Quantized interlevel character in quantum systems

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A Quantized Inter-level Character in Quantum Systems

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For a quantum system subject to external parameters, the Berry phase is an intra-level property, which is gauge invariant module 2π for a closed loop in the parameter space and generally is non-quantized. In contrast, we define a inter-band character Θ for a closed loop, which is gauge invariant and quantized as integer values. It is a quantum mechanical analogy of the Euler character based on the Gauss-Bonnet theorem for a manifold with a boundary. The role of the Gaussian curvature is mimicked by the difference between the Berry curvatures of the two levels, and the counterpart of the geodesic curvature is the quantum geometric potential which was proposed to improve the quantum adiabatic condition. This quantized inter-band character is also generalized to quantum degenerate systems.

Introduction.— The study on time-dependent systems has greatly facilitated the exploration of novel physics [1–11]. In particular, the research of the quantum adiabatic evolution has led to a variety of important results, such as the quantum adiabatic theorem [12–14], the Landau-Zener transition [15, 16], the Gell-Mann-Low theorem [17], and the Berry phase and holonomy [18, 19]. It gives rise to many applications in quantum control and quantum computation [20–28]. Another noteworthy example is the Berry phase and the corresponding gauge structure, which have been applied to condensed matter physics on revealing novel phenomena, including the quantized charge pumping [29, 30], quantum spin Hall effect [31–33], quantum anomalous Hall effect [34], and electric polarization [35, 36].

The Berry phase equals the surface integral of the Berry curvature over an area enclosed by a loop in the parameter space, while the first Chern number corresponds to integrating the Berry curvature over a closed surface. According to the generalized Gauss-Bonnet theorem, the Chern number is quantized. The Chern number is very helpful in characterizing the topological phase different from the ordinary "phase" associated to the symmetry breaking of local order parameters. For example, the first Chern number characterizes the quantization of Hall conductance [37, 38]. The Berry phase also has a deep relation to the gauge field and differential geometry, where it is viewed as a holonomy of the Hermitian line bundle [19]. It can also be calculated by a line integral over a loop. The integration result is independent of the linear velocity on the loop, implying the geometric property of the Berry phase. Wilczek and Zee further introduced the non-Abelian Berry phase [39], a generalization of the original Abelian one [18]. The non-Abelian Berry phase is presented in the quantum degenerate system with a $U(N)$ gauge field, which also has a deep relation to the topology, such as the Wilson loop [40] and the second Chern number.

The Berry phase is a consequence of the projection of the Hilbert space to a particular level. Around a closed loop, its value actually is gauge dependent but remains invariant module 2π. On the other hand, the inter-level connection, i.e., the projection of the time-derivative of the state-vector of one level to that of another one, is not well-studied. An interesting application is the quantum geometric potential, which has been applied to modify the quantum adiabatic condition (QAC) [41], and its effect on quantum adiabatic evolution has been experimentally detected [42].

In this article, we construct a gauge invariant inter-level character Θ based on the quantum geometric potential. It is quantized in terms of integers, which can be viewed as a counterpart of the Euler characteristic number for a manifold with boundary. The Gauss-Bonnet theorem says that there are two contributions to the Euler characteristic numbers including the surface integral of the Gaussian curvature and the loop integral of the geodesic curvature along the boundary. The quantum geometric potential plays the role of the geodesic curvature, and the Berry curvature difference between two levels is the analogy to the Gaussian curvature. We also generalized the quantum geometric potential to the case of degenerate quantum systems, and the quantized character Θ can be constructed accordingly.

Gauge invariant in non-degenerate quantum systems — For non-degenerate quantum systems, an inter-level gauge invariant, referred as "quantum geometric potential", was introduced in literature [41]. Without loss of generality, we start with a non-degenerate N-level Hamiltonian $\hat{H}(\vec{\lambda}(t))$ controlled by a real l-vector $\vec{\lambda}(t) = \{\lambda_1(t), \lambda_2(t), \cdots, \lambda_l(t)\}$ as a function of time t. At each fixed t, a set of orthonormal eigenfunctions $|\phi_m(\vec{\lambda})\rangle$ associated with the eigenvalues $E_m(\vec{\lambda})$ are determined by $\hat{H}(\vec{\lambda})|\phi_m(\vec{\lambda})\rangle = E_m(\vec{\lambda})|\phi_m(\vec{\lambda})\rangle$, $(m = 1, 2, \cdots, N)$. The Berry connection for each energy level is defined as $\mathcal{A}^{\mu}_m = i\langle\phi_m(\vec{\lambda})|\partial_{\lambda_\mu}|\phi_m(\vec{\lambda})\rangle$ $(\mu = 1, 2, \cdots, l)$. Consequently, quantum geometric potential arises as,

$$\Delta_{\mathrm{ND},mn} = \mathcal{A}_n - \mathcal{A}_m + \frac{d}{dt}\arg\langle\phi_m|\dot{\phi}_n\rangle, \qquad (1)$$

where ND denotes the non-degenerate systems, and the "$\cdot$" illustrates the time-derivative. In addition, $\mathcal{A}_m \equiv$

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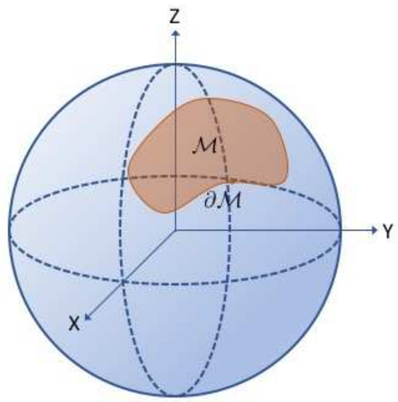

FIG. 1: The region $\mathcal{M}$ on the $\mathbb{S}^2$ Bloch sphere with a smooth boundary $\partial\mathcal{M}$.

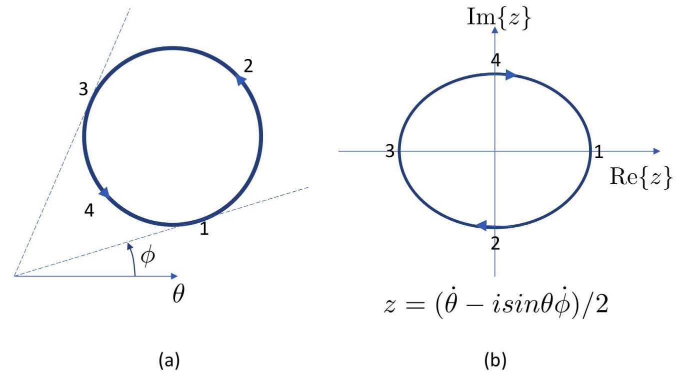

FIG. 2: (a) The top view of a closed curve on the Bloch sphere in the vicinity of the north pole. θ and ϕ represent the radial and angular coordinates, respectively. (b) The corresponding curve $z(t)$ in the complex plane with $z(t) = \langle\phi_+|\dot{\phi}_-\rangle = (\dot{\theta} - i\sin\theta\dot{\phi})/2$.

$\mathcal{A}^\mu_m\dot{\lambda}_\mu$ (in this paper the repeated indices imply the summation). The adiabatic solution to the time-dependent Schrödinger equation, $i\partial_t|\eta^a_m(\vec{\lambda}(t))\rangle = \hat{H}(\vec{\lambda}(t))|\eta^a_m(\vec{\lambda}(t))\rangle$ is

$$|\eta^a_m(t)\rangle = \exp\{-i\int_0^t E_m(\tau)d\tau\}|\tilde{\phi}^a_m(t)\rangle, \qquad (2)$$

with $|\tilde{\phi}^a_m(t)\rangle = \exp\{\int i\mathcal{A}_m dt\}|\phi^a_m(t)\rangle$, if the initial state $|\eta^a_m(0)\rangle = |\phi^a_m(0)\rangle$. Then $\Delta_{\mathrm{ND},mn}$ can be also defined as

$$\Delta_{\mathrm{ND},mn} = \frac{d}{dt}\arg\langle\tilde{\phi}_m|\dot{\tilde{\phi}}_n\rangle. \qquad (3)$$

$\Delta_{\mathrm{ND},mn}$ is gauge invariant under an arbitrary local $U(1)\otimes U(1)$ gauge transform with $|\phi_{m(n)}(t)\rangle \to e^{i\alpha_{m(n)}(t)}|\phi_{m(n)}(t)\rangle$ where $\alpha_{m(n)}(t)$ are smooth scalar functions. In the spin-$\frac{1}{2}$ system coupled to an external time-dependent magnetic field, Δ_{ND} is equivalent to the geodesic curvature of the path of the magnetic field orientation on the Bloch sphere, implying its geometric implications. When applying $\Delta_{\mathrm{ND},mn}$ to the time-dependent system, an improved QAC for the non-degenerate system can be established for $n \neq m$ [41],

$$\frac{\left|\langle\phi_m|\dot{\phi}_n\rangle\right|}{|E_m(t) - E_n(t) + \Delta_{\mathrm{ND},mn}(t)|} \ll 1, \qquad (4)$$

which indicates $E_m(t) - E_n(t) + \Delta_{\mathrm{ND},mn}(t)$ is more appropriate to describe the instantaneous energy gaps.

A quantized character in non-degenerate system— We introduce a new quantized gauge invariant character Θ based on the quantum geometric potential as an analogy to Gauss-Bonnet theorem with boundary. For simplicity, we begin with a two-level system controlled by a real 3-vector $\vec{\lambda}(t)$. At each time t, there exist a pair of eigenfunctions $|\phi_\pm(\vec{\lambda}(t))\rangle$ associated with the eigenvalues $E_\pm(\vec{\lambda}(t))$. Define $\omega = (\mathcal{A}^\mu_- - \mathcal{A}^\mu_+)d\lambda^\mu$, and $\mathcal{F} = d\omega$ with d being the exterior derivative. Explicitly, $\mathcal{F}$ is carried out as $\mathcal{F} = \mathcal{F}_- - \mathcal{F}_+$, where $\mathcal{F}_\pm = \frac{1}{2}F^{\mu\nu}_\pm d\lambda^\mu \wedge d\lambda^\nu$ with $F^{\mu\nu}_\pm = \partial^\mu\mathcal{A}^\nu_\pm - \partial^\nu\mathcal{A}^\mu_\pm$. A novel quantized character Θ is defined as

$$\begin{aligned} 2\pi\Theta &= \int_{\mathcal{M}}\mathcal{F} - \int_{\partial\mathcal{M}}\Delta_{\mathrm{ND}}dt \\ &= \Phi_+ - \Phi_- - \int_{\partial\mathcal{M}} d\,\arg\langle\phi_+|\dot{\phi}_-\rangle, \end{aligned} \qquad (5)$$

where Δ_{ND} is the gauge invariant in Eq. (1) for the non-degenerate systems, and $\Phi_\pm = \int_{\partial\mathcal{M}}\mathcal{A}^\mu_\pm d\lambda_\mu - \int_{\mathcal{M}}\mathcal{F}_\pm$. Since $\mathcal{F}$ and Δ_{ND} are both locally gauge invariant, Θ is also gauge invariant.

To show the quantization of Θ, we first consider a simple example of a two-level problem with the Hamiltonian $\hat{H}(t) = B\hat{n}(t)\cdot\vec{\sigma}$. Here $\hat{n}$ is a 3D unit vector, and the whole parameter space is the Bloch sphere. If $\hat{n}(t)$ concludes a region $\mathcal{M}$ on the Bloch sphere with a smooth boundary $\partial\mathcal{M}$ (Fig. 1), then Θ is quantized. Consider the transition term $\langle\phi_+|\dot{\phi}_-\rangle$ from the ground state to the excited state, which is a complex number. The corresponding $\mathcal{F}$ is the Berry curvature difference between the ground and excited states. To explicitly calculate Θ, we can work in a give gauge that $|\phi_-(\theta,\phi)\rangle = (\sin\frac{\theta}{2}e^{-i\phi}, -\cos\frac{\theta}{2})^T$ and $|\phi_+(\theta,\phi)\rangle = (\cos\frac{\theta}{2}e^{-i\phi}, \sin\frac{\theta}{2})^T$. Under this gauge, $\Phi_+ = 2\pi$ if $\partial\mathcal{M}$ encloses the north pole, and $\Phi_- = -2\pi$ if it encloses the south pole. Otherwise $\Phi_\pm = 0$. Meanwhile $\arg\langle\phi_+|\dot{\phi}_-\rangle = \arg\Big((\dot{\theta} - i\sin\theta\dot{\phi})/2\Big)$. When $\vec{\lambda}(t)$ completes a close loop $\partial\mathcal{M}$, correspondingly, $z(t) = \langle\phi_+|\dot{\phi}_-\rangle$ defines a close curve in complex plane. The winding number of $z(t)$ relative to the origin is defined as $W[z] = \int_{\partial\mathcal{M}} d\,\arg\langle\phi_+|\dot{\phi}_-\rangle$ as shown in Fig. 2. If $\partial\mathcal{M}$ does not enclose the north or south pole, $\Phi_\pm$ do not contribute, and $W[\langle\phi_+|\dot{\phi}_-\rangle]$ contributes -2π, such that $\Theta = 1$. After a similar analysis for other situations, one can conclude that $\Theta = 1$ for any region $\mathcal{M}$ on the sphere.

For a general non-degenerate model, we can define the quantized character Θ between any two different energy

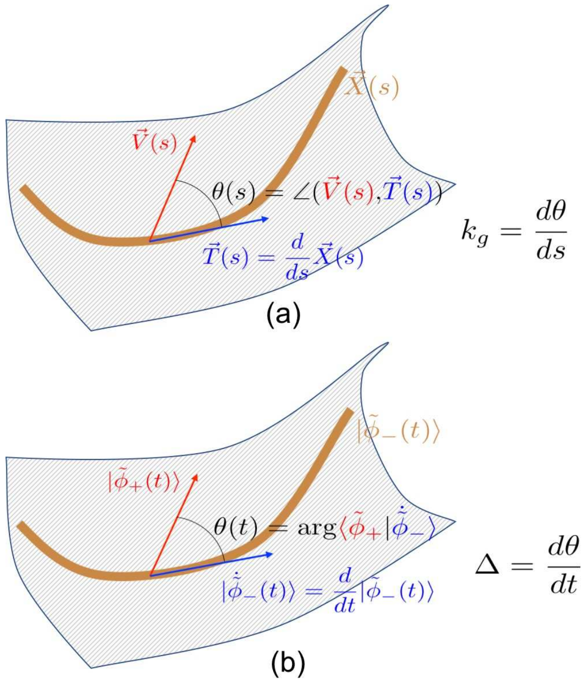

FIG. 3: (a) A curve $\vec{X}(s)$ is plotted on a 2D manifold (shaded area) in the 3D real space. $\vec{V}(s)$ lives in the tangent space, and is parallelly transported along the curve. $\vec{T}(s) = \frac{d}{ds}\vec{X}(s)$ is the velocity vector, and θ is the angle between $\vec{V}$ and $\vec{T}$. The geodesic curvature $k_g = d\theta/ds$. (b) The trajectory of $|\tilde{\phi}_-(t)\rangle$ is sketched in the Hilbert space. $|\tilde{\phi}_+(t)\rangle$ is a parallelly transported "tangent" vector along the "curve". $|\dot{\tilde{\phi}}_-(t)\rangle$ is the velocity vector, which is the derivative of of the "curve". The gauge invariant $\Delta = d\theta/dt$, where $\theta = \arg\langle\tilde{\phi}_+|\dot{\tilde{\phi}}_-\rangle$.

levels $E_\pm$ associated with a closed curve in the parameter space. According to the Stokes theorem, $\Phi_\pm$ count the singularities of Berry connections $\mathcal{A}^\mu_\pm$ in the region $\mathcal{M}$, e.g. the number of the Dirac strings, hence, they are quantized. The winding number of $z(t)$ relative to the origin is also quantized. Therefore, Θ is quantized for any situation.

Below we demonstrate the similarities between the quantized character Θ and the Euler number in the Gauss-Bonnet theorem. For a 2D compact Riemannian manifold $\mathcal{M}$ with a smooth boundary $\partial\mathcal{M}$, the Gauss-Bonnet theorem reads

$$\int_{\mathcal{M}} G dA + \int_{\partial\mathcal{M}} k_g ds = 2\pi\chi(\mathcal{M}), \tag{6}$$

where G, k_g and $\chi(\mathcal{M})$ are the Gaussian curvature, geodesic curvature of $\partial\mathcal{M}$, and the Euler number of $\mathcal{M}$, respectively. For quantum systems (e.g. a spin-1/2 problem in an external magnetic field), each point in the parameter space has an associated Hilbert space, i.e., the bundle. The Gauss-Bonnet theorem is generalized to characterize the bundle by the Chern number.

The gauge invariant Δ_{ND} defined in Eq. (1) is the analogy to the geodesic curvature k_g in Eq. (6). To explain this, we plot a curve $\vec{X}(s)$ on a 2D manifold in $\mathbb{R}^3$ as shown in the Fig. 3a, which is parameterized by the arc length s. $\vec{X}(s)$ represents the displacement vector for a point on the curve, then k_g is a geometric quantity depending on both the manifold and the curve. The geodesic curvature k_g reflects the deviation of the curve from the local geodesics. Choose a vector function $\vec{V}(s)$ living in the tangent space at the position $\vec{X}(s)$ and is parallelly transported along the curve. Then $k_g = d\theta/ds$, where θ is the angle between the velocity vector $\vec{T} = d\vec{X}/ds$ and $\vec{V}(s)$.

The similarity between Δ_{ND} and k_g is illustrated in Fig. 3 b. Following Eq. 3, the trajectory of $|\tilde{\phi}_-(t)\rangle$, which has taken into account the Berry phase, is viewed as a curve with the parameter time t in the Hilbert space. $|\dot{\tilde{\phi}}_-(t)\rangle$ is the analogy of the "tangent" vector, and $|\tilde{\phi}_+(t)\rangle$ corresponds to the parallel-transported vector field along the curve. Consequently, the gauge invariant term $\Delta_{\mathrm{ND}} = d\theta/dt$ is the time derivative of the angle $\theta = \arg\langle\tilde{\phi}_+|\dot{\tilde{\phi}}_-\rangle$ over time. Therefore, Eq. (5) can be viewed as a quantum analogy to the Gauss-Bonnet theorem described in Eq. (6).

Recall the proof of the Gauss-Bonnet theorem in differential geometry, we can observe the similarity to our theorem described in Eq. (5). To prove the Gauss-Bonnet theorem, one first decompose the geodesic curvature into two parts. One is the derivative of the angle between the velocity vector $\vec{T}$ and the local coordinates, which contributes an integer winding number when the curve $\vec{X}$ completes a loop since $\vec{T}$ has to come back to itself. The other part is a loop integral of a 1-form. Through the Stokes theorem, it equals the negative of the surface integral of the Gaussian curvature. Hence, this proof scheme is very similar to the proof to the quantization of Θ defined in Eq. (5).

There exist fundamental differences between the gauge invariant Δ_{ND} and the usual Berry connection. The integral of Δ_{ND} over a close loop is gauge invariant and single-valued. In contrast, the Berry connection is *not* gauge invariant locally, and the Berry phase for a closed loop evolution is gauge invariant but multiple valued module 2π. The Berry connection and the Berry phase are intra-subspace quantities associated with one energy level, while Δ_{ND} is an inter-subspace property associated with two different energy levels.

A quantized character in degenerate systems — The gauge invariant quantized character Θ studied above can also be extended to the degenerate systems. For this purpose, the gauge invariant Δ_{ND} is generalized to the case with degeneracy, which is defined between two eigenspaces associated with two different degenerate energy levels. We first consider a special case that a Hamiltonain $\hat{H}(\vec{\lambda})$ possessing N energy levels $E_m(\vec{\lambda})$ ($m = 1, 2, \cdots, N$), each of which is L-fold degenerate. The situation for energy levels possessing different degeneracies is discussed in Appendix C.

For each energy level m, there is a set of instantaneous orthonormal eigenstates $|\phi_m^a(\vec{\lambda})\rangle$, satisfying $\hat{H}(\vec{\lambda})|\phi_m^a(\vec{\lambda})\rangle = E_m(\vec{\lambda})|\phi_m^a(\vec{\lambda})\rangle$ ($a = 1, 2, \cdots, L$). If the system evolves adiabatically starting from the initial state $|\eta_m^a(\vec{\lambda}(0))\rangle = |\phi_m^a(\vec{\lambda}(0))\rangle$, then the adiabatic solution to the time-dependent Schrödinger equation, $i\partial_t|\eta_m^a(\vec{\lambda}(t))\rangle = \hat{H}(\vec{\lambda}(t))|\eta_m^a(\vec{\lambda}(t))\rangle$ is

$$|\eta_m^a(t)\rangle = \exp\{-i\int_0^t E_m(\tau)d\tau\}|\tilde{\phi}_m^a(t)\rangle \tag{7}$$

with $|\tilde{\phi}_m^a(t)\rangle = |\phi_m^b(t)\rangle[\Omega_m(t)]^{ba}$. The non-Abelian Berry phases Ω_m and the correspoinding Berry connections $\mathcal{A}_m^\mu$ are defined as

$$\Omega_m(t) = \mathcal{P}\left\{\exp\left\{i\int_{\vec{\lambda}(0)}^{\vec{\lambda}(t)} \mathcal{A}_m^\mu d\lambda^\mu\right\}\right\}, \tag{8}$$

$$\mathcal{A}_m^\mu(\vec{\lambda})^{ab} = i\langle\phi_m^a(\vec{\lambda})|\partial_{\lambda^\mu}|\phi_m^b(\vec{\lambda})\rangle, \tag{9}$$

where $\mathcal{P}$ means path-ordering [39]. The exact time-dependent solution can be expanded as $|\psi(t)\rangle = c_m^a(t)|\eta_m^a(t)\rangle$, then one obtains

$$\dot{c}_m^a(t) = -\sum_{n\neq m}\exp\left\{i\int_0^t \epsilon_{mn}(\tau)d\tau\right\}(\Omega_m^\dagger T_{mn}\Omega_n)^{ab}c_n^b(t), \tag{10}$$

where $\epsilon_{mn}(\tau) = E_m(\tau) - E_n(\tau)$ (details in the Appendix A). The transition matrices T_{mn} are followed by

$$T_{mn}^{ab} = \langle\phi_m^a(\vec{\lambda})|\partial_t|\phi_n^b(\vec{\lambda})\rangle, \tag{11}$$

where a and b denote the row and column indices of the matrix T_{mn}, respectively, with m and n being energy level labels.

To figure out the gauge invariant in the degenerate case, we extract the "phase" from $\Omega_m^\dagger T_{mn}\Omega_n$, i.e., the counterpart of $\Delta_{\mathrm{ND,mn}}(t)$ in Eq. (1). The "phase" of T is defined as $\theta_T = \frac{-i}{L}\mathrm{Tr}[\ln(UV^\dagger)]$, where U and V are unitary matrices from $T's$ singular value decomposition, $T_{mn} = U_{mn}S_{mn}V_{mn}^\dagger$, and S_{mn} is a diagonal real matrix with non-negative elements. We assume all the singular values of T are positive (The details are in the Appendix B). The "phase" of Ω_m is $\frac{1}{n}\mathrm{Tr}\{\int\mathcal{A}_m d\tau\}$ where $\mathcal{A}_m = \mathcal{A}_m^\mu\dot{\lambda}^\mu$, i.e., because Ω_m can be expressed as $\exp\{\int\frac{i}{n}\mathrm{Tr}\{\mathcal{A}_m\}d\tau\}\bar{\Omega}_m$ where $\det\bar{\Omega}_m = 1$. Then the gauge invariant in the degenerate systems is defined as

$$\Delta_{\mathrm{D},mn} = \frac{1}{L}\mathrm{Tr}\left\{\mathcal{A}_n - \mathcal{A}_m - i\frac{d}{dt}\ln(U_{mn}V_{mn}^\dagger)\right\}, \tag{12}$$

or, in a compact form

$$\Delta_{\mathrm{D},mn} = -\frac{i}{L}\mathrm{Tr}\{\dot{X}_{mn}X_{mn}^\dagger\} \tag{13}$$

with $X_{mn}(\vec{\lambda}(t)) = \Omega_m^\dagger U_{mn}V_{mn}^\dagger\Omega_n$ (here "D" denotes the degenerate systems). The "phase" of $\Omega_m^\dagger T_{mn}\Omega_n$ is defined as $\int i\Delta_{\mathrm{D},mn}d\tau$, and Eq. (10) can be rewritten as

$$\begin{aligned}\dot{c}_m^a &= -\sum_{n\neq m}\exp\left\{i\int_0^t(\epsilon_{mn}(\tau) + \Delta_{\mathrm{D,mn}}(\tau))d\tau\right\}\\ &\times(\bar{\Omega}_m^\dagger\bar{U}_{mn}S_{mn}\bar{V}_{mn}^\dagger\bar{\Omega}_n)^{ab}c_n^b(t).\end{aligned} \tag{14}$$

Similar as $\Delta_{\mathrm{ND},mn}$ in non-degenerate situations, $\Delta_{\mathrm{D},mn}$ provides a proper correction for the instantaneous energy gaps for the degenerate systems. With the introduction of $\Delta_{\mathrm{D},mn}$, a modified QAC is discussed in Appendix A.

$\Delta_{\mathrm{D},mn}$ is $U(L)\otimes U(L)$ gauge invariant under any two independent $U(L)$ gauge transformations W_m and W_n (details in the Appendix C):

$$\begin{aligned}|\phi_m^a(\vec{\lambda})\rangle &\to |\phi_m^b(\vec{\lambda})\rangle(W_m(\vec{\lambda}))^{ba},\\ |\phi_n^a(\vec{\lambda})\rangle &\to |\phi_n^b(\vec{\lambda})\rangle(W_n(\vec{\lambda}))^{ba}.\end{aligned} \tag{15}$$

Then the quantized character Θ can be defined between any two eigenspaces associated with eigenvalues $E_\pm$. Δ in Eq. (5) is replaced by Δ_{D}, and $\mathcal{F}$ is defined as $\frac{1}{L}\mathrm{Tr}\{\mathcal{F}_- - \mathcal{F}_+\}$, where $\mathcal{F}_\pm = \frac{1}{2}F_\pm^{\mu\nu}d\lambda^\mu\wedge d\lambda^\nu$ with $F_\pm^{\mu\nu} = \partial^\mu\mathcal{A}_\pm^\nu - \partial^\nu\mathcal{A}_\pm^\mu - i\left[\mathcal{A}_\pm^\mu, \mathcal{A}_\pm^\nu\right]$ being the non-Abelian Berry curvatures. $z(t) = \exp\{\frac{1}{L}\mathrm{Tr}\ln(UV^\dagger)\}\}$ defines a closed curve in the complex plane, when $\vec{\lambda}$ completes a close loop. Therefore, $W[z] = \int\frac{-i}{L}\mathrm{Tr}\{\ln UV^\dagger)\}$ is a winding number of z relative to the origin of the complex plane, which is quantized and play the counterpart of $\int_{\partial\mathcal{M}} d\arg\langle\phi_+|\dot{\phi}_-\rangle$ in non-degenerate case. Therefore Eq. (5) still holds for degenerate system.

Discussion and conclusions— Based on the gauge invariant quantum geometric potential, we define a new quantized character Θ for both non-degenerate and degenerate quantum systems. It is a quantum analogy to the Gauss-Bonnet theorem for a manifold with boundary. This character is fundamentally different from the Chern number which is quantized for the bundle based on a manifold without boundary. Furthermore, Θ is an inter-level index, while the Chern number is an intra-band (level) property.

We speculate that this quantized inter-level character Θ can be further applied to the study of quantizations of physical observables in topological physics and quantum adiabatic condition. Since it is an inter-band quantity, it may have applications in studying non-equilibrium properties including inter-band transitions, non-adiabatic processes and dynamical properties involving with multiple bands.

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Appendix A: Time Evolving Equation for Degenerate system

As discussed in the article, the solution to the time dependent Schrödinger equation can be expanded by $|\eta_m^a\rangle$ defined in Eq. (7) in the main text as

$$|\psi(t)\rangle = c_m^a(t)|\eta_m^a(t)\rangle, \tag{A1}$$

or with $|\tilde{\phi}_m^a\rangle = |\phi_m^b(t)\rangle(\Omega_m(t))^{ba}$ as

$$|\psi(t)\rangle = c_m^a(t)\exp\{-i\int_0^t E_m(\tau)d\tau\}|\tilde{\phi}_m^a\rangle, \tag{A2}$$

where Ω_m is defined in Eq. (9) in the main text. It can be shown that $\langle\tilde{\phi}_m^a|\dot{\tilde{\phi}}_m^a\rangle = 0$, because

$$\begin{aligned}\langle\tilde{\phi}_m^a|\dot{\tilde{\phi}}_m^a\rangle &= (\Omega_m^\dagger)^{ac}\langle\phi_m^c|\dot{\phi}_m^b\rangle(\Omega_m)^{ba} + (\Omega_m^\dagger)^{ac}\langle\phi_m^c|\phi_m^b\rangle(\dot{\Omega}_m)^{ba} \\ &= (\Omega_m^\dagger)^{ac}(-i\mathcal{A}_m)^{cb}(\Omega_m)^{ba} + (\Omega_m^\dagger)^{ac}\delta^{cb}(i\mathcal{A}_m)^{bd}(\Omega_m)^{da} = 0.\end{aligned} \tag{A3}$$

Solving the time dependent Schrödinger equation $i\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$:

$$i\{\dot{c}_m^a|\tilde{\phi}_m^a\rangle - iE_m(t)c_m^a|\tilde{\phi}_m^a\rangle + c_m^a|\dot{\tilde{\phi}}_m^a\rangle\}\exp\{-i\int_0^t E_m(\tau)d\tau\} = E_m^a c_m^a \exp\{-i\int_0^t E_m(\tau)d\tau\}|\tilde{\phi}_m^a\rangle. \tag{A4}$$

Left multiply $\langle\tilde{\phi}_m^a|$ to the equation above, one obtains

$$i\{\dot{c}_m^a - iE_m(t)\}\exp\{-i\int_0^t E_m(\tau)d\tau\} + \sum_{b,n,n\neq m} ic_n^b(t)\langle\tilde{\phi}_m^a|\dot{\tilde{\phi}}_n^b\rangle\exp\{-i\int_0^t E_n(\tau)d\tau\} = E_m(t)c_m^a(t)\exp\{-i\int_0^t E_m(\tau)d\tau\}. \tag{A5}$$

Then one arrives at

$$\dot{c}_m^a(t) = -\sum_{n,n\neq m}(\exp\{i\int_0^t \epsilon_{mn}(\tau)d\tau\}\langle\tilde{\phi}_m^a|\dot{\tilde{\phi}}_n^b\rangle)c_n^b(t). \tag{A6}$$

Therefore the time evolving equation of Eq. (10) in the main text can be obtained,

$$\dot{c}_m^a(t) = -\sum_{n\neq m}\exp\{i\int_0^t \epsilon_{mn}(\tau)d\tau\}(\Omega_m^\dagger T_{mn}\Omega_n)^{ab}c_n^b(t), \tag{A7}$$

with $\epsilon_{mn}(\tau) = E_+(\tau) - E_-(\tau)$. Therefore

$$\dot{c}_m^a = -\sum_{n\neq m}\exp\left\{i\int_0^t(\epsilon_{mn}(\tau) + \Delta_{\mathrm{D},mn}(\tau))d\tau\right\} \times (\bar{\Omega}_m^\dagger\bar{U}_{mn}S_{mn}\bar{V}_{mn}^\dagger\bar{\Omega}_n)^{ab}c_n^b(t). \tag{A8}$$

With the gauge invariant Δ_D in the degenerate systems Eq. (12), we can further revise the QAC for the quantum degenerate systems. For an adiabatic process, all the $c_m^b(t)$'s are nearly time-independent, because $|\eta_m^b(t)\rangle$ are already the adiabatic evolution states. If one further assumes that $\epsilon_{mn}(t)$, $\Delta_{\mathrm{D},mn}(t)$, S_{mn} and $(\bar{\Omega}_m^\dagger\bar{U}_{mn}S_{mn}\bar{V}_{mn}^\dagger\bar{\Omega}_n)^{ab}(t)$ are slow varying variables, and the system is initially prepared in the states $|\eta_k^a(0)\rangle$, then the time-evolving part is approximately controlled by $\exp\{i(\epsilon_{mn} + \Delta_{\mathrm{D},mn})t\}$. With these conditions, the QAC for the degenerate systems can be expressed as $\forall m \neq n$

$$\frac{\max(S_{mn})}{|\epsilon_{mn} + \Delta_{\mathrm{D},mn}|} \ll 1, \tag{A9}$$

where $\max(S_{mn})$ is the maximum value of the singular values of the transition matrix T_{mn}. Physically, the $\max(S_{mn})$ represents the most possible channel in the process of transition.

To illustrate how the degenerate QAC Eq. (A9) works, we construct a two-level toy model as follows:

$$H(t) = \begin{bmatrix}\vec{n}_1(t)\cdot\vec{\sigma} & \\ & \vec{n}_2(t)\cdot\vec{\sigma}\end{bmatrix}. \tag{A10}$$

If $\vec{n}_1 = \vec{n}_2 = (\sin\theta\cos(\omega t), \sin\theta\sin(\omega t), \cos\theta)$, then H is simply a double copy of Rabi model. $\Delta_{\rm D}$ can be calculated by Eq. (12), and the result is $(1-2\cos^2(\theta/2))\omega$. After extracting the phase term $i\int_0^t \Delta_{\rm D}(\tau)d\tau$, the remaining part $\bar{\Omega}_+^\dagger \bar{U} S \bar{V}^\dagger \bar{\Omega}_-$ is a constant, and S is also a contant matrix $\sin(\theta)\omega/2 \cdot \mathbb{I}_{2\times 2}$, so that we can use Eq. (A9) to judge the adiabaticity as

$$\frac{|\sin(\theta)\omega/2|}{|2+(1-2\cos^2(\theta/2))\omega|} \ll 1. \tag{A11}$$

When $\theta \to 0^+$, Eq. (A11) breaks down if $\omega \simeq 2$, because the denominator goes to zero. This is expected since when ω matches the energy gap, the resonance happens so that the system is not adiabatic anymore.

Besides $\Delta_{\rm D}$, one can also define other gauge invariants within the general time-dependent problem described above. Every single element of the matrix, $(\Omega_m^\dagger T_{mn} \Omega_n)^{ab}$ can be evaluated as $\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle$, and it is also gauge invariant as long as the initial basis are fixed. Similar as what we do in the non-degenerate case, we can separate the phase factor from $\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle$ as

$$\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle = \exp\{i\int_0^t \Delta_{mn}^{ab} d\tau\} |\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle| \tag{A12}$$

with $\Delta_{mn}^{ab} = \frac{d}{dt}\arg(\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle)$. Then Eq. (10) can be rewritten by using Δ^{ab} as

$$\dot{c}_m^a(t) = -\sum_{m\neq n} \exp\{i\int_0^t (\epsilon_{mn}(\tau) + \Delta_{mn}^{ab}(\tau))d\tau\} |\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle| c_n^b(t). \tag{A13}$$

If one further assume $\epsilon_{mn}(t) = \epsilon_{mn}$, $|\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle|$ and Δ_{mn}^{ab} are slow varying varibles, the adiabatic condition can be deduced as

$$\frac{|\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle|}{|\epsilon_{mn} + \Delta_{mn}^{ab}|} \ll 1 \quad \forall a, b, m \neq n. \tag{A14}$$

$|\tilde{\phi}_m^a\rangle$ are adiabatically evolved basis, so that the meaning of QAC Eq. (A14) is that all the transitions between any two adiabatically evolved basis with different energies are all very weak, so that this degenerate system can evolve adiabatically.

Appendix B: Ambiguity of the Singular Value Decomposition (SVD)

For a general $l \times l$ matrix C, when applying SVD to it, one will obtain $(C)^{ab} = (U)^{ad}(\Lambda)^d(V^\dagger)^{db}$, with l non-negative singular values Λ_d (a, b and d vary from $1 \to l$) and U and V being unitary matrices. SVD has its intrinsic ambiguity that comes from the unitary matrices U and V. In the case that all the singular values are positive, one can insert two diagonal matrices as:

$$(C)^{ab} = (U)^{ad}(\Lambda)^d(V^\dagger)^{db} = (U)^{ad}e^{i\lambda_d}(\Lambda)^d e^{-i\lambda_d}(V^\dagger)^{db} \tag{B1}$$

with λ_d being any real numbers. After the insertion, one can define $(U')^{ad} = (U)^{ad}e^{i\lambda_d}$ and $(V')^{ad} = (V)^{ad}e^{i\lambda_d}$, so that $C = U'\Lambda V'^\dagger$ which is also a valid SVD of C. Therefore SVD has its intrinsic ambiguity of the choice of the unitary matrices, but there is neither ambiguity of the singular values nor ambiguity of the product of U and $V^\dagger$ in this case.

When the singular values of a matrix C contain a zero or multiple zeros, there are further ambiguities. For example, if C is decomposed as $C = U\Lambda V^\dagger$ and the n^{th} singular value is zero, then one can also insert two diagonal matrices as

$$(C)^{ab} = (U)^{ad}(\Lambda)^d(V^\dagger)^{db} = (U)^{ad}e^{i\lambda_d}(\Lambda)^d e^{-i\lambda'_d}(V^\dagger)^{db} \tag{B2}$$

with λ_d and λ'_d being any real numbers and $\lambda_d = \lambda'_d$ if $d \neq n$. Because the n^{th} singular value is zero, λ_n and λ'_n do not have to be equal. Define $(U')^{ad} = (U)^{ad}e^{i\lambda_d}$ and $(V')^{ad} = (V)^{ad}e^{i\lambda'_d}$, so that $C = U'\Lambda V'^\dagger$, however $UV^\dagger \neq U'V'^\dagger$.

Appendix C: Proof of the Gauge Invariance of the Quantum Geometric Potential $\Delta_{\rm D}$

As mentioned in the article, $\Delta_{\rm D}$ is gauge invariant under any independent $U(L)$ gauge transformations W_m

$$|\phi_m^a(\vec{\lambda})\rangle \rightarrow |\phi_m^b(\vec{\lambda})\rangle (W_m(\vec{\lambda}))^{ba}. \tag{C1}$$

Under the gauge transformations above, $\mathcal{A}_m$, T_{mn} and $U_{mn}V_{mn}^\dagger$ transform as follows:

$$\begin{aligned} \mathcal{A}_m^\mu &\rightarrow W_m^\dagger \mathcal{A}_m^\mu W_m + iW_m^\dagger \partial_{\lambda^\mu} W_m & \text{(C2)}\\ T_{mn} &\rightarrow W_m^\dagger T_{mn} W_n & \text{(C3)}\\ U_{mn}V_{mn}^\dagger &\rightarrow W_m^\dagger U_{mn}V_{mn}^\dagger W_n. & \text{(C4)} \end{aligned}$$

(U_{mn} and $V_{mn}^\dagger$ are the unitary matrices come from the SVD of T_{mn}; $\mathcal{A}_m$ and T_{mn} are introduced in Eq. (9) and Eq. (11) in the main text). $\Delta_{\rm D}$ is carried out as

$$\Delta_{{\rm D},mn} = \frac{1}{L}{\rm Tr}\{(\mathcal{A}_n - \mathcal{A}_m) + i\frac{d}{dt}(-\ln(U_{mn}V_{mn}^\dagger))\}, \tag{C5}$$

and under the gauge transformations W_m

$$\Delta_{{\rm D},mn} \xrightarrow{W_m} \frac{1}{L}{\rm Tr}\{(W_n^\dagger \mathcal{A}_n W_n + iW_n^\dagger \dot{W}_n - W_m^\dagger \mathcal{A}_m W_m - iW_m^\dagger \dot{W}_m) + i\frac{d}{dt}(-\ln(U_{mn}V_{mn}^\dagger) - \ln(W_m^\dagger) - \ln(W_n))\}. \tag{C6}$$

We have used the fact that ${\rm Tr}\{\ln(AB)\} = {\rm Tr}\{\ln(A)\} + {\rm Tr}\{\ln(B)\}$ if $A, B \in U(L)$ in the equation above. $W_m^\dagger \mathcal{A}_m W_m$ are similarity transformations, so that the trace remains the same as before. If $A \in U(L)$, then ${\rm Tr}\{\ln(A)\} = \ln(\det(A))$, so that $\frac{d}{dt}{\rm Tr}\{\ln(A)\} = \frac{d}{dt}{\rm Tr}\{\ln(\Lambda)\}$ with $V\Lambda V^\dagger = A$ and Λ being diagonal. If $V\Lambda V^\dagger = A \in U(L)$, then

$${\rm Tr}\{A^\dagger \dot{A}\} = {\rm Tr}\{V\Lambda^\dagger(V^\dagger \dot{V})\Lambda V^\dagger + V\dot{V}^\dagger + V\Lambda^\dagger \dot{\Lambda} V^\dagger\} = {\rm Tr}\{\Lambda^\dagger \dot{\Lambda}\} = {\rm Tr}\{\Lambda^{-1}\dot{\Lambda}\} = \frac{d}{dt}{\rm Tr}\{\ln(\Lambda)\}, \tag{C7}$$

so that if $A \in U(L)$, $\frac{d}{dt}{\rm Tr}\{\ln(A)\} = {\rm Tr}\{A^\dagger \dot{A}\}$. Then Eq. (C6) can be simplified as

$$\Delta_{\rm D} \xrightarrow{W_m} \Delta_{\rm D} + \frac{1}{L}{\rm Tr}\{-i\frac{d}{dt}(\ln(W_n^\dagger) + \ln(W_n) + \ln(W_m^\dagger) - \ln(W_m^\dagger))\} = \Delta_{\rm D}. \tag{C8}$$

Therefore $\Delta_{\rm D}$ is gauge invariant under a $U(L) \times U(L)$ gauge transformation.

As for the case that the degeneracies of these two eigenspaces are different, one can still define the gauge invariant as

$$\Delta_{{\rm D},mn} = -\frac{i}{\min(L_m, L_n)}{\rm Tr}\{\dot{X}_{mn}X_{mn}^\dagger\}, \tag{C9}$$

where X is $\Omega_m^\dagger U_{mn}V_{mn}^\dagger \Omega_n$, and L_m and L_n are the degeneracies of these two eigenspaces (suppose $L_m < L_n$). As mentioned in the main text of this article, $V^\dagger V = \mathbb{I}_{L_m \times L_m}$ is an identity matrix, while $VV^\dagger$ is not. $\mathcal{A}_m$, T_{mn} and $U_{mn}V_{mn}^\dagger$ transform as same as Eq. (C2), Eq. (C3) and Eq. (C4), so that under the gauge transformation:

$$\begin{aligned} \Delta_{{\rm D},mn} &= -\frac{i}{L_m}{\rm Tr}\{-i\mathcal{A}_m + \frac{d}{dt}(U_{mn}V_{mn}^\dagger)(V_{mn}U_{mn}^\dagger) + iU_{mn}V_{mn}^\dagger \mathcal{A}_n V_{mn}U_{mn}^\dagger\} & \text{(C10)}\\ &\xrightarrow{W_m} -\frac{i}{L_m}{\rm Tr}\{-iW_m^\dagger \mathcal{A}_m W_m + W_m^\dagger \dot{W}_m + \dot{W}_m^\dagger W_m + \frac{d}{dt}(U_{mn}V_{mn}^\dagger)(V_{mn}U_{mn}^\dagger) & \text{(C11)}\\ &\quad + U_{mn}V_{mn}^\dagger \dot{W}_n W_n^\dagger V_{mn}U_{mn}^\dagger + W_m^\dagger U_{mn}V_{mn}^\dagger W_n(iW_n^\dagger \mathcal{A}_n W_n - W_n^\dagger \dot{W}_n)W_n^\dagger V_{mn}U_{mn}^\dagger W_m\} & \text{(C12)}\\ &= -\frac{i}{L_m}{\rm Tr}\{-iW_m^\dagger \mathcal{A}_m W_m + \frac{d}{dt}(U_{mn}V_{mn}^\dagger)(V_{mn}U_{mn}^\dagger) + iW_m^\dagger U_{mn}V_{mn}^\dagger \mathcal{A}_n V_{mn}U_{mn}^\dagger W_m\} & \text{(C13)}\\ &= \Delta_{{\rm D},mn}. & \text{(C14)} \end{aligned}$$

Therefore the gauge invariance is verified. Note that some terms in the equations above, like $U_{mn}V_{mn}^\dagger \mathcal{A}_n V_{mn}U_{mn}^\dagger$ and $U_{mn}V_{mn}^\dagger \dot{W}_n W_n^\dagger V_{mn}U_{mn}^\dagger$ are in fact not similarity transformations of $\mathcal{A}_n$ and $\dot{W}_n W_n^\dagger$.

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