Berry phase of a two-level system

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We study a two-level system

$$\begin{aligned} H &= \boldsymbol{B} \cdot \boldsymbol{\sigma} \\ &= B \left(\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta \right) \cdot \boldsymbol{\sigma} \\ &= B \begin{pmatrix} \cos\theta & e^{-\mathrm{i}\phi} \sin\theta \\ e^{\mathrm{i}\phi} \sin\theta & \cos\theta \end{pmatrix}, \end{aligned} \tag{1}$$

where $\boldsymbol{\sigma} \coloneqq (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices, and $\boldsymbol{B} = B \left(\sin\theta \cos\phi, \sin\theta \cos\phi, \cos\theta \right)$ is a parameter in polar coordinates ($B > 0$, $0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$). Since B merely sets an energy scale, we assign $B = 1$ below. We consider the Berry phase of the lower level $\left| \downarrow \right\rangle = \left| \downarrow (\theta, \phi) \right\rangle$ with the eigenenergy $E = -B = -1$ in two-dimensional (θ, ϕ) space.

Owing to the spinor structure, the Berry curvature should be uniform in (θ, ϕ) space. Thus, let us first focus on the behavior around $\theta = 0$ and expand

$$\boldsymbol{B} \simeq (n_x, n_y, 1) \quad \left(\left| n_x \right|, \left| n_x \right| \ll 1 \right). \tag{2}$$

With this parametrization, the lower level $\left| \downarrow \right\rangle = \left| \downarrow (n_x, n_y) \right\rangle$ is given as

$$\left| \downarrow (n_x, n_y) \right\rangle \simeq \begin{pmatrix} \left(n_x - \mathrm{i} n_y \right)/2 \\ -1 \end{pmatrix}. \tag{3}$$

Accordingly, the Berry connection is obtained as

$$A_{n_x} = \mathrm{i} \left\langle \downarrow \right| \partial_{n_x} \left| \downarrow \right\rangle = \frac{\mathrm{i}}{4} \left(n_x + \mathrm{i} n_y \right), \tag{4}$$

$$A_{n_y} = \mathrm{i} \left\langle \downarrow \right| \partial_{n_y} \left| \downarrow \right\rangle = \frac{1}{4} \left(n_x + \mathrm{i} n_y \right), \tag{5}$$

yielding the Berry curvature

$$F = \partial_{n_x} A_{n_y} - \partial_{n_y} A_{n_x} = \frac{1}{2}. \tag{6}$$

Then, the Chern number is given as

$$C = \oint \frac{d\theta d\phi}{2\pi} F = 1, \tag{7}$$

which is indeed quantized, consistent with the general discussion.

The nonzero Chern number necessitates singularities in the Berry connection $\boldsymbol{A}$ somewhere in two-dimensional (θ, ϕ) space. To confirm such singularities, we express the lower level $\left| \downarrow \right\rangle = \left| \downarrow (\theta, \phi) \right\rangle$, with one possible gauge choice, as

$$\left| \downarrow (\theta, \phi) \right\rangle = \begin{pmatrix} e^{-\mathrm{i}\phi} \sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix}. \tag{8}$$

The corresponding Berry connection is obtained as[*1]

$$A_\theta = \mathrm{i} \langle \downarrow | \partial_\theta | \downarrow \rangle = 0, \tag{10}$$

$$A_\phi = \mathrm{i} \langle \downarrow | \left(\frac{\partial_\phi}{\sin\theta} \right) | \downarrow \rangle = \frac{\sin^2(\theta/2)}{\sin\theta} = \frac{1}{2}\tan(\theta/2), \tag{11}$$

which indeed diverges at $\theta = \pi$. Additionally, the Berry curvature is given as

$$F = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (A_\phi \sin\theta) = \frac{1}{2}, \tag{12}$$

which is consistent with Eq. (6). Alternatively, let us take another gauge choice,

$$|\downarrow(\theta,\phi)\rangle = \begin{pmatrix} \sin(\theta/2) \\ -e^{\mathrm{i}\phi}\cos(\theta/2) \end{pmatrix}. \tag{13}$$

The corresponding Berry connection is obtained as

$$A_\theta = \mathrm{i} \langle \downarrow | \partial_\theta | \downarrow \rangle = 0, \tag{14}$$

$$A_\phi = \mathrm{i} \langle \downarrow | \left(\frac{\partial_\phi}{\sin\theta} \right) | \downarrow \rangle = -\frac{\cos^2(\theta/2)}{\sin\theta} = -\frac{1}{2\tan(\theta/2)}, \tag{15}$$

which diverges at $\theta = 0$.

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As an application, let us consider a continuous Dirac model in two dimensions:

$$H(\boldsymbol{k}) = k_x\sigma_x + k_y\sigma_y + m\sigma_z \qquad \left(\boldsymbol{k} \in \mathbb{R}^2\right) \tag{16}$$

with a mass parameter $m \in \mathbb{R}$. The occupied band is represented as Eq. (8) with

$$\phi(\boldsymbol{k}) \coloneqq \tan^{-1}\frac{k_y}{k_x} \in [0, 2\pi), \quad \theta(\boldsymbol{k}) \coloneqq \tan^{-1}\frac{\sqrt{k_x^2 + k_y^2}}{m} \in [0, \pi]. \tag{17}$$

To calculate the Berry connection, we employ $k \coloneqq \sqrt{k_x^2 + k_y^2} \in [0, \infty)$ and $\phi \in [0, 2\pi)$, leading to

$$A_k = \mathrm{i} \langle \downarrow | \partial_k | \downarrow \rangle = 0, \quad A_\phi = \mathrm{i} \langle \downarrow | \left(\frac{\partial_\phi}{k} \right) | \downarrow \rangle = \frac{\sin^2(\theta/2)}{k} = \frac{1}{2k}\left(1 - \frac{m}{\sqrt{k^2+m^2}}\right). \tag{18}$$

Consequently, the Berry curvature is given as

$$F = \frac{1}{k}\frac{\partial}{\partial k}(kA_\phi) = \frac{m}{2(k^2+m^2)^{3/2}}, \tag{19}$$

and the Chern number is accordingly obtained as

$$C = \oint \frac{d^2k}{2\pi} F = \frac{m}{2}\int_0^\infty \frac{kdk}{(k^2+m^2)^{3/2}} = \frac{\operatorname{sgn} m}{2}\int_0^\infty \frac{xdx}{(x^2+1)^{3/2}} = \frac{\operatorname{sgn} m}{2}. \tag{20}$$

[*1] The gradient in polar coordinates on the unit sphere reads

$$\nabla = \boldsymbol{e}_\theta \partial_\theta + \boldsymbol{e}_\phi \frac{\partial_\phi}{\sin\theta}. \tag{9}$$