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Geometric tensor and the topological characterization of the Bloch band in a two-band lattice model

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ABSTRACT

We investigate the quantum Riemannian metric and the Euler characteristic number of the Bloch states manifold in a two-band lattice model, where a topological phase transition from the normal to the Chern insulator occurs. We derive the topological Euler number of the band from the Gauss–Bonnet theorem on the closed Bloch states manifold in the first Brillouin zone, where the Riemannian metric of the states manifold is established by the real part of the quantum geometric tensor in the 2D quasi-momentum space. Meanwhile, we show that the imaginary part of the geometric tensor corresponds to the Berry curvature which leads to the Chern number characterization of the band insulator. We discuss the topological numbers induced by the geometric tensor analytically in the case of two-band Hamiltonian and characteristic the zero-temperature phase diagram by the Euler number and first Chern number, respectively.

1. Introduction

The geometric and topological properties have been key ingredient in understanding the novel states in quantum condensed matters. Since the finding of the Berry phase and its holonomy interpretation in the $U(1)$ line bundle with the parallel transport of the quantum states in the cyclic adiabatic evolutions [1,2], many important findings on the topological nature of the quantum matter have come into physics, i.e., the quantized Hall conductance [3–5], adiabatic pumping [6,7], topological insulators and superconductivity [8–12], and recently the fractional Chern insulators in flat bands [13–15]. As a more general covariant tensor than the Berry curvature on the Hilbert space geometry, the quantum geometric tensor (QGT) [16–24] defined on the manifold of quantum states is naturally expected to shed some light on the understanding of quantum phase transitions (QPTs) in many-body systems [25–27]. Historically, the real part of QGT as a Riemannian metric was first proposed by Provost and Valee in order to define a local $U(1)$ gauge invariant quantum distance between two quantum states in some parameterized Hilbert space. This effort results to a Riemannian structure of the quantum states manifold, and the corresponding Riemannian metric is given by the real part of the geometric tensor. Remarkably, its imaginary part was later found is nothing but the Berry curvature.

Recent studies [19,20,28] have shown that the ground-state geometric tensor can provide a unified approach of the fidelity susceptibility [29] and the Berry curvature to witness the QPTs [30–33]. It is shown that the underlying mechanism is the singular and scaling behavior of the QGT in the vicinity of the critical points. Particularly, the Riemannian metric as the real part of the QGT is recognized as the leading term of the fidelity [34] which is the overlap of two ground states associated to infinitesimally close parameters. Generally, the Riemannian metric will exhibit the divergent behavior in the quantum critical region in the thermodynamic limit. In the approach of Berry phase, it was argued that a non-contractible ground-state Berry phase in the loop over the parameter space is associated to QPTs. This fact indicates that the critical points associated to the divergence of the Berry curvature in the thermodynamic limit. Particularly, a scaling analysis of this QGT in the vicinity of the critical points has been performed. On the other hand, the previous studies on the ground state QGT are mainly focused on the local properties, *i.e.*, fidelity susceptibility and the partial derivatives of Berry phase near the critical points, and then only the phase boundaries can be witnessed by this approach.

Very recently, a topological Euler number [35,36], derived from the real part of the QGT, has been introduced to characterize the topological nature of the Bloch band in gapped fermionic systems. The Euler number endows the band insulators with a new

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topological number index in addition to the Chern number. In this approach, the Euler number can be derived from the Gauss–Bonnet theorem on the closed Bloch states manifold in the first Brillouin zone, where the Riemannian metric of the states manifold is established by the real part of the quantum geometric tensor in the quasi-momentum space.

In this work, we choose a 2D lattice model as an example which exhibits a non-trivial topological phase transition with time-reversal symmetry broken. This model was first introduced by Qi et al. [37] and can be physically realized in $Hg_{1-x}Mn_xTe/Cd_{1-x}Mn_xTe$ quantum wells with a proper amount of Mn spin polarization [38]. We discuss the geometric tensor exactly in the two-band system, which gives the Riemannian metric and Berry curvature of band, respectively. Then we obtain the topological Euler number of the band from the Gauss–Bonnet theorem on the closed Bloch states manifold in the first Brillouin zone, which is based on the Riemannian metric of the Bloch states manifold given by the real part of the QGT. As a comparison, the first Chern number is also obtained by the integral of the Berry curvature as the imaginary part of the geometric tensor over the first Brillouin zone. Finally, we give the phase diagram of the model distinguished by the Euler number and the first Chern number, respectively.

2. Riemannian metric, Berry curvature and the quantum geometric tensor

To begin with, we introduce the notions of the quantum Riemannian metric and the geometric tensor on the quantum states manifold. The Riemannian metric can be derived from a gauge invariant distance between two states on the U(1) line bundle. Following the steps introduced by Provost and Vallee, we first consider a family $\{\varphi(s)\}$ of normalized vectors of Hilbert space which is based on an n-dimensional parameter $s=(s_1,\ldots,s_n)\in\mathbb{R}^n$. The distance between two close vectors in the family $\{\varphi(s)\}$ can be developed up to second order as follows:

$$\|\varphi(s+ds)-\varphi(s)\|^2=\sum_{\mu\nu}\langle\partial_\mu\varphi(s)|\partial_\nu\varphi(s)\rangle\, ds^\mu\, ds^\nu. \tag{1}$$

Separating the Hermitian product into the real and the imaginary parts $\langle\partial_\mu\varphi(s)|\partial_\nu\varphi(s)\rangle=\gamma_{\mu\nu}+i\sigma_{\mu\nu}$, and we have $\gamma_{\mu\nu}(s)=\gamma_{\mu\nu}(s)$, $\sigma_{\mu\nu}(s)=\;-\sigma_{\mu\nu}(s)$. Thus its imaginary parts $\sigma_{\mu\nu}$ will be canceled out in the summation of the quantum distance, and then Eq. (1) reads

$$\|\varphi(s+ds)-\varphi(s)\|^2=\sum_{\mu\nu}\gamma_{\mu\nu}(s)ds^\mu\, ds^\nu. \tag{2}$$

However, the quantities $\gamma_{ij}(s)$ cannot be regarded as a metric to measure the quantum distance because it is not gauge invariant in the $U(1)$ gauge transformation of $\varphi(s)$. This can be clearly seen as follows: For the same physical states $\varphi(s)$ and $\varphi'(s)=e^{i\alpha(s)}\varphi(s)$ define on the same point in the parameter space, we have $\gamma_{\mu\nu}{}'(s)=\mathrm{Re}\langle\partial_\mu\varphi'(s)|\partial_\nu\varphi'(s)\rangle$, which is generally different from $\gamma_{\mu\nu}(s)$. More precisely, we have to make the metric tensor invariant to ensure an invariant quantum distance under the $U(1)$ gauge transformation of the same physical states. It can be verified that a $U(1)$ gauge-invariant metric tensor can be constructed as

$$g_{\mu\nu}(s)=\gamma_{\mu\nu}(s)-A_\mu(s)A_\nu(s), \tag{3}$$

where $A_{\mu(\nu)}(s)=i\langle\varphi(s)|\partial_{\mu(\nu)}\varphi(s)\rangle$ is nothing but the Berry–Simon connection. It can be verified that this quantity defined by Eq. (3) is a symmetric positive-definite Riemannian metric.

Now we introduce the quantum geometric tensor:

$$Q_{\mu\nu}=\langle\partial_\mu\varphi(s)|[\mathbf{1}-\mathcal{P}(s)]|\partial_\nu\varphi(s)\rangle, \tag{4}$$

where $\mathcal{P}(s):=|\varphi(s)\rangle\langle\varphi(s)|$ is the projection operator. The geometric tensor can be rewritten as $Q_{\mu\nu}=g_{\mu\nu}-iF_{\mu\nu}/2$, where

$$g_{\mu\nu}=\mathrm{Re}\,Q_{\mu\nu} \tag{5}$$

can be verified as a Riemannian metric (the Fubini-Study metric on the Projective Hilbert space), which establishes a Riemannian manifold of the Bloch states, and then the quantum distance can be written as $dS^2=\sum_{\mu,\upsilon}\mathrm{Re}\,Q_{\mu\nu}dk^\mu\, dk^\upsilon$. The term $\mathcal{F}_{\mu\nu}=-2\,\mathrm{Im}\,Q_{\mu\nu}$ which has been canceled out in the summation of the distance due to its antisymmetry, but can be associated to a 2-form $\mathcal{F}=\sum_{\mu,\upsilon}\mathcal{F}_{\mu\nu}dk^\mu\wedge dk^\nu$, which is nothing but the Berry curvature.

3. The model

Historically, a two-band lattice model with a nonzero Chern number was first proposed as by Haldane [23] which was a honeycomb lattice model with imaginary next-nearest-neighbor hopping. Haldane find the two different symmetries breaking about the space reflection and the time-reversal can be classified by the Chern numbers which reflect the topology of the ground-state.

The Bloch Hamiltonian is generally given by $H(k)=\varepsilon(k)I_{2\times2}+\sum_{\alpha=1}^3 d_\alpha(k)\sigma^\alpha$, where $I_{2\times2}$ is the 2×2 identity matrix and σ^α the three Pauli matrix. The diagonalization of $H(k)$ is straightforward and the eigenvalues can be written as $E_\pm(k)=\varepsilon(k)\pm\sqrt{\sum_{\alpha=1}^3 d_\alpha^2(k)}$, and eigenvectors as

$$u(k)_+=\begin{pmatrix}\cos\,\theta/2\\ e^{i\Phi}\,\sin\,\theta/2\end{pmatrix}, u(k)_-=\begin{pmatrix}-\sin\,\theta/2\\ e^{i\Phi}\,\cos\,\theta/2\end{pmatrix} \tag{6}$$

where $\Phi=\arctan d_1(k)/\sqrt{d_1^2(k)+d_2^2(k)}$, and $\theta=\arccos d_3(k)/\sqrt{d_1^2(k)+d_2^2(k)+d_3^2(k)}$.

Here we choose the following two-band model as an example because it is one of the simplest models that exhibit the topological non-trivial states. In this model, the Bloch Hamiltonian is

$$H(k)=\sin\,k_x\sigma^1+\sin\,k_y\sigma^2+(m+\cos\,k_x+\cos\,k_y)\sigma^3, \tag{7}$$

that is, the coefficients are given by $\varepsilon(k)=0$, $d_1=\sin\,k_x$, $d_2=\sin\,k_y$ and $d_3=m+\cos\,k_x+\cos\,k_y$. This model exhibits a non-trivial topological quantum phase transition from the normal insulator to Chern insulator, which was first introduced by Qi et al. [37] and can be physically realized in $Hg_{1-x}Mn_xTe/Cd_{1-x}Mn_xTe$ quantum wells with a proper amount of Mn spin polarization [38].

In the thermodynamic limit, the QGT of the Bloch band can be naturally defined on the 2D quasi-momentum space $\boldsymbol{k}=(k_x,k_y)$, and the QGT of the lower Bloch band can be obtained by substituting $u(k)_-$ into Eq. (4), then we have

$$Q_{xy}=\frac{1}{4}(\partial_{kx}\theta\partial_{ky}\theta+\partial_{kx}\Phi\partial_{ky}\Phi\,\sin^2\theta)+\frac{1}{4}i\,\sin\,\theta(\partial_{kx}\Phi\partial_{ky}\theta-\partial_{ky}\Phi\partial_{kx}\theta). \tag{8}$$

The corresponding Riemannian metric and Berry curvature can be obtained by using the relation $g_{xy}=\mathrm{Re}\,Q_{xy}$ and $F_{xy}=-2\,\mathrm{Im}\,Q_{xy}$. The direct calculations of geometric tensor Q_{xy} is tedious, however, it can be verified that the determinant of the Riemannian metric can be expressed as (for details see Appendix A)

$$\det g=(\mathrm{Im}\,Q_{xy})^2=\left(\frac{\hat{\boldsymbol{d}}\cdot\partial_{k_x}\hat{\boldsymbol{d}}\times\partial_{k_y}\hat{\boldsymbol{d}}}{4}\right)^2=\frac{(m\,\cos\,k_x\cos\,k_y+\cos\,k_x+\cos\,k_y)^2}{16[(m+\cos\,k_x+\cos\,k_y)^2+\sin^2k_x+\sin^2k_y]^3} \tag{9}$$