Dr. Nicolai Lang
Institute for Theoretical Physics III, University of Stuttgart

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Problem 3.1: Gauge-invariant computation of the Berry phase

[**Written** | 3 pt(s)]

ID: ex_gauge_invariant_computation_berry_phase:tqp25

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

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

where summation over repeated indices is implied.

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 derive an equivalent expression for Eq. (1) that circumvents this problem by removing the derivative from the states.

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

a) Use Stokes' theorem to show that **1**pt(s)

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

Here, Σ is a 2D submanifold in parameter space such that its boundary $\partial\Sigma = \Gamma$ and $\mathrm{d}\boldsymbol{\sigma}$ denotes the oriented surface element on Σ.

b) Use the completeness of the instantaneous eigenbasis to derive **1**pt(s)

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

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

c) Now show that **1**pt(s)

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

and use this to derive the final expression

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

Note that the choice of a continuous gauge is no longer a requirement to evaluate this expression as it is manifestly gauge invariant.

However, if the gap closes at some points in parameter space, Σ must not cross these points (the denominator would vanish). Then there *is* an ambiguity in choosing Σ for a given path Γ and the choice of Σ determines the outcome of the integral.

Problem 3.2: Spin in a magnetic field revisited

[**Oral** | 6 pt(s)]

ID: ex_spin_magnetic_field:tqp25

Learning objective

In Problem 2.2 you studied the Berry phase that is collected by a spin-$\frac{1}{2}$ that adiabatically follows a varying magnetic field. Here you redo this calculation for arbitrary spins S using the manifestly gauge-invariant method derived in Problem 3.1. You will find that integer and half-integer spins behave differently.

Consider a single spin $S \in \frac{1}{2}\mathbb{N}_0$ in an external magnetic field $\boldsymbol{B}$. This is described by the Hamiltonian

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

where $\boldsymbol{S} = (S_x, S_y, S_z)^T$ is the spin operator. As in Problem 2.2, $\boldsymbol{B}$ plays the role of a slowly varying, tunable parameters (in the lecture called $\mathbf{\Gamma}$), i.e., the parameter space is isomorphic to $\mathbb{R}^3$.

a) Derive the instantaneous eigenstates and eigenenergies of the Hamiltonian (6). **1**pt(s)

For which choice of parameters $\boldsymbol{B}$ are the ground states non-degenerate?

In the following, we fix one of the non-degenerate eigenstates and denote it by $|m^*(\boldsymbol{B})\rangle$ with $m^* \in \{-S, -S+1, \ldots, S\}$. Let us consider a closed path $\Gamma : t \mapsto \boldsymbol{B}(t)$ with $t \in [0, T]$ in parameter space that does not touch the origin so that $\boldsymbol{B}(t) \neq \mathbf{0}$ for all $t \in [0, T]$.

b) Show that the Berry phase along this path can be computed as **1**pt(s)

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

where Σ denotes a 2D surface in parameter space that does not touch the origin ($\boldsymbol{B} = \mathbf{0}$) and is bounded by the parameter path Γ ($\partial\Sigma = \Gamma$).

Hint: Use the results from Problem 3.1.

c) Evaluate the matrix elements in the expression (7) for the Berry phase for arbitrary $\boldsymbol{B}$. **3**pt(s)

Use this to show that the Berry phase evaluates to

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

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

Hint: Use the raising and lowering operators $S^\pm = S_x \pm iS_y$ to evaluate the matrix elements in the case where $\boldsymbol{B} = \boldsymbol{B}_0 := B\boldsymbol{e}_z$ points in the direction of the quantization axis. Then use that $\boldsymbol{S}$ is a *vector operator* to derive the matrix elements for arbitrary, rotated $\boldsymbol{B}$.

d) Finally, consider a path Γ that traces out a great circle in parameter space and calculate the collected Berry phase when adiabatically traversing the path. **1**pt(s)

Compare the phase collected by *half-integer* spins and *integer* spins.

Problem 3.3: Sum of Chern numbers

[**Written** | 2 pt(s)]

ID: ex_sum_chern_numbers:tqp25

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.

Consider a lattice model with M bands labeled by $n \in \{1,\dots,M\}$ and Bloch functions $|u_{n\boldsymbol{k}}\rangle$.

In the lecture, we introduced the *Berry curvature* on the Brillouin zone for the n-th band as

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

and defined the *Chern number* of the n-th band as

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

Here we use the short-hand notation $\tilde{\partial}_i := \partial_{k_i}$ for $i \in \{x,y\}$.

Show that the sum of the Berry curvature over all bands vanishes,

$$\sum_{n=1}^{M}\mathcal{F}^{[n]}_{ij}(\boldsymbol{k}) = 0 \quad \text{for every } \boldsymbol{k}\in T^2. \tag{11}$$

Use this to show that the sum of the Chern numbers over all bands vanishes as well,

$$\sum_{n=1}^{M} C^{[n]} = 0\,. \tag{12}$$

Hint: Use that the Bloch functions for fixed $\boldsymbol{k}$ form a complete, orthonormal basis of $\mathcal{H}(\boldsymbol{k})$.