

Quantized interlevel character in quantum systems

Chao Xu, Jianda Wu,^{*} and Congjun Wu

Department of Physics, University of California, San Diego, California 92093, USA



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For a quantum system subject to external parameters, the Berry phase is an intralevel property, which is gauge invariant module 2π for a closed loop in the parameter space and generally is nonquantized. In contrast, we define an interband 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 interband character is also generalized to quantum degenerate systems.

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I. INTRODUCTION

The study of time-dependent systems has greatly facilitated the exploration of novel physics [1–11]. In particular, research on 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 has given 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 to reveal 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 as different from the ordinary “phase” associated with 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 interlevel connection, i.e., the projection of the time derivative of the state vector of one level to that of another one, has not been 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 interlevel 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, i.e., 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.

II. GAUGE INVARIANT IN NONDEGENERATE QUANTUM SYSTEMS

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

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

^{*}Present address: Max-Planck-Institut für Physik Komplexer Systeme, 01187 Dresden, Germany.

where ND denotes the nondegenerate systems, and the “.” illustrates the time derivative. In addition, $\mathcal{A}_m \equiv \mathcal{A}_m^\mu \dot{\lambda}_\mu$ (in this paper, the repeated indices imply the summation). The adiabatic solution to the time-dependent Schrödinger equation, $i \partial_t |\eta_m^a(\vec{\lambda}(t))\rangle = \hat{H}(\vec{\lambda}(t)) |\eta_m^a(\vec{\lambda}(t))\rangle$, is

$$|\eta_m^a(t)\rangle = \exp \left\{ -i \int_0^t E_m(\tau) d\tau \right\} |\tilde{\phi}_m^a(t)\rangle, \quad (2)$$

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

$$\Delta_{\text{ND},mn} = \frac{d}{dt} \arg(\tilde{\phi}_m | \dot{\tilde{\phi}}_n). \quad (3)$$

$\Delta_{\text{ND},mn}$ is gauge invariant under an arbitrary local $U(1) \otimes U(1)$ gauge transform with $|\phi_{m(n)}(t)\rangle \rightarrow e^{i\alpha_{m(n)}(t)} |\phi_{m(n)}(t)\rangle$, 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 $\Delta_{\text{ND},mn}$ to the time-dependent system, an improved QAC for the nondegenerate system can be established for $n \neq m$ [41],

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

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

III. A QUANTIZED CHARACTER IN NONDEGENERATE SYSTEM

We introduce a quantized gauge-invariant character Θ based on the quantum geometric potential as an analogy to the 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 exists a pair of eigenfunctions $|\phi_\pm(\vec{\lambda}(t))\rangle$ associated with the eigenvalues $E_\pm(\lambda(t))$. 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 $\mathcal{F}_\pm = \frac{1}{2} F_\pm^{\mu\nu} d\lambda^\mu \wedge d\lambda^\nu$ with $F_\pm^{\mu\nu} = \partial^\mu \mathcal{A}_\pm^\nu - \partial^\nu \mathcal{A}_\pm^\mu$. A quantized character Θ is defined as

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

where Δ_{ND} is the gauge invariant in Eq. (1) for the nondegenerate systems, and $\Phi_\pm = \int_{\partial\mathcal{M}} \mathcal{A}_\pm^\mu d\lambda_\mu - \int_{\mathcal{M}} \mathcal{F}_\pm$. 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 three-dimensional (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}

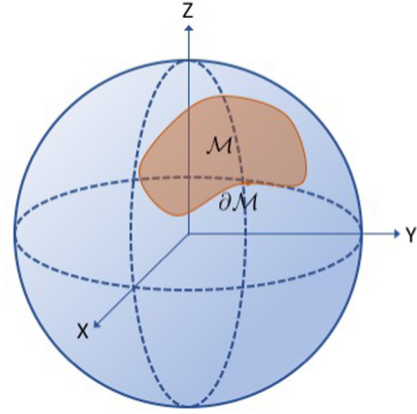


FIG. 1. The region \mathcal{M} on the S^2 Bloch sphere with a smooth boundary $\partial\mathcal{M}$.

is the Berry-curvature difference between the ground and excited states. To explicitly calculate Θ , we can work in a given gauge where $|\phi_-(\theta, \phi)\rangle = (\sin \frac{\theta}{2} e^{-i\phi}, -\cos \frac{\theta}{2})^T$ 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, $\arg(\phi_+ | \dot{\phi}_-) = \arg[(\dot{\theta} - i \sin \theta \dot{\phi})/2]$. When $\vec{\lambda}(t)$ completes a close loop $\partial\mathcal{M}$, correspondingly, $z(t) = \langle \phi_+ | \dot{\phi}_- \rangle$ defines a close curve in the complex plane. The winding number of $z(t)$ relative to the origin is defined as $W[z] = \int_{\partial\mathcal{M}} d \arg(\phi_+ | \dot{\phi}_-)$, as shown in Fig. 2. If $\partial\mathcal{M}$ does not enclose the north or south pole, Φ_\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 nondegenerate model, we can define the quantized character Θ between any two different energy levels E_\pm associated with a closed curve in the parameter space. According to the Stokes theorem, Φ_\pm count the singularities of Berry connections \mathcal{A}_\pm^μ 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

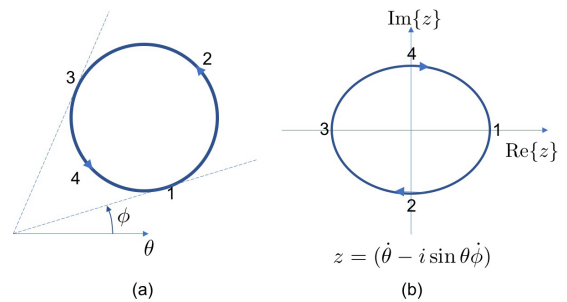


FIG. 2. (a) The top view of a closed curve on the Bloch sphere in the vicinity of the north pole. θ and ϕ represent the radial and angular coordinates, respectively. (b) The corresponding curve $z(t)$ in the complex plane with $z(t) = \langle \phi_+ | \dot{\phi}_- \rangle = (\dot{\theta} - i \sin \theta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

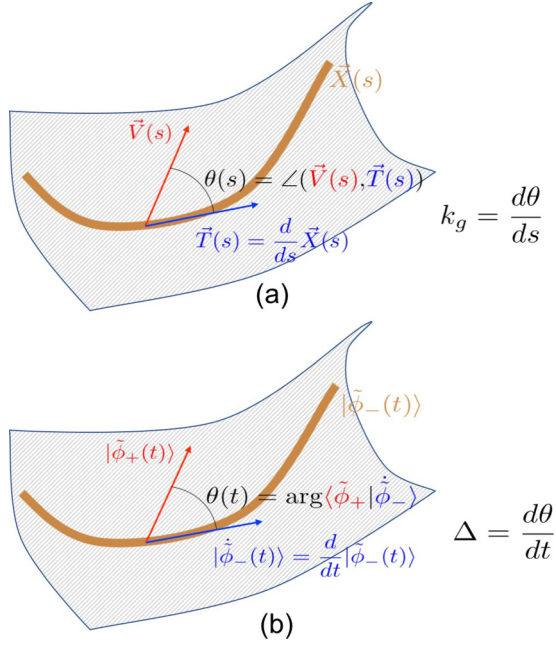


FIG. 3. (a) A curve $\vec{X}(s)$ is plotted on a 2D manifold (shaded area) in the 3D real space. $\vec{V}(s)$ lives in the tangent space, and is parallel transported along the curve. $\vec{T}(s) = \frac{d}{ds}\vec{X}(s)$ is the velocity vector, and θ is the angle between \vec{V} and \vec{T} . The geodesic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

theorem. For a 2D compact Riemannian manifold \mathcal{M} with a smooth boundary $\partial\mathcal{M}$, the Gauss-Bonnet theorem reads

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

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 Fig. 3(a), 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 parallel 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. $|\tilde{\phi}_-(t)\rangle$ 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 $\Delta_{\text{ND}} = d\theta/dt$ is the time derivative of the angle $\theta = \arg(\tilde{\phi}_+|\tilde{\phi}_-)$ 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, and we can observe the similarity to our theorem described in Eq. (5). To prove the Gauss-Bonnet theorem, one first decomposes 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 closed 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 intrasubspace quantities associated with one energy level, while Δ_{ND} is an intersubspace property associated with two different energy levels.

IV. 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 Hamiltonian $\hat{H}(\vec{\lambda})$ possesses N energy levels $E_m(\vec{\lambda})$ ($m = 1, 2, \dots, N$), 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 $\hat{H}(\vec{\lambda})|\phi_m^a(\vec{\lambda})\rangle = E_m(\vec{\lambda})|\phi_m^a(\vec{\lambda})\rangle$ ($a = 1, 2, \dots, L$). 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

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

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 corresponding Berry connections \mathcal{A}_m^μ are defined as

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

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

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

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

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

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

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 $\Delta_{\text{ND},mn}(t)$ in Eq. (1). The phase of T is defined as $\theta_T = \frac{-i}{L} \text{Tr}[\ln(UV^\dagger)]$, 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 (details are given in Appendix B). The phase of Ω_m is $\frac{1}{n} \text{Tr}[\int \mathcal{A}_m d\tau]$, where $\mathcal{A}_m = \mathcal{A}_m^\mu \lambda^\mu$, i.e., because Ω_m can be expressed as $\exp(\int \frac{i}{n} \text{Tr}\{\mathcal{A}_m\} d\tau) \bar{\Omega}_m$, where $\det \bar{\Omega}_m = 1$. Then the gauge invariant in the degenerate systems is defined as

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

or, in a compact form,

$$\Delta_{\text{D},mn} = -\frac{i}{L} \text{Tr}\{\dot{X}_{mn} X_{mn}^\dagger\}, \quad (13)$$

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 $\int i \Delta_{\text{D},mn} d\tau$, and Eq. (10) can be rewritten as

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

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

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

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

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 $\frac{1}{L} \text{Tr}\{\mathcal{F}_- - \mathcal{F}_+\}$, where $\mathcal{F}_\pm = \frac{1}{2} F_\pm^{\mu\nu} d\lambda^\mu \wedge d\lambda^\nu$ with $F_\pm^{\mu\nu} = \partial^\mu \mathcal{A}_\pm^\nu - \partial^\nu \mathcal{A}_\pm^\mu - i[\mathcal{A}_\pm^\mu, \mathcal{A}_\pm^\nu]$ being the non-Abelian Berry curvatures. $z(t) = \exp\{\frac{1}{L} \text{Tr} \ln(UV^\dagger)\}$ defines a closed curve in the complex plane, when $\vec{\lambda}$ completes a closed loop. Therefore, $W[z] = \int \frac{-i}{L} \text{Tr}[\ln(UV^\dagger)]$ is a winding number of z relative to the origin of the complex plane, which is quantized and plays the

counterpart of $\int_{\partial \mathcal{M}} \text{darg}(\phi_+ | \phi_-)$ in the nondegenerate case. Therefore, Eq. (5) still holds for the degenerate system.

V. DISCUSSION AND CONCLUSIONS

Based on the gauge-invariant quantum geometric potential, we define a quantized character Θ for both nondegenerate 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 interlevel index, while the Chern number is an intraband (level) property.

We speculate that this quantized interlevel 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 interband quantity, it may have applications in studying nonequilibrium properties, including interband transitions, nonadiabatic processes, and dynamical properties involving multiple bands.

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APPENDIX A: TIME-EVOLVING EQUATION FOR DEGENERATE SYSTEM

As discussed in this 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

$$|\psi(t)\rangle = c_m^a(t) |\eta_m^a(t)\rangle, \quad (A1)$$

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

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

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

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

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

$$\begin{aligned} i \{ \dot{c}_m^a |\tilde{\phi}_m^a\rangle - i E_m(t) c_m^a |\tilde{\phi}_m^a\rangle + c_m^a |\dot{\tilde{\phi}}_m^a\rangle \} \exp \left\{ -i \int_0^t E_m(\tau) d\tau \right\} \\ = E_m^a c_m^a \exp \left\{ -i \int_0^t E_m(\tau) d\tau \right\} |\tilde{\phi}_m^a\rangle. \end{aligned} \quad (A4)$$

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

$$\begin{aligned} & i \{ \dot{c}_m^a - i E_m(t) \} \exp \left\{ -i \int_0^t E_m(\tau) d\tau \right\} + \sum_{b,n,n \neq m} i c_n^b(t) \langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle \exp \left\{ -i \int_0^t E_n(\tau) d\tau \right\} \\ & = E_m(t) c_m^a(t) \exp \left\{ -i \int_0^t E_m(\tau) d\tau \right\}. \end{aligned} \quad (\text{A5})$$

Then one arrives at

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

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

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

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

$$\begin{aligned} \dot{c}_m^a & = - \sum_{n \neq m} \exp \left\{ i \int_0^t [\epsilon_{mn}(\tau) + \Delta_{D,mn}(\tau)] d\tau \right\} \\ & \times (\tilde{\Omega}_m^\dagger \tilde{U}_{mn} S_{mn} \tilde{V}_{mn}^\dagger \tilde{\Omega}_n)^{ab} c_n^b(t). \end{aligned} \quad (\text{A8})$$

With the gauge invariant Δ_D in the degenerate systems given by 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 $\epsilon_{mn}(t)$, $\Delta_{D,mn}(t)$, S_{mn} , and $(\tilde{\Omega}_m^\dagger \tilde{U}_{mn} S_{mn} \tilde{V}_{mn}^\dagger \tilde{\Omega}_n)^{ab}(t)$ 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 $\exp\{i(\epsilon_{mn} + \Delta_{D,mn})t\}$. With these conditions, the QAC for the degenerate systems can be expressed as ($\forall m \neq n$)

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

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 probable channel in the process of transition.

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

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

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 the Rabi model. Δ_D can be calculated by Eq. (12) and the result is $[1 - 2 \cos^2(\theta/2)]\omega$. After extracting the phase term $i \int_0^t \Delta_D(\tau) d\tau$, the remaining part $\tilde{\Omega}_+^\dagger \tilde{U} S \tilde{V}^\dagger \tilde{\Omega}_-$ is a constant, and S is also a constant matrix $\sin(\theta)\omega/2 \cdot \mathbb{I}_{2 \times 2}$, so that we can use Eq. (A9) to judge the

adiabaticity as

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

When $\theta \rightarrow 0^+$, 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 no longer adiabatic.

Besides Δ_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 is fixed. Similar to what we do in the nondegenerate case, we can separate the phase factor from $\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle$ as

$$\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle = \exp \left\{ i \int_0^t \Delta_{mn}^{ab} d\tau \right\} |\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle|, \quad (\text{A12})$$

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

$$\begin{aligned} \dot{c}_m^a(t) & = - \sum_{m \neq n} \exp \left\{ i \int_0^t [\epsilon_{mn}(\tau) + \Delta_{mn}^{ab}(\tau)] d\tau \right\} \\ & \times |\langle \tilde{\phi}_m^a | \dot{\tilde{\phi}}_n^b \rangle| c_n^b(t). \end{aligned} \quad (\text{A13})$$

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

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

$|\tilde{\phi}_m^a\rangle$ is the adiabatically evolved basis, so that the meaning of QAC given by Eq. (A14) is that all the transitions between any two adiabatically evolved bases 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 $1 \rightarrow l$) 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

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

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

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

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. We 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, $U V^{\dagger} \neq U' V'^{\dagger}$.

APPENDIX C: PROOF OF THE GAUGE INVARIANCE OF THE QUANTUM GEOMETRIC POTENTIAL Δ_{D}

As mentioned in this article, Δ_{D} is gauge invariant under any independent $U(L)$ gauge transformations W_m ,

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

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

$$\mathcal{A}_m^{\mu} \rightarrow W_m^{\dagger} \mathcal{A}_m^{\mu} W_m + i W_m^{\dagger} \partial_{\lambda^{\mu}} W_m, \quad (\text{C2})$$

$$T_{mn} \rightarrow W_m^{\dagger} T_{mn} W_n, \quad (\text{C3})$$

$$U_{mn} V_{mn}^{\dagger} \rightarrow W_m^{\dagger} U_{mn} V_{mn}^{\dagger} W_n. \quad (\text{C4})$$

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

$$\Delta_{\text{D},mn} = \frac{1}{L} \text{Tr} \left\{ (\mathcal{A}_n - \mathcal{A}_m) + i \frac{d}{dt} [-\ln(U_{mn} V_{mn}^{\dagger})] \right\}, \quad (\text{C5})$$

and under the gauge transformations W_m ,

$$\begin{aligned} \Delta_{\text{D},mn} \xrightarrow{W_m} & \frac{1}{L} \text{Tr} \left\{ (W_n^{\dagger} \mathcal{A}_n W_n + i W_n^{\dagger} \dot{W}_n \right. \\ & - W_m^{\dagger} \mathcal{A}_m W_m - i W_m^{\dagger} \dot{W}_m) + i \frac{d}{dt} [-\ln(U_{mn} V_{mn}^{\dagger}) \\ & \left. - \ln(W_m^{\dagger}) - \ln(W_n) \right\}. \end{aligned} \quad (\text{C6})$$

We have used the fact that $\text{Tr}\{\ln(AB)\} = \text{Tr}\{\ln(A)\} + \text{Tr}\{\ln(B)\}$ 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 $\text{Tr}\{\ln(A)\} = \ln[\det(A)]$, so that $\frac{d}{dt} \text{Tr}\{\ln(A)\} = \frac{d}{dt} \text{Tr}\{\ln(\Lambda)\}$ with $V \Lambda V^{\dagger} = A$ and Λ being diagonal. If $V \Lambda V^{\dagger} = A \in U(L)$, then

$$\begin{aligned} \text{Tr}\{A^{\dagger} \dot{A}\} &= \text{Tr}\{V \Lambda^{\dagger} (\dot{V}^{\dagger} V) \Lambda V^{\dagger} + V \dot{V}^{\dagger} + V \Lambda^{\dagger} \dot{\Lambda} V^{\dagger}\} \\ &= \text{Tr}\{\Lambda^{\dagger} \dot{\Lambda}\} = \text{Tr}\{\Lambda^{-1} \dot{\Lambda}\} = \frac{d}{dt} \text{Tr}\{\ln(\Lambda)\}, \end{aligned} \quad (\text{C7})$$

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

$$\begin{aligned} \Delta_{\text{D}} \xrightarrow{W_m} & \Delta_{\text{D}} + \frac{1}{L} \text{Tr} \left\{ -i \frac{d}{dt} [\ln(W_n^{\dagger}) + \ln(W_n) \right. \\ & \left. + \ln(W_m^{\dagger}) - \ln(W_m) \right\} = \Delta_{\text{D}}. \end{aligned} \quad (\text{C8})$$

Therefore, Δ_{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

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

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, $V^{\dagger} V = \mathbb{I}_{L_m \times L_m}$ is an identity matrix, while $V V^{\dagger}$ is not. \mathcal{A}_m , T_{mn} , and $U_{mn} V_{mn}^{\dagger}$ transform the same as Eqs. (C2)–(C4), so that under the gauge transformation,

$$\Delta_{\text{D},mn} = -\frac{i}{L_m} \text{Tr} \left\{ -i \mathcal{A}_m + \frac{d}{dt} (U_{mn} V_{mn}^{\dagger}) (V_{mn} U_{mn}^{\dagger}) + i U_{mn} V_{mn}^{\dagger} \mathcal{A}_n V_{mn} U_{mn}^{\dagger} \right\} \quad (\text{C10})$$

$$\xrightarrow{W_m} -\frac{i}{L_m} \text{Tr} \left\{ -i W_m^{\dagger} \mathcal{A}_m W_m + W_m^{\dagger} \dot{W}_m + \dot{W}_m^{\dagger} W_m + \frac{d}{dt} (U_{mn} V_{mn}^{\dagger}) (V_{mn} U_{mn}^{\dagger}) \right\} \quad (\text{C11})$$

$$+ U_{mn} V_{mn}^{\dagger} \dot{W}_n W_n^{\dagger} V_{mn} U_{mn}^{\dagger} + W_m^{\dagger} U_{mn} V_{mn}^{\dagger} W_n (i W_n^{\dagger} \mathcal{A}_n W_n - W_n^{\dagger} \dot{W}_n) W_n^{\dagger} V_{mn} U_{mn}^{\dagger} W_m \quad (\text{C12})$$

$$= -\frac{i}{L_m} \text{Tr} \left\{ -i W_m^{\dagger} \mathcal{A}_m W_m + \frac{d}{dt} (U_{mn} V_{mn}^{\dagger}) (V_{mn} U_{mn}^{\dagger}) + i W_m^{\dagger} U_{mn} V_{mn}^{\dagger} \mathcal{A}_n V_{mn} U_{mn}^{\dagger} W_m \right\} \quad (\text{C13})$$

$$= \Delta_{\text{D},mn}. \quad (\text{C14})$$

Therefore, the gauge invariance is verified. Note that some terms in the equations above, such as $U_{mn} V_{mn}^{\dagger} \mathcal{A}_n V_{mn} U_{mn}^{\dagger}$ 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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