 1, m_j, 0, m_{j+1}, \ldots, 0, m_l),
\]

then

\[
\mathcal{I}_\Psi \left( \sum_j E_j \Psi \dagger X E_j P(\sigma)^{-1} \right) \xi
\]

\[
= \frac{1}{2} \text{Tr} \left( \sum_j E_j X \dagger \Psi E_j \xi - \xi E_j \Psi \dagger X E_j \right)
\]

\[
= \frac{1}{2} \text{Tr} (X \dagger \Psi \xi - \xi \Psi \dagger X)
\]

\[
= J_\Psi (X) \xi
\]

for every \( X \) in \( T\Psi \mathcal{S}(\sigma) \) and every \( \xi \) in \( \mathfrak{u}(\sigma) \). Thus,

\[
\mathcal{A}_\Psi (X) = \sum_j E_j \Psi \dagger X E_j P(\sigma)^{-1}.
\]

Observe that the orthogonal projection of \( T\Psi \mathcal{S}(\sigma) \) onto \( V\Psi \mathcal{S}(\sigma) \) is given by the connection form followed by the infinitesimal generator given by equation (3). Therefore, the vertical and horizontal projections of \( X \) in \( T\Psi \mathcal{S}(\sigma) \) are \( X^\perp = \Psi \mathcal{A}_\Psi (X) \) and \( X^\parallel = X - \Psi \mathcal{A}_\Psi (X) \), respectively.

### 3. Applications of geometric framework for mixed quantum states

We have introduced a geometrical framework for mixed quantum states represented by density operators which has so far resulted in an operational geometric phase and higher order geometric phases, a geometric uncertainty relation, a dynamic distance measure and an energy estimate and a classification of optimal Hamiltonians for mixed quantum states. In this section we will briefly discuss these applications of our framework.

#### 3.1. Operational geometric phases for non-degenerate and degenerate mixed quantum states

Geometric phases are very important tools both in classical and quantum physics. Uhlmann [10–13] was among the
first to develop a theory for geometric phase for parallel transported mixed states. The theory is based on the concept of purification. Another approach to geometric phase for parallel transported non-degenerate mixed states, based on quantum interferometry, was proposed by Sjöqvist et al [14]. This phase has been verified in several experiments, and according to Slater [15] it generally yields different outcomes than that of Uhlmann.

Recently, we have introduced an operational geometric phase [5] for mixed quantum states based on spectral weighted traces of holonomies, and we have shown that it generalizes the interferometric definition of Sjöqvist et al. The operational geometric phase is a direct application of the Riemannian structure of our geometric framework. We also introduce higher order geometric phases for mixed quantum states. Our operational geometric phase applies to general unitary evolutions of non-degenerate and also degenerate mixed states. The operational geometric phase is defined by

\[ \gamma_{\rho}(\tau) = \arg \text{Tr}(\Psi_{\parallel}(\tau) \Pi(\rho) \Psi_{\parallel}(\tau)) = \arg \text{Tr}(\Psi_{\parallel}(0) \Psi_{\parallel}(\tau)), \]

where \( \Pi(\rho) \Psi_{\parallel} = \Psi_{\parallel}(\tau) \) and \( \Psi_{\parallel} \) is the horizontal lift of \( \rho \) extending from \( \Psi_{0} \):

\[ \Psi_{\parallel}(t) = \Psi(t) \exp\left(-\int_{0}^{t} A_{\Psi}(\tau) \, d\tau\right). \]

Here \( \exp_{\ast} \) is the positive time-ordered exponential. For more details about the construction of the operational geometric phase and higher order geometric phases we refer the reader to our recent paper [5].

3.2. Dynamic distance measure

Distance measures are very important tools in quantum information processing. Recently we have proposed a new distance measure for mixed quantum states that we call the dynamic distance measure. The dynamic distance measure is defined in terms of a measurable quantity, which make it very suitable for applications.

Let \( \rho_{0} \) and \( \rho_{1} \) be isospectral density operators and consider a von Neumann equation

\[ i\dot{\rho} = [H, \rho], \quad \rho(t_{0}) = \rho_{0}, \quad \rho(t_{1}) = \rho_{1}. \]

We define

\[ D(H, \rho_{0}, \rho_{1}) = \int_{t_{0}}^{t_{1}} \sqrt{\text{Tr}(H^{2}\rho) - \text{Tr}(H\rho)^{2}} \, dt, \]

provided \( H \) is such that a solution curve \( \rho \) to (8) exists, and we define the dynamic distance between \( \rho_{0} \) and \( \rho_{1} \) by

\[ \text{Dist}(\rho_{0}, \rho_{1}) = \inf_{H} D(H, \rho_{0}, \rho_{1}), \]

where the infimum is taken over all Hamiltonian \( H \) for which the boundary value problem (8) is solvable. In fact, it is the distance function associated with the metric \( g \). We have also compared our dynamic distance measure with the well-known Bures distance [16–19], and it turns out that the dynamic measure is bounded from below, but is in general not equal to, the Bures distance. The reason is that Uhlmann’s definition of parallel transport is different from ours.

4. Conclusion

Recently, we have used the framework presented in section 2 to derive a geometric uncertainty relation for observables acting on mixed quantum states. For pure states the uncertainty relation reduces to the geometric interpretation of the Robertson–Schrödinger uncertainty relation by Ashtekar and Schilling [3]. But in general the two relations are not equivalent. This is due to the multiple dimensions of the gauge group for general mixed states. More information about our result, especially a comparison with the Robertson–Schrödinger uncertainty relation, can be found in [6].

We have introduced a geometrical framework for general quantum states represented by density operators on finite dimensional quantum systems in mixed states that evolve unitarily. Our geometrical framework enable us to establish relation between geometrical structures and general quantum systems. This correspondence between geometry and quantum physics gives new insight in our understanding of the foundations of quantum mechanics and quantum information with many applications. We have shown that our geometric framework has already resulted in a new operational geometric phase and higher order geometric phases and a new dynamic distance measure. There are other applications of our framework that worth mentioning such as quantum speed limit and optimal quantum control for mixed quantum states. Unfortunately, there is no space left here to discuss these issues. Interested reader may see our paper [8] for further information and a detailed discussion of the subject. We believe our geometric framework could result in many other interesting applications in the field of quantum dynamics, quantum information, quantum computations, quantum control and quantum optics.

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References

[1] Bengtsson I and Życzkowski K 2008 Geometry of Quantum States—An Introduction to Entanglement (Cambridge: Cambridge University Press)
[2] Grabowski J, Ku M and Marmo G 2005 Geometry of quantum systems: density states and entanglement J. Phys. A: Math. Gen. 38 10217
[3] Ashtekar A and Schilling T A 1998 Geometrical formulation of quantum mechanics On Einstein’s Path ed A Harvey (Berlin: Springer) pp 23–65
[4] Nielsen M A and Chuang I L 2010 Quantum Computation and Quantum Information (Cambridge: Cambridge University Press)
[5] Andersson O and Heydari H 2013 Operational geometric phase for mixed quantum states New J. Phys. 15 053006
[6] Andersson O and Heydari H 2013 Geometric uncertainty relation for mixed quantum states, arXiv:1302.2074
[7] Andersson O and Heydari H 2013 Dynamic distance measure on spaces of isospectral mixed quantum states Entropy 15 3688–97
[8] Andersson O and Heydari H 2013 Geometry of quantum dynamics and a time–energy uncertainty relation for mixed states, arXiv:1302.1844
[9] Andersson O and Heydari H 2014 Geometrical structures of quantum phase space of mixed quantum states, in preparation
[10] Uhlmann A 1976 The ‘transition probability’ in the state space of a *-algebra Rep. Math. Phys. 9 273–9
[11] Uhlmann A 1986 Parallel transport and ‘quantum holonomy’ along density operator Rep. Math. Phys. 74 229–40
[12] Uhlmann A 1989 On Berry phases along mixtures of states Ann. Phys. 501 63–9
[13] Uhlmann A 1991 A gauge field governing parallel transport along mixed states Lett. Math. Phys. 21 229–36
[14] Sjöqvist E, Pati A K, Ekert A, Anandan J S, Ericsson M, Oi D K L and Vedral V 2000 Geometric phases for mixed states in interferometry Phys. Rev. Lett. 85 2845–9
[15] Slater P B 2002 Mixed state holonomies Lett. Math. Phys. 60 123–33
[16] Bures D 1969 An extension of Kakutani’s theorem on infinite product measures to the tensor product of semifinite w*-algebras Trans. Am. Math. Soc. 135 199–212
[17] Uhlmann A 1992 The metric of Bures and the geometric phase Groups and Related Topics (Mathematical Physics Studies vol 13) (Dordrecht: Kluwer) pp 267–74
[18] Dittmann J 1993 On the Riemannian geometry of finite dimensional mixed states Sem. S. Lie 3 73–87
[19] Dittmann J 1999 Explicit formulae for the Bures metric J. Phys. A: Math. Gen. 32 2663–70