Physics Letters A 380 (2016) 2888–2891

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

A new method to calculate Berry phase in one-dimensional quantum anomalous Hall insulator

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ARTICLE INFO

Article history:
Received 5 May 2016
Received in revised form 16 June 2016
Accepted 26 June 2016
Available online 1 July 2016
Communicated by R. Wu

Keywords:
Berry phase
Chern number
Quantum anomalous Hall insulator
Su–Schrieffer–Heeger model

ABSTRACT

Based on the residue theorem and degenerate perturbation theory, we derive a new, simple and general formula for Berry phase calculation in a two-level system for which the Hamiltonian is a real symmetric matrix. The special torus topology possessed by the first Brillouin zone ($1BZ$) of this kind of systems ensures the existence of a nonzero Berry phase. We verify the correctness of our formula on the Su–Schrieffer–Heeger (SSH) model. Then the Berry phase of one-dimensional quantum anomalous Hall insulator (1DQAHI) is calculated analytically by applying our method, the result being $-\frac{\pi}{2}-\frac{\pi}{4}\,\mathrm{sgn}(B)[\mathrm{sgn}(\Delta-4B)+\mathrm{sgn}(\Delta)]$. Finally, illuminated by this idea, we investigate the Chern number in the two-dimensional case, and find a very simple way to determine the parameter range of the non-trivial Chern number in the phase diagram.

1. Introduction

The Berry phase entered the lexicon of physics some 30 years ago [1]. Since then, numerous applications and experimental confirmations of this phase have been found in various physical systems [2–6]. A classical result showed in Berry's work [1] was that for a closed loop the Berry phase associated with the ground state is the half of the solid angle swept out [7]. This geometric phase is connected with a classical angle, namely, the Hannay angle [8], by a simple and elegant expression in the semiclassical limit [9]. However, compared with the case of three-dimensional variable space, where Pauli matrix σ_y naturally contains imaginary number i, this result is difficult to understand if being directly translated to one-dimensional lattice case [1,10,11]. In the case of a two-level systems such as SSH model, their Hamiltonian can be described by a real symmetric matrix and be parametrized by a closed curve in a plane. In the general definition, the Berry phase is calculated through integrating over the $1BZ$ [12–16]. The essential difficulty exists in the progress where canceling imaginary unit i is not trivial. A natural solution is to use the residue theorem. Nevertheless, due to the energy degenerate, calculating residues is technically challenging. Fortunately, by methods of degenerate perturbation theory, we can find an ingenious way to do this [1,10].

The purpose of this Letter is to discuss a more convenient method to calculate and understand Berry phases in some general systems such as anomalous Hall effect [17], topological semimetal [18,19] and crystalline insulator [20]. The mathematical and physical structures that Berry phase entails are very rich. For example, the integral of the Berry curvature, which is related to Berry phase in a two-dimensional system, over a close surface is guaranteed to be an integer multiple of 2π. The integer, known as the Chern number, is a topological invariant. Moreover, the adoption of the Berry-phase concepts has established a link between the anomalous Hall effect and the topological nature of the Hall currents. The ideas and techniques in the Letter could contribute to the understanding of these topological materials. Berry phase plays a fundamental role in determining all kinds of special property in topological materials. Compared with standard mathematically demanding approach, this Letter offers a natural and compact method to calculate the Berry phase in general one-dimensional case.

The structure of this Letter is as follows. In Sec. 2, by the method of topological transformation, we derive a general formula to calculate Berry phase in a two-level system. We verify the formula with SSH model in Sec. 3. The Berry phase of a positive-energy wave function in 1DQAHI is calculated in Sec. 4. In Sec. 5, we consider the positional relationships between degenerate points and the torus which is topologically equivalent to the $1BZ$ in the two-dimensional case. Inspired by the discussion in the above sections, we present an easy method to determine the parameter range of the non-trivial Chern number in the phase diagram.

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http://dx.doi.org/10.1016/j.physleta.2016.06.047
0375-9601/

2. Berry phase in two-level system with real symmetric matrix

One can take a general two-level system in solid physics, whose Hamiltonian reads

$$H(k)=\begin{pmatrix} h(k) & g(k) \\ g(k) & -h(k) \end{pmatrix}. \tag{1}$$

Here, k is an arbitrary parameter, yet one usually chooses it as wave vector which is in $1BZ$. In one-dimensional case, $k\in[-\pi,\pi]$. The real matrix elements h and g are the periodic functions of k. Then eigenvalue of energy is $E_\pm\equiv\pm r=\pm\sqrt{h^2+g^2}$. $\Psi_\pm$ is corresponding to eigen vectors. The wave function of positive energy reads

$$\Psi_+=\begin{pmatrix} \frac{g}{\sqrt{g^2+(r-h)^2}} \\ \frac{r-h}{\sqrt{g^2+(r-h)^2}} \end{pmatrix}. \tag{2}$$

Especially, if there exists k_0, which makes $g=h=0$, namely, energies are degenerate. One can use $|\uparrow>$, $|\downarrow>$ to label two basic vectors.

The Hamiltonian, eigenvalue of energies and wave functions satisfy

$$\begin{aligned} &H(k=\pi)\equiv H(k=-\pi); \\ &E(k=\pi)=E(k=-\pi); \\ &|\Psi(k=\pi)|=|\Psi(k=-\pi)|. \end{aligned} \tag{3}$$

Therefore, the point $-\pi$ is physically equivalent to π in one-dimensional case. That is to say, $1BZ$ is topologically equivalent to a close circle.

The Berry phase is defined by following formula, which reads,

$$\gamma_+\equiv-\gamma_-=i\int_{1BZ}<\Psi_+|\frac{d}{dk}|\Psi_+>dk. \tag{4}$$

For convenience, the Berry phase related positive energy also reads,

$$\begin{aligned} \gamma_+&=i\int_{1BZ}<\Psi_+|\frac{dh}{dk}\frac{\partial}{\partial h}+\frac{dg}{dk}\frac{\partial}{\partial g}|\Psi_+>dk \\ &=i\int_{\partial C^+}<\Psi_+|dh\frac{\partial}{\partial h}+dg\frac{\partial}{\partial g}|\Psi_+>. \end{aligned} \tag{5}$$

Here, the point (g,h) satisfies the equation of the close curve ∂C, that reads,

$$\partial C: F(g,h)=0. \tag{6}$$

The symbol ∂C^+ is corresponding to anti-clockwise rotation of wave vector k.

If there are not degenerate points in zone C, or on curve ∂C,

$$\begin{aligned} \gamma_+&=i\int_{\partial C^+}\left(\frac{g}{\sqrt{g^2+(r-h)^2}},\quad\frac{r-h}{\sqrt{g^2+(r-h)^2}}\right) \\ &\quad\times\begin{pmatrix} \frac{[g(r-h)^2]dh+\{r[(r-h)^2+g^2]-g^2(2r-h)\}dg}{r[\sqrt{g^2+(r-h)^2}]^3} \\ \frac{[-g^2(r-h)]dh+\{g[g^2+(r-h)^2]-g(2r-h)(r-h)\}dg}{r[\sqrt{g^2+(r-h)^2}]^3} \end{pmatrix} \\ &=\int_{\partial C^+}0dh+0dg=0. \end{aligned} \tag{7}$$

Next, let us calculate the residue number of integrand function. We can make a topological transformation to turn the curve ∂C into the circle ∂S, reads

$$z=c(\omega),\ z\equiv\mathrm{Re}\,z+i\,\mathrm{Im}\,z,\ \omega\equiv h+ig. \tag{8}$$

Here $c(\omega)$ are the suitable continuous function of ω, to make z satisfy the equation of circle ∂S, that reads,

$$z-z_0=Re^{ik}. \tag{9}$$

Here, z_0 is the circle point, and R is the radius. Therefore,

$$\gamma_+=i\int_{1BZ}<\Psi_+|\frac{d}{dk}|\Psi_+>dk=i\int_{\partial S^+}<\Psi'_+(z)|\frac{d}{dz}|\Psi'_+(z)>dz. \tag{10}$$

Here, $|\Psi'_\pm(z)>$ are wave functions of argument z. If $z=0+i0$, it is a degenerate point.

Basing on degenerate perturbation theory [10], one can obtain a wonderful result that reads,

$$\begin{aligned} &|\Psi'_\pm(z)>=\cos\chi_\pm|\uparrow>+\sin\chi_\pm|\downarrow>; \\ &|\Psi'_+(-z)>=\cos\chi'_+|\uparrow>+\sin\chi'_+|\downarrow>. \end{aligned} \tag{11}$$

Here, $2\chi_+=2\chi_--\pi$, $2\chi_+=2\chi'_+-\pi$. So $\chi'_+=\chi_-$. Therefore, one can get

$$|\Psi'_+(-z)>=|\Psi'_-(z)>. \tag{12}$$

Because of the orthogonality of eigen vectors, which reads,

$$<|\Psi'_+(z)|\Psi'_-(z)>=0,\ <|\Psi'_+(z)|\Psi'_+(z)>=1. \tag{13}$$

The value of the integrand function near the degenerate point $(0,0)$ reads,

$$\begin{aligned} &(<\Psi'_+|\frac{d}{dz}|\Psi'_+>)_{(0.0)} \\ &\equiv\lim_{z\to0}\frac{<\Psi'_+(z)|\Psi'_+(z)>-<\Psi'_+(z)|\Psi'_+(-z)>}{2z} \\ &=\lim_{z\to0}\frac{<\Psi'_+(z)|\Psi'_+(z)>-<\Psi'_+(z)|\Psi'_-(z)>}{2z}=\frac{1}{2z}. \end{aligned} \tag{14}$$

Hence, we have an important result that the residue number reads,

$$\mathrm{Res}(<\Psi'_+|\frac{d}{dz}|\Psi'_+>)|_{(z=0)}=\frac{1}{2}. \tag{15}$$

There conclusions are list as follows (i), (ii) and (iii).

(i) $(0,0)$ is not in $C\cup\partial C$, the Berry phase reads,

$$\gamma_+=0. \tag{16}$$

(ii) $(0,0)\in C$, the Berry phase reads,

$$\gamma_+=i(2\pi i)\,\mathrm{Res}(<\Psi'_+|\frac{d}{dz}|\Psi'_+>)|_{(z=0)}=-\pi. \tag{17}$$

(iii) $(0,0)\in\partial C$, the Berry phase reads

$$\gamma_+=i(\pi i)\,\mathrm{Res}(<\Psi'_+|\frac{d}{dz}|\Psi'_+>)|_{(z=0)}=-\frac{\pi}{2}. \tag{18}$$

3. Berry phase in SSH model

Let us inspect the case of SSH model introduced to describe electrons in 1D polyacetylene [21,22]. Researchers have found that the SSH model is a very important and useful model to explain diverse physical phenomena. For example, by means of the particle–boson coupling taken from SSH model, ones can study the sharp transition for single polarons [23]. Using the inversion symmetry which is the bosonic analogue of the SSH model, ones can analyze interacting ultracold bosonic atoms in a one-dimensional superlattice potential with alternating tunneling rates [24]. SSH model is