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Problem 1: Gauge-invariant computation of the Berry phase

Learning objective

In the lecture we introduced the Berry phase and provided an expression in terms of the Berry curvature that depends on derivatives of the parameter-dependent eigenstates. This restricts the gauges to be continuous in the parameters—a condition that is often impossible to satisfy in numerical studies. Here you derive an equivalent expression that is manifestly gauge-invariant and therefore useful for numerical computations of Berry phases and Chern numbers.

Consider a Hamiltonian $H(\mathbf{\Gamma})$ with instantaneous (non-degenerate) eigenbasis $\{|n(\mathbf{\Gamma})\rangle\}$ and eigenenergies $E_n(\mathbf{\Gamma})$; in the following we focus on one of the eigenstates and denote it as $|v(\mathbf{\Gamma})\rangle$. In the lecture, the Berry phase on the subspace spanned by $|v(\mathbf{\Gamma})\rangle$ along a closed path Γ was defined as the contour integral

$$\gamma(\Gamma) = i \oint_\Gamma \langle v(\mathbf{\Gamma})| \, \partial_{\mathbf{\Gamma}} \, |v(\mathbf{\Gamma})\rangle \, \mathrm{d}\mathbf{\Gamma} \,. \tag{1}$$

The basis can be changed by gauge transformations $|v(\mathbf{\Gamma})\rangle \mapsto e^{i\xi(\mathbf{\Gamma})} |v(\mathbf{\Gamma})\rangle$ but the gauges in Eq. (1) are not arbitrary: they must be sufficiently smooth since $\partial_{\mathbf{\Gamma}} |v(\mathbf{\Gamma})\rangle$ needs to be well-defined on the contour.

In numerical studies one often determines the instantaneous eigenbasis for different parameters $\mathbf{\Gamma}$ independently. Since each computation can pick an arbitrary phase for the basis states, it is typically not guaranteed that the resulting gauge is continuous. In the following, you will derive an equivalent expression that circumvents this problem by removing the derivative from the states.

Here we will focus on the case of a three-dimensional parameter space $\mathbf{\Gamma} \in \mathbb{R}^3$ so that Stoke's theorem takes its "usual" form.

a) Use Stoke's theorem to show that

$$\gamma(\Gamma) = i \int_\Sigma \varepsilon_{ijk} \left\langle \partial_{\Gamma_j} v(\mathbf{\Gamma}) \middle| \partial_{\Gamma_k} v(\mathbf{\Gamma}) \right\rangle \mathrm{d}\sigma_i \tag{2}$$

where Σ is a 2D submanifold in the parameter space such that $\partial\Sigma = \Gamma$; $\mathrm{d}\boldsymbol{\sigma}$ is the oriented surface element on Σ and summation over repeated indices is implied.

b) Use the completeness of the instantaneous eigenstates to derive

$$\gamma(\Gamma) = i \sum_{n \neq v} \int_\Sigma \varepsilon_{ijk} \left\langle \partial_{\Gamma_j} v(\mathbf{\Gamma}) \middle| n(\mathbf{\Gamma}) \right\rangle \langle n(\mathbf{\Gamma}) | \partial_{\Gamma_k} v(\mathbf{\Gamma}) \rangle \, \mathrm{d}\sigma_i \,. \tag{3}$$

(*Hint:* Use that $\partial_{\Gamma_i} \langle n(\mathbf{\Gamma}) | n(\mathbf{\Gamma}) \rangle = 0$.)

c) Now show that

$$\langle n(\mathbf{\Gamma})|\partial_{\Gamma_k} v(\mathbf{\Gamma})\rangle = \frac{\langle n(\mathbf{\Gamma})|\,[\partial_{\Gamma_k} H(\mathbf{\Gamma})]\,|v(\mathbf{\Gamma})\rangle}{E_v(\mathbf{\Gamma}) - E_n(\mathbf{\Gamma})} \tag{4}$$

to derive the final expression

$$\gamma(\Gamma) = i \sum_{n\neq v} \int_\Sigma \frac{\langle v(\mathbf{\Gamma})|\,[\partial_{\mathbf{\Gamma}} H(\mathbf{\Gamma})]\,|n(\mathbf{\Gamma})\rangle \times \langle n(\mathbf{\Gamma})|\,[\partial_{\mathbf{\Gamma}} H(\mathbf{\Gamma})]\,|v(\mathbf{\Gamma})\rangle}{(E_v(\mathbf{\Gamma}) - E_n(\mathbf{\Gamma}))^2}\, \mathrm{d}\boldsymbol{\sigma}\,. \tag{5}$$

Note that the choice of a continuous gauge is no longer a requirement to evaluate this expression as it is manifestly gauge invariant. However, there *is* an ambiguity in choosing Σ for a given path Γ if the gap closes at some point(s) in parameter space because Σ must not cross these points (denominator!); the choice of Σ then determines the outcome of the integral.

Problem 2: Spin in a magnetic field revisited

> **Learning objective**
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> In a previous problem you studied the Berry phase that is collected by a spin-$\frac{1}{2}$ that adiabatically follows a varying magnetic field. Here you will redo this calculation using the gauge-invariant method derived in Problem 1 for arbitrary spins S. You will find that integer and half-integer spins behave differently.

Consider a single spin $S \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \dots\}$ in the magnetic field $\boldsymbol{B}$ described by the spin operator $\boldsymbol{S}$ and the Hamiltonian

$$H(\boldsymbol{B}) = \boldsymbol{B}\cdot\boldsymbol{S} \tag{6}$$

where again $\boldsymbol{B}$ plays the role of slowly varying parameters.

a) Derive the instantaneous (formal) eigenstates and eigenenergies of Eq. (6).

   How does $B = |\boldsymbol{B}|$ affect potential degeneracies?

b) Fix one of the non-degenerate manifolds of eigenstates, say $|m^*(\boldsymbol{B})\rangle$ with $m^* \in \{-S, -S+1, \dots, S-1, S\}$, and consider a closed loop $\Gamma : t \mapsto \boldsymbol{B}$ in the parameter space of magnetic fields that does not touch the origin, $\boldsymbol{B}(t) \neq \mathbf{0}$ for all $t \in [0, T]$.

   Show that the Berry phase can be computed as

$$\gamma(\Gamma) = i \sum_{m\neq m^*} \int_\Sigma \frac{\langle m^*(\boldsymbol{B})|\,\boldsymbol{S}\,|m(\boldsymbol{B})\rangle \times \langle m(\boldsymbol{B})|\,\boldsymbol{S}\,|m^*(\boldsymbol{B})\rangle}{B^2(m^*-m)^2}\, \mathrm{d}\boldsymbol{\sigma}\,. \tag{7}$$

   (*Hint:* Use the results of Problem 1.)

c) Use the eigenbasis for $\boldsymbol{B} = B\boldsymbol{e}_z$ to evaluate Eq. (7) and show that

$$\gamma(\Gamma) = -\int_\Sigma \frac{m^*}{B^3}\,\boldsymbol{B}\cdot \mathrm{d}\boldsymbol{\sigma} = -m^*\,\Omega_\Sigma \tag{8}$$

   with the solid angle Ω_Σ defined by the projection of Σ onto the unit sphere.

   (*Hint:* Use $S^\pm = S_x \pm iS_y$ and that $\boldsymbol{S}$ is a vector operator.)

d) Let Γ trace out a great circle and compare the Berry phase collected by half-integer and integer spins when adiabatically rotated once around an arbitrary axis orthogonal to their quantization axis.

Problem 3: Sum of Chern numbers

Learning objective

It is a well-known (and useful) fact that the sum of Chern numbers over all bands of a lattice model vanishes identically. Here you show this statement.

For a lattice model with M bands and Bloch functions $|u_{n\boldsymbol{k}}\rangle$, we introduced the Berry curvature on the Brillouin zone as ($\tilde{\partial}_i = \partial_{k_i}$, $i = x, y$)

$$\mathcal{F}_{ij}^{[n]}(\boldsymbol{k}) = \tilde{\partial}_j \mathcal{A}_i^{[n]} - \tilde{\partial}_i \mathcal{A}_j^{[n]} = -i \left\langle \tilde{\partial}_j u_{n\boldsymbol{k}} \middle| \tilde{\partial}_i u_{n\boldsymbol{k}} \right\rangle + i \left\langle \tilde{\partial}_i u_{n\boldsymbol{k}} \middle| \tilde{\partial}_j u_{n\boldsymbol{k}} \right\rangle \tag{9}$$

and the Chern number of band $n = 1, \ldots, M$ as

$$C^{[n]} = -\frac{1}{2\pi} \int_{T^2} \mathcal{F}_{xy}^{[n]} \, \mathrm{d}^2 k \,. \tag{10}$$

Show that

$$\sum_{n=1}^{M} C^{[n]} = 0 \tag{11}$$

by showing that the total Berry curvature of all bands $\sum_{n=1}^{M} \mathcal{F}_{ij}^{[n]}(\boldsymbol{k})$ vanishes for every $\boldsymbol{k}$.

(*Hint:* Use the completeness of the Bloch functions for fixed $\boldsymbol{k}$.)