Quantum Geometric Tensor for Mixed States Based on the Covariant Derivative

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The quantum geometric tensor (QGT) is a fundamental quantity for characterizing the geometric properties of quantum states and plays an essential role in elucidating various physical phenomena. The traditional QGT, defined only for pure states, has limited applicability in realistic scenarios where mixed states are common. To address this limitation, we generalize the definition of the QGT to mixed states using the purification bundle and the covariant derivative. Notably, our proposed definition reduces to the traditional QGT when mixed states approach pure states. In our framework, the real and imaginary parts of this generalized QGT correspond to the Bures metric and the mean gauge curvature, respectively, endowing it with a broad range of potential applications. Additionally, using our proposed mixed-state QGT, we derive the geodesic equation applicable to mixed states. This work establishes a unified framework for the geometric analysis of both pure and mixed states, thereby deepening our understanding of the geometric properties of quantum states.

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1. Introduction. The quantum geometric tensor (QGT), a crucial concept connecting quantum mechanics and geometry, has achieved increasing attention recently.[1–6] The study of the QGT is based on the projective Hilbert space,[7,8] which is defined as the set of density operators for pure states. When this space is equipped with a positive-definite Riemannian metric and a symplectic form, it manifests as a Kähler manifold.[8] The QGT combines these two geometric structures, thereby becoming a powerful tool for characterizing the geometric properties of quantum states.[9,10] To date, the QGT has played a crucial role in understanding numerous physical phenomena, such as superfluidity in flat bands,[11,12] orbital susceptibility,[13,14] excitonic Lamb shift,[15] the nonadiabatic anomalous Hall effect,[13] quantum phase transitions,[16,17] quantum fluctuations,[18] and topological matter.[19–21]

Traditionally, the QGT has been defined solely for pure states. This limitation restricts its application in practical scenarios where mixed states, arising from decoherence or finite-temperature effects, are inevitable. To address this limitation, significant efforts have been made to develop meaningful definitions for a mixed-state quantum geometric tensor (MSQGT). For example, based on the Uhlmann bundle,[22–24] an MSQGT was proposed with its real part corresponding to the well-known Bures metric[24] or quantum Fisher information matrix.[25] This metric, related to fidelity,[26,27] is widely used to quantify the distance between quantum states.[26–28] However, the imaginary part of this MSQGT invariably vanishes,[24] contrasting with the pure-state QGT,[9,10] whose imaginary part is the generally non-vanishing Berry curvature. Based on the Sjöqvist distance,[29–31] another type of MSQGT was introduced and can be regarded as the sum of the classical Fisher–Rao metric and the weighted pure-state QGT.[30] Although this type of MSQGT can be reduced to the pure-state QGT, its real part does not equal the Bures metric, thereby limiting its applications.

In order to overcome these limitations, we introduce a new definition of MSQGT based on the covariant derivative. This definition not only maintains consistency with the QGT for pure states but also features a real part that equals the Bures metric, thereby offering a wide range of potential applications. Furthermore, leveraging the advantages of the covariant derivative, the geodesic equation for the space measured by the Bures metric can be readily derived. Moreover, through a systematic investigation of the horizontal lift, we identify a new local gauge-invariant quantity with potential for experimental verification.

The rest of this paper is organized as follows. Section 2 introduces the purification bundle, based on the purification of mixed states, and defines its connection. In Section 3, we define the covariant derivative based on this connection. Utilizing the gauge transformation properties of the covariant derivative, we then provide the definition of our MSQGT and analyze the characteristics of its real and imaginary parts. A key advantage of our MSQGT, emphasized in Section 4, is its reduction to the traditional pure-state QGT as mixed states approach pure states. Section 5, as an important application of the covariant derivative, introduces a method for determining geodesics in the space measured by the Bures metric. In Section 6, we investigate the holonomy of closed curves and introduce a novel gauge-invariant quantity. Finally, Section 7 con-

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cludes this paper. Detailed derivations are provided in the Supplementary Materials (SM).

2. Definition of the Purification Bundle and Its Connection. For any mixed state of a quantum system S with dimension N, it is always possible to purify the state by incorporating an environment system E with the same dimension.[27] The purification of the mixed state ρ_S is represented by a pure state $|\psi\rangle$ for the combined system $S+E$, such that $\mathrm{Tr}_E(|\psi\rangle\langle\psi|) = \rho_S$. As stated by the Hughston–Jozsa–Wootters (HJW) theorem,[32] any two purifications of a density matrix can be connected by a unitary transformation acting on E.

As depicted in Fig. 1, the non-uniqueness of purification is naturally described within the framework of fiber bundle theory. Specifically, a bundle can be constructed by assigning the space of full-rank mixed states as the base manifold M, the space of purifications as the bundle manifold P, and the unitary group $\mathrm{U}(N)$ as the structure group. The projection map π: $P \to M$ is defined by the partial trace over the environment. Consequently, the fiber bundle constructed in this manner is termed the purification bundle. In this bundle, each fiber comprises all pure states of the composite system $S+E$ that reduce to the same mixed state; different points within a fiber are connected by a unitary operator acting on E.

Another essential concept in fiber bundle theory is the connection, which dictates how fibers are glued together. In the purification bundle, where the bundle manifold comprises pure states, it is possible to determine the connection through an inner product. For any pair of tangent vectors $|X\rangle$ and $|Y\rangle$ in the tangent space of the point $|\psi_p\rangle$ in the bundle manifold, we can define a new inner product as follows:

$$(|X\rangle, |Y\rangle) = \mathrm{Re}\langle X|Y\rangle\,, \tag{1}$$

where $\langle X|Y\rangle$ represents the standard Hilbert space inner product. We will establish the concept of horizontal vector based on this new inner product.

In the fiber bundle theory, a vertical curve is defined as a curve that lies along a fiber. Thus, by the HJW theorem, any vertical curve through $|\psi_p\rangle$ in the purification bundle can be locally generated by a Hermitian operator, i.e.,

$$C_V(t) = I_S \otimes \exp(\mathrm{i}H_E t)|\psi_p\rangle\,, \tag{2}$$

where H_E can be any Hermitian operator acting on E and t represents the curve's parameter. To simplify notation, we will omit I_S in the remainder of this paper. Since the vertical vector is the tangent vector of a vertical curve, any vertical vector at $|\psi_p\rangle$ can be written as

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} C_V(t) = \mathrm{i}H_E|\psi_p\rangle\,. \tag{3}$$

By combining the vertical vectors and the new inner product defined in Eq. (1), we can define the connection for the purification bundle. Specifically, for a general curve $|\psi(t)\rangle$, we can define its connection $\mathcal{A}_t$ by

$$\mathrm{i}\mathcal{A}_t|\psi(t)\rangle = (|\partial_t\psi(t)\rangle)_V\,, \tag{4}$$

where $|\partial_t\psi(t)\rangle$ denotes the tangent vector of the curve $|\psi(t)\rangle$ and $(|\partial_t\psi(t)\rangle)_V$ is its vertical component. According to Eq. (3), to ensure that $\mathrm{i}\mathcal{A}_t|\psi(t)\rangle$ is vertical, the connection $\mathcal{A}_t$ must be a Hermitian operator on the environment.

Based on Eq. (4), we can derive the expression for the connection. Since the inner product of a horizontal tangent vector with a vertical one is zero, we obtain

$$(\mathrm{i}H_E|\psi\rangle, |\partial_t\psi\rangle) = (\mathrm{i}H_E|\psi\rangle, \mathrm{i}\mathcal{A}_t|\psi\rangle)\,. \tag{5}$$

This identity must be satisfied for any Hermitian operator H_E acting on the environment. Utilizing the Schmidt decomposition, the state $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_{i=0}^{N-1} \sqrt{p_i}|\xi_i\rangle|v_i\rangle\,, \tag{6}$$

where $\{|\xi_i\rangle\}$ and $\{|v_i\rangle\}$ denote the orthonormal bases for S and E, respectively. Then any Hermitian operator acting on E can be decomposed as a real linear combination of the following operators: $h_{ik} = |v_i\rangle\langle v_k| + |v_k\rangle\langle v_i|$, $g_{ik} = \mathrm{i}|v_i\rangle\langle v_k| - \mathrm{i}|v_k\rangle\langle v_i|$, so that the set $\{h_{ik}, g_{ik}\}$ forms a basis for the space of Hermitian operators acting on E. Substituting this basis into Eq. (5) one obtains

$$\mathcal{A}_t = -\mathrm{i}\left(\sum_{i=0}^{N-1}|\partial_t v_i\rangle\langle v_i| + \sum_{i,k=0}^{N-1}\frac{2\sqrt{p_i p_k}}{p_i+p_k}\langle\xi_k|\partial_t\xi_i\rangle|v_i\rangle\langle v_k|\right). \tag{7}$$

To analyze how the connection transforms under local gauge transformations, consider applying a local gauge transformation to a given curve as follows:

$$|\psi(t)\rangle \to |\psi'(t)\rangle = U_E(t)|\psi(t)\rangle\,, \tag{8}$$

where $U_E(t)$ is a unitary operator acting on E. The new curve $|\psi'(t)\rangle$ has the Schmidt decomposition,

$$|\psi'(t)\rangle = \sum_{i=0}^{N-1}\sqrt{p_i}|\xi_i\rangle U_E(t)|v_i\rangle. \tag{9}$$

Inserting this result into Eq. (7) provides the local gauge transformation rule for the connection as

$$\mathcal{A}_t \to \mathcal{A}'_t = U_E(t)\mathcal{A}_t U_E^\dagger(t) - \mathrm{i}\partial_t U_E(t) U_E^\dagger(t)\,. \tag{10}$$

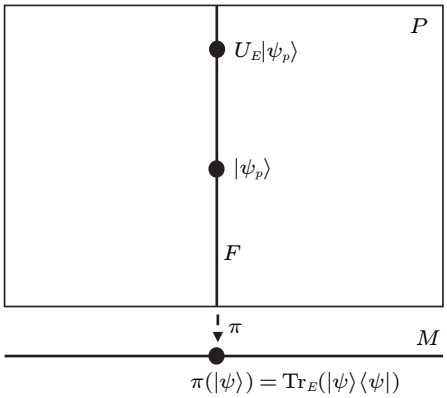

Fig. 1. Illustration of the purification bundle. P and M represent the bundle manifold and base manifold, respectively. π is the projection map. $|\psi_p\rangle$ and $U_E|\psi_p\rangle$ belong to the same fiber F in the bundle manifold. $|\psi\rangle$ represents any point that lies on the fiber F.

It is important to note that the expression for the connection in Eq. (7) presents significant challenges for numerical calculations. These challenges primarily stem from the fact that the Schmidt decomposition of $|\psi\rangle$ includes an inherent arbitrariness: for any phase ϕ_i, both $\mathrm{e}^{\mathrm{i}\phi_i}|\xi_i\rangle$ and $\mathrm{e}^{-\mathrm{i}\phi_i}|v_i\rangle$ remain valid Schmidt bases for $|\psi\rangle$. Consequently, the derivative of the Schmidt basis in Eq. (7) cannot be determined uniquely. To address this issue, we reformulate Eq. (7) into an expression that does not depend on the Schmidt decomposition,

$$\mathcal{A}_t = -\mathrm{i}\mathscr{L}_{(\mathrm{Tr}_S|\psi\rangle\langle\psi|)}[\mathrm{Tr}_S(|\partial_t\psi\rangle\langle\psi| - |\psi\rangle\langle\partial_t\psi|)]\,. \tag{11}$$

The operator function $\mathscr{L}$ in this equation is defined as

$$\mathscr{L}_\sigma(O) = \sum_{i,k}\frac{\langle i|O|k\rangle}{q_i+q_k}|i\rangle\langle k|\,, \tag{12}$$

where σ is any mixed state and $|i\rangle$ denotes an eigenstate of σ, with q_i being the eigenvalue associated with $|i\rangle$. The equivalence between Eq. (7) and Eq. (11) is demonstrated in SM.

Consider a curve $\rho(t)$ on the base manifold and a curve $|\psi(t)\rangle$ on the bundle manifold, where t denotes the curve parameter. If, for each t, the state $|\psi(t)\rangle$ purifies $\rho(t)$, we say that $|\psi(t)\rangle$ is a lift of $\rho(t)$. Moreover, if the tangent vector of $|\psi(t)\rangle$ remains horizontal at every point along the curve, then $|\psi(t)\rangle$ is called a horizontal lift. According to Eq. (4), the condition for a curve to be a horizontal lift is that its connection vanishes. For a horizontal lift $|\psi(t)\rangle$, the following relation holds:

$$\begin{aligned}\big(|\psi(t)\rangle, |\psi(t+\mathrm{d}t)\rangle\big) &= |\langle\psi(t)|\psi(t+\mathrm{d}t)\rangle| \\ &= F\big(\rho(t), \rho(t+\mathrm{d}t)\big)\,,\end{aligned} \tag{13}$$

where $F(A,B) = \mathrm{Tr}\Big(\sqrt{\sqrt{A}\,B\,\sqrt{A}}\Big)$ represents the fidelity between states A and B. A detailed derivation of Eq. (13) is provided in the SM.

3. Covariant Derivative and the Definition of the MSQGT. We define the covariant derivative $|D_t\psi\rangle$ as the horizontal component of a tangent vector. Based on Eq. (4), the covariant derivative can be expressed by

$$|D_t\psi\rangle = |\partial_t\psi\rangle - (|\partial_t\psi\rangle)_V = |\partial_t\psi\rangle - \mathrm{i}\mathcal{A}_t|\psi\rangle\,. \tag{14}$$

Suppose the mixed quantum states on the base manifold are parameterized by a set of parameters $\boldsymbol{x} = (x^1, x^2, ..., x^\mu, ..)^\top$. Then we can obtain that the covariant derivative shares properties similar to those of the ordinary derivative, including

$$D_\mu\langle\psi|\psi\rangle = \langle D_\mu\psi|\psi\rangle + \langle\psi|D_\mu\psi\rangle = 0, \tag{15}$$

$$\begin{aligned}D_\mu D_\nu\langle\psi|\psi\rangle &= \langle D_\mu D_\nu\psi|\psi\rangle + \langle\psi|D_\mu D_\nu\psi\rangle \\ &\quad + \langle D_\mu\psi|D_\nu\psi\rangle + \langle D_\nu\psi|D_\mu\psi\rangle = 0,\end{aligned} \tag{16}$$

where $D_\mu = \frac{\partial}{\partial x^\mu} - \mathrm{i}\mathcal{A}_\mu$ and the second-order covariant derivative is defined as

$$\begin{aligned}|D_\mu D_\nu\psi\rangle &= |\partial_\mu\partial_\nu\psi\rangle - \mathrm{i}\partial_\mu\mathcal{A}_\nu|\psi\rangle - \mathrm{i}\mathcal{A}_\nu|\partial_\mu\psi\rangle \\ &\quad - \mathrm{i}\mathcal{A}_\mu|\partial_\nu\psi\rangle - \mathcal{A}_\mu\mathcal{A}_\nu|\psi\rangle\,.\end{aligned} \tag{17}$$

Moreover, under the local gauge transformation in Eq. (8), the covariant derivative transforms as

$$|D_\mu\psi\rangle \to |D'_\mu\psi'\rangle = |\partial_\mu\psi'\rangle - \mathrm{i}\mathcal{A}'_\mu|\psi'\rangle = U_E(\boldsymbol{x})|D_\mu\psi\rangle. \tag{18}$$

Thus, the covariant derivative transforms in the same manner as $|\psi\rangle$, which makes it frequently used in constructing gauge-invariant quantities.

Utilizing the covariant derivative, we can develop a gauge-invariant metric for the base manifold. The metric is defined as

$$Q_{\nu\mu} = \langle D_\nu\psi|D_\mu\psi\rangle. \tag{19}$$

This metric is precisely our new MSQGT and its gauge invariance can be readily examined using Eq. (18). Substituting Eqs. (6) and (7) into this definition yields

$$\begin{aligned}Q_{\nu\mu} &= \sum_{i=0}^{N-1}\partial_\nu\sqrt{p_i}\,\partial_\mu\sqrt{p_i} + \sum_{i=0}^{N-1}p_i\langle\partial_\nu\xi_i|\partial_\mu\xi_i\rangle \\ &\quad - \sum_{i,k=0}^{N-1}\frac{4p_i^2p_k}{(p_i+p_k)^2}\langle\partial_\nu\xi_i|\xi_k\rangle\langle\xi_k|\partial_\mu\xi_i\rangle\,.\end{aligned} \tag{20}$$

A detailed derivation of this expression can be found in the SM.

Denote the real and imaginary parts of our MSQGT by g and σ respectively, then $Q_{\nu\mu} = g_{\nu\mu} + \mathrm{i}\sigma_{\mu\nu}$. It can be inferred that $g_{\nu\mu}$ is symmetric, whereas the $\sigma_{\nu\mu}$ is antisymmetric under the exchange of indices ν and μ, consistent with the pure-state QGT. The details of this derivation can be found in the SM. Considering the symmetry, the expression for the real part can be rewritten as

$$\begin{aligned}g_{\nu\mu} &= \sum_{i=0}^{N-1}\partial_\nu\sqrt{p_i}\,\partial_\mu\sqrt{p_i} + \sum_{i=0}^{N-1}p_i\mathrm{Re}\langle\partial_\nu\xi_i|\partial_\mu\xi_i\rangle \\ &\quad - \sum_{i,k=0}^{N-1}\frac{2p_ip_k}{p_i+p_k}\mathrm{Re}(\langle\partial_\nu\xi_i|\xi_k\rangle\langle\xi_k|\partial_\mu\xi_i\rangle).\end{aligned} \tag{21}$$

This expression coincides with that for the Bures metric.[25,33]

Similar to the pure-state QGT, the imaginary part of our MSQGT is closely related to the gauge curvature. The gauge curvature of the purification bundle is defined as the covariant exterior derivative of the connection,

$$T_{\mu\nu} = D_\mu\mathcal{A}_\nu - D_\nu\mathcal{A}_\mu = \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu - \mathrm{i}[\mathcal{A}_\mu, \mathcal{A}_\nu]\,. \tag{22}$$

Since $[D_\nu, D_\mu]|\psi\rangle = |D_\nu D_\mu\psi\rangle - |D_\mu D_\nu\psi\rangle = -\mathrm{i}(\partial_\nu\mathcal{A}_\mu - \partial_\mu\mathcal{A}_\nu)|\psi\rangle - [\mathcal{A}_\nu, \mathcal{A}_\mu]|\psi\rangle$ holds for any purification $|\psi\rangle$, one can establish the following relation between the covariant derivative and the curvature:

$$\mathrm{i}[D_\nu, D_\mu] = \partial_\nu\mathcal{A}_\mu - \partial_\mu\mathcal{A}_\nu - \mathrm{i}[\mathcal{A}_\nu, \mathcal{A}_\mu] = T_{\nu\mu}\,. \tag{23}$$

By combining this relation with Eqs. (6) and (7), we can derive that

$$\sigma_{\nu\mu} = \frac{1}{2}\langle\psi|\mathrm{i}[D_\mu, D_\nu]|\psi\rangle = \frac{1}{2}\langle\psi|T_{\nu\mu}|\psi\rangle\,. \tag{24}$$

The details of this derivation are provided in the SM. Hence, the imaginary part of the MSQGT corresponds to the mean gauge curvature.

Finally, it is noteworthy that while the expression for the MSQGT derived in Eq. (20) possesses theoretical significance, its practical utility for numerical computation is limited. This limitation originates from the inherent phase ambiguity in the eigenstates of a density matrix, which renders their derivatives non-unique. Therefore, directly calculating the MSQGT from Eq. (20) is not feasible, and an expression independent of this phase arbitrariness must be derived. Considering $\rho = \sum_i p_i|\xi_i\rangle\langle\xi_i|$, it can be easily shown that the MSQGT in Eq. (20) is equal to the following expression:

$$Q_{\nu\mu} = \sum_{i,k=0}^{N-1} \frac{p_i}{(p_i + p_k)^2} \langle\xi_i|\partial_\nu\rho|\xi_k\rangle\langle\xi_k|\partial_\mu\rho|\xi_i\rangle \,. \tag{25}$$

The proof is provided in the SM. Clearly, this expression is unaffected by phase arbitrariness, giving it a wider range of applications.

4. Relation between Mixed-State and Pure-State QGTs. Although Eqs. (20) and (25) were originally derived for full-rank density matrices, they can be asymptotically extended to pure-state cases. Specifically, when ρ approaches a pure state $|\xi_0\rangle\langle\xi_0|$, the MSQGT reduces to

$$Q_{\nu\mu} \to \langle\partial_\nu\xi_0|\partial_\mu\xi_0\rangle - \langle\partial_\nu\xi_0|\xi_0\rangle\langle\xi_0|\partial_\mu\xi_0\rangle \,, \tag{26}$$

which precisely reproduces the traditional pure-state QGT.[9,10] This agreement confirms the inherent consistency between our MSQGT and the pure-state QGT. A detailed derivation is provided in the SM.

To further investigate the relation, we explicitly compute the MSQGT for a qubit system under the following parametrization:

$$\rho(\theta,\phi) = \frac{I + \boldsymbol{r}\cdot\boldsymbol{\sigma}}{2} \,, \tag{27}$$

where I is the identity, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denotes the vector composed of the Pauli matrices, and $\boldsymbol{r} = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$ is a three-dimensional vector called the Bloch vector.

We first analyze the case with $r = 0.9$. Both the real and imaginary components of the MSQGT are numerically computed and presented in Fig. 2. Clearly, the real components of $Q_{\theta\phi}$ display symmetry ($\mathrm{Re}Q_{\theta\phi} = \mathrm{Re}Q_{\phi\theta}$) under the exchange of θ and ϕ, while the imaginary component of $Q_{\theta\phi}$ is antisymmetric ($\mathrm{Im}Q_{\theta\phi} = -\mathrm{Im}Q_{\phi\theta}$). The diagonal elements of the imaginary part of the MSQGT vanish ($\mathrm{Im}Q_{\theta\theta} = \mathrm{Im}Q_{\phi\phi} = 0$) due to the antisymmetry. Furthermore, the MSQGT exhibits ϕ-independence under this parametrization.

Finally, we compare the pure-state QGT and our MSQGT for various purities in Fig. 3 (only the θ-dependence is presented, as the QGT is independent of ϕ, as indicated in Fig. 2). Clearly, as the purity increases, the MSQGT approaches the traditional pure-state QGT. This confirms the theoretical prediction that the two definitions are consistent.

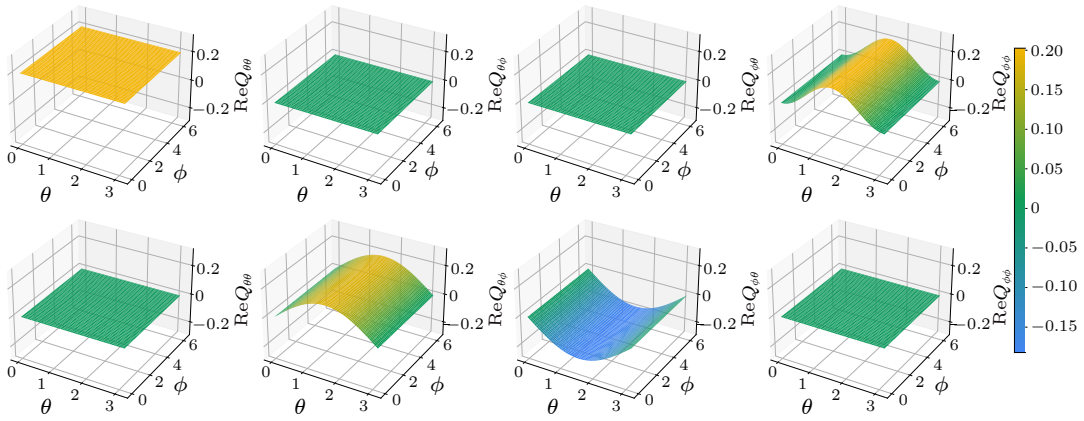

Fig. 2. Quantum geometric tensor for mixed qubit states with a fixed purity equal to 0.95.

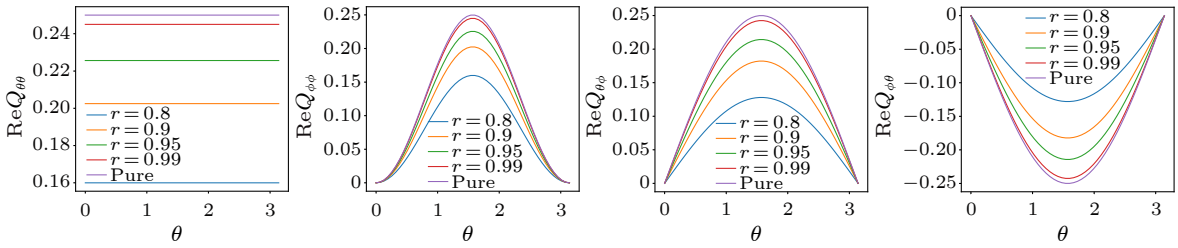

Fig. 3. Comparison between the MSQGT and pure-state QGT.

5. Geodesics under the Metric of the MSQGT. The real part of the newly defined MSQGT serves as the Bures metric on the base manifold. This naturally raises the question of how to determine geodesics with respect to the Bures metric. In this section, we derive the corresponding geodesic equation by exploiting the intrinsic properties of the covariant derivative and provide a general method to solve it.

Given an arbitrary curve $|\psi(t)\rangle$ on the bundle manifold with $t \in [0, T]$, its projection onto the base manifold has a length

$$l = \int_0^T \sqrt{g_{tt}\mathrm{d}t^2} = \int_0^T \sqrt{\langle D_t\psi|D_t\psi\rangle}\,\mathrm{d}t\,. \tag{28}$$

Varying the curve length yields

$$\begin{aligned}\delta l &= \int_0^T \frac{(\delta\langle D_t\psi|)|D_t\psi\rangle + \langle D_t\psi|(\delta|D_t\psi\rangle)}{2\sqrt{\langle D_t\psi|D_t\psi\rangle}}\mathrm{d}t \\ &= \int_0^T \frac{(|D_t\psi\rangle, \delta|D_t\psi\rangle)}{\sqrt{\langle D_t\psi|D_t\psi\rangle}}\mathrm{d}t\,.\end{aligned} \tag{29}$$

Given that the length is invariant under reparametrization, t can always be rescaled such that

$$\langle D_t\psi|D_t\psi\rangle = 1\,. \tag{30}$$

Therefore, it is sufficient to consider the variation

$$\delta l = \int_0^T (|D_t\psi\rangle, \delta|D_t\psi\rangle)\mathrm{d}t\,. \tag{31}$$

To ensure that $\delta l = 0$ for any $|\delta\psi\rangle$, $|\psi(t)\rangle$ must satisfy the condition

$$|D_tD_t\psi\rangle = -|\psi\rangle\,. \tag{32}$$

Details of this derivation are provided in the SM. This equation represents the geodesic equation under the Bures metric. It is important to note that this equation is valid only when the condition $\langle D_t\psi|D_t\psi\rangle = 1$ is satisfied. In the case where $|\psi\rangle$ is a horizontal lift with its connection vanishing, the geodesic equation can be further simplified to

$$|\partial_t\partial_t\psi\rangle = -|\psi\rangle, \quad \text{(for horizontal lift of geodesics)}. \tag{33}$$

The general solution to this equation is given by

$$|\psi(t)\rangle = \cos(t)|\psi(0)\rangle + \sin(t)\left|\psi\left(\frac{\pi}{2}\right)\right\rangle, \tag{34}$$

where $|\psi(0)\rangle$ and $|\psi(\pi/2)\rangle$ are constant quantum states whose determination requires appropriate boundary conditions.

Given two mixed states ρ_A and ρ_B separated by a Bures angle θ with $\theta < \pi/2$ (the geodesic connecting two points separated by $\pi/2$ is not unique), let $|\psi(t)\rangle$ denote the horizontal lift of the geodesic between them, and $|\psi(t_A)\rangle$ and $|\psi(t_B)\rangle$ be purifications of ρ_A and ρ_B, respectively. Without loss of generality, we can choose $t_A = 0$. To determine $|\psi(t)\rangle$ completely, we need to determine $|\psi(\pi/2)\rangle$. Since the Bures angle between two points equals the path length of the geodesic connecting them, according to Eqs. (28) and (30), we can obtain that

$$\theta = l(\rho_A, \rho_B) = \int_0^{t_B} \sqrt{\langle D_t\psi(t)|D_t\psi(t)\rangle}\,\mathrm{d}t = t_B\,. \tag{35}$$

So $t_B = \theta$. Combining these conditions, $|\psi(\pi/2)\rangle$ can be determined by solving the following equations:

$$\begin{aligned}&\mathrm{Tr}_E[|\psi(\theta)\rangle\langle\psi(\theta)|] = \rho_B, \\ &\mathrm{Tr}_S\left[|\psi(0)\rangle\left\langle\psi\left(\frac{\pi}{2}\right)\right| - \left|\psi\left(\frac{\pi}{2}\right)\right\rangle\langle\psi(0)|\right] = 0, \\ &\left[|\psi(0)\rangle, \left|\psi\left(\frac{\pi}{2}\right)\right\rangle\right] = 0.\end{aligned} \tag{36}$$

In these equations, the second equation ensures that $|\psi(t)\rangle$ is a horizontal lift and the third guarantees $\langle D_t\psi(t)|D_t\psi(t)\rangle = 1$. After solving $|\psi(\pi/2)\rangle$, the geodesic connecting ρ_A and ρ_B can be obtained by projecting $|\psi(t)\rangle$ onto the base manifold.

As an example, we consider a qubit system and discuss the shape of geodesics in its Bloch sphere representation. One possible solution of the geodesic equation is

$$\begin{aligned}|\psi(t)\rangle =& \cos(t)\Big(\sqrt{\frac{1+r}{2}}\,|00\rangle + \sqrt{\frac{1-r}{2}}\,|11\rangle\Big) \\ &+ \sin(t)\Big(-\sqrt{\frac{1-r}{2}}\,|00\rangle + \sqrt{\frac{1+r}{2}}\,|11\rangle\Big),\end{aligned} \tag{37}$$

where $|ij\rangle$ is the abbreviation of state $|i\rangle_S|j\rangle_E$, and r can be chosen as any number between 0 and 1. Projecting $|\psi(t)\rangle$ onto the base manifold yields

$$\rho(t) = \mathrm{Tr}_E(|\psi(t)\rangle\langle\psi(t)|) = \frac{I + \cos(2t+\varphi)\sigma_z}{2} \tag{38}$$

with $\cos\varphi = r$. Clearly, the geodesic described by $\rho(t)$ corresponds to the z-axis. Considering the spherical symmetry of the Bloch sphere, we conclude that all diameters of the Bloch sphere are geodesics.

Besides, another type of solution to the geodesic equation is

$$\begin{aligned}|\psi'(t)\rangle =& \cos(t)\Big(\sqrt{\frac{1+r}{2}}\,|00\rangle + \sqrt{\frac{1-r}{2}}\,|11\rangle\Big) \\ &+ \sin(t)\Big(\sqrt{\frac{1-r}{2}}\,|01\rangle + \sqrt{\frac{1+r}{2}}\,|10\rangle\Big).\end{aligned} \tag{39}$$

By projecting it to the base manifold, we can obtain another geodesic

$$\rho'(t) = \frac{I + \sin(2t)\sigma_x + r\cos(2t)\sigma_z}{2}\,. \tag{40}$$

The geodesic traced by $\rho'(t)$ forms an ellipse described by the equation

$$x^2 + \frac{z^2}{r^2} = 1, \quad \forall r \in (0, 1], \tag{41}$$

where x and z denote the x- and z-components of the Bloch vector corresponding to ρ'. Therefore, ellipses with a major axis length of 1 represent another category of geodesics in the Bloch sphere. It is important to note that diameters can also be considered as ellipses, characterized by a minor axis length of 0. It is an interesting finding that geodesics under the Bures metric are typically ellipses rather than great circular arcs. Reduction to circular arcs occurs only when the two states involved are both pure.

6. Holonomy in the Purification Bundle. As shown in Fig. 4, we consider a closed curve C on the base manifold. While the curve on the base manifold is closed, the starting and ending points of its horizontal lift typically do not

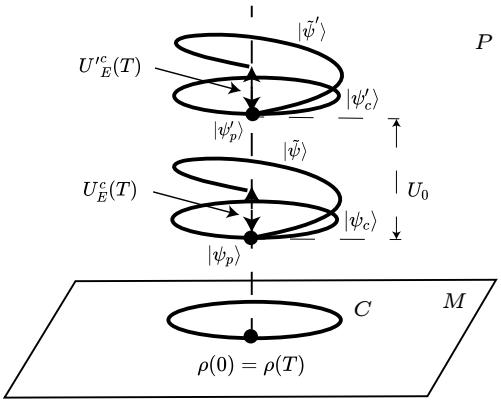

Fig. 4. Illustration of the holonomy associated with the closed curve C. The curves $|\tilde{\psi}\rangle$ and $|\tilde{\psi}'\rangle$ denote two horizontally lifted curves passing through the states $|\psi_p\rangle$ and $|\psi'_p\rangle$, respectively. Correspondingly, the holonomies associated with these horizontal lifts are denoted by $U^c_E(T)$ and $U'^c_E(T)$. The curves $|\psi_c\rangle$ and $|\psi'_c\rangle$ describe two closed reference curves passing through $|\psi_p\rangle$ and $|\psi'_p\rangle$, respectively and they differ by a constant unitary transformation U_0.

coincide. Instead, they differ by a unitary operator acting on E, referred to as the holonomy.

To obtain the expression for the holonomy, we select a closed reference path $|\psi_c(t)\rangle$ in the bundle manifold, with its projection being the closed curve C. Let us examine the horizontal lift of the curve C originating from $|\psi_c(0)\rangle$. As depicted in Fig. 4, we denote this horizontal lift as $|\tilde{\psi}(t)\rangle$, and it satisfies $|\tilde{\psi}(0)\rangle = |\psi_c(0)\rangle$. The distinction between $|\psi_c(t)\rangle$ and $|\tilde{\psi}(t)\rangle$ is represented by $U^c_E(t)$, i.e.,

$$|\tilde{\psi}(t)\rangle = U^c_E(t)|\psi_c(t)\rangle. \tag{42}$$

Using $\mathcal{A}^c_t$ and $\mathcal{A}_t$ to denote the connections related to curves $|\psi_c(t)\rangle$ and $|\tilde{\psi}(t)\rangle$, respectively. Referring to Eq. (10), it follows that

$$\mathcal{A}_t = U^c_E(t)\mathcal{A}^c_t U^c_E(t)^\dagger - \mathrm{i}\partial_t U^c_E(t) U^c_E(t)^\dagger . \tag{43}$$

Since $|\tilde{\psi}(t)\rangle$ is a horizontal lift, it implies that $\mathcal{A}_t = 0$. Therefore, we have

$$\mathrm{i}\partial_t U^c_E(t) = U^c_E(t)\mathcal{A}^c_t . \tag{44}$$

By solving this equation, we derive

$$U^c_E(T) = \left[\mathcal{P}\exp\left(\mathrm{i}\int_0^T \mathcal{A}^c_\tau \,\mathrm{d}\tau\right)\right]^\dagger , \tag{45}$$

where $\mathcal{P}$ represents the path ordering. Given that the reference curve is closed, we have $|\psi_c(0)\rangle = |\psi_c(T)\rangle$, where T represents the parameter corresponding to the ending point. According to Eq. (42), we can obtain that

$$|\tilde{\psi}(T)\rangle = U^c_E(T)|\psi_c(T)\rangle = U^c_E(T)|\psi_c(0)\rangle = U^c_E(T)|\tilde{\psi}(0)\rangle. \tag{46}$$

Clearly, $U^c_E(T)$ represents the transformation between the starting and ending points of the horizontal lift, thereby precisely characterizing the holonomy of the closed curve C. Importantly, it should be emphasized that the holonomy $U^c_E(T)$ does not depend on the choice of reference curve but is determined solely by the chosen horizontal lift. Since only one horizontal lift of a closed curve exists through a given point,[34] the holonomy $U^c_E(T)$ depends only on the starting point of the selected horizontal lift.

It is worth noting that the holonomy is not invariant under gauge transformations. To illustrate this, as depicted in Fig. 4, we choose an alternative reference closed curve given by $|\psi'_c(t)\rangle = U_0|\psi_c(t)\rangle$ in the bundle manifold to compute the holonomy, where U_0 is a t-independent unitary operator. Based on Eqs. (10) and (45), the holonomy for the horizontal lift passing through $|\psi'_c(0)\rangle$ is

$$\begin{aligned} U'^c_E(T) &= \left[\mathcal{P}\exp\left(\mathrm{i}\int_0^T U_0\mathcal{A}^c_\tau U_0^\dagger \,\mathrm{d}\tau\right)\right]^\dagger \\ &= U_0\left[\mathcal{P}\exp\left(\mathrm{i}\int_0^T \mathcal{A}^c_\tau \,\mathrm{d}\tau\right)\right]^\dagger U_0^\dagger \\ &= U_0 U^c_E(T) U_0^\dagger . \end{aligned} \tag{47}$$

The equation describes the gauge transformation law for the holonomy. It is noteworthy that in the U(1) gauge case, where U_0 is a complex number rather than a matrix, the holonomy becomes gauge-invariant and is recognized as the Aharonov–Anandan geometric phase.[35]

Although the holonomy is generally not gauge invariant, the mean holonomy (or overlap between the starting and ending points of a horizontal lift of a closed curve) is gauge-invariant. Its expression is

$$O_C = \langle\tilde{\psi}(0)|\tilde{\psi}(T)\rangle = \langle\tilde{\psi}(0)|U^c_E(T)|\tilde{\psi}(0)\rangle. \tag{48}$$

Under the gauge transformation of U_0, this quantity becomes

$$O'_C = \langle\tilde{\psi}(0)|U_0^\dagger U_0 U^c_E(T) U_0^\dagger U_0|\tilde{\psi}(0)\rangle = O_C . \tag{49}$$

Thus, the mean holonomy is indeed gauge-invariant. Its phase is known as the Uhlmann phase.[36]

7. *Conclusion.* In this paper, we propose a new definition for the MSQGT. Our MSQGT converges to the traditional pure-state QGT when mixed states approach pure states. Its real part corresponds to the well-known Bures metric, while its imaginary part corresponds to the mean gauge curvature. Furthermore, we derive the geodesic equation under the Bures metric and provide some solutions for qubit systems. Finally, we investigate the holonomy in the purification bundle and obtain a new gauge-invariant quantity. Our approach, based on the covariant derivative on the purification bundle, is a powerful tool for studying the gauge-invariant quantity and local geometrical properties of quantum states. This research enhances the understanding of the relationship between geometry and quantum mechanics and holds potential applications in diverse fields such as quantum information processing, quantum metrology, and quantum control. Future research is expected to focus on experimentally measuring the MSQGT and the mean holonomy related to a closed curve. Additionally, investigating the connections between the MSQGT and other fundamental concepts in quantum theory is a topic of further interest.

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