# TA 12. Berry phase: Magnetic monopoles in parameter space

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This tutorial is mostly based on Shimon's notes, Section 4.3 of the Adiabatic theorem chapter, and Section 1.5 of [1606.06687].

## 1 Introduction: connection of Berry phase with gauge potentials

You studied during lectures the Berry phase as a physical phase, arising in the context of adiabatic changes in the parameter space $\vec{R}$ of the Hamiltonian $H(\{x_i, p_i\}; \vec{R})$, where $\{x_i, p_i\}$ are the dynamical variables of the system, whereas $\vec{R}$ are the parameters of the Hamiltonian (for example, a fixed, not dynamical external magnetic field).

There are several connection of Berry phase with gauge potentials. Let's first recall some quantities which are useful in discussing the Berry phase. At first, the physical Berry phase reads

$$\gamma = \oint_C \mathcal{A}_i \, \mathrm{d}R_i \ , \ \mathcal{A}_i = \mathrm{i} \left\langle \psi(\vec{R}) \middle| \frac{\partial}{\partial R_i} \middle| \psi(\vec{R}) \right\rangle \ , \tag{1.1}$$

where $C$ is a *closed* contour in parameter space, $\psi(\vec{R})$ is the parameter-dependent wavefunction, and $\mathcal{A}_i$ is called the connection, which is the analogous of a vector potential in gauge theories. To better see this last point, notice that, under a overall phase change of the wavefunction, the connection changes,

$$\psi' = \mathrm{e}^{\mathrm{i}\chi(\vec{R})}\psi \implies \mathcal{A}'_i = \mathcal{A}_i + \partial_i \chi \ ; \tag{1.2}$$

the analogy with the vector potential is apparent, and one can see the phase change of the wavefunction as a gauge transformation. Physics should be invariant with respect to this gauge transformation, and in fact it is possible to recast the Berry phase as depending on the curvature (analogous of the field strength) $\mathcal{F}_{ij}$, by means of the generalized Stokes theorem

$$\gamma = \int_S \mathcal{F}_{ij} \, \mathrm{d}S_{ij} \ , \ \mathcal{F}_{ij} = \frac{\partial \mathcal{A}_i}{\partial R_j} - \frac{\partial \mathcal{A}_j}{\partial R_i} \ , \tag{1.3}$$

where $S$ is a two-dimensional surface in the parameter space bounded by $C$. Notice that, in a 3D parameter space (the one we will be interested in the following), we can write

$$\gamma = \int_S \boldsymbol{\nabla} \times \vec{\mathcal{A}} \cdot \mathrm{d}\vec{S} \ , \tag{1.4}$$

which is the (hopefully) familiar Stokes theorem.

## 2 Berry connection for a 2 level system

Let's discuss the Berry phase in the context of a two level system; the hermitian Hamiltonian can generically be written as

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{pmatrix} = \frac{1}{2}(H_{11} + H_{22})\mathbb{1} + \begin{pmatrix} (H_{11} - H_{22})/2 & H_{12} \\ H_{12}^* & (H_{22} - H_{11})/2 \end{pmatrix} =: H_1 + H_2 \ ; \tag{2.1}$$

we will focus on $H_2$, since it will have the same eigenstates and just shifted eigenvalues as the full $H$; in fact

$$(H_1 + H_2) \left|\lambda\right\rangle = \lambda \left|\lambda\right\rangle \implies H_2 \left|\lambda\right\rangle = \left(\lambda - \frac{1}{2}(H_{11} + H_{22})\right) \left|\lambda\right\rangle \ . \tag{2.2}$$

We will rewrite $H_2$ as

$$H_2 =: \begin{pmatrix} Z & X + \mathrm{i}Y \\ X - \mathrm{i}Y & -Z \end{pmatrix} \ . \tag{2.3}$$

Notice that $H$ can be seen as the Hamiltonian of a spin 1/2 particle in a magnetic field, $H \sim B + \vec{B} \cdot \vec{\sigma}$. This is the physical system you can have in mind in the following, where $\vec{R} = \{X, Y, Z\}$ can be seen as the cartesian components of an external magnetic field.

The eigenvalues of $H_2$ are

$$\det(H_2 - E\mathbb{1}) = 0 \implies E = \pm\sqrt{X^2 + Y^2 + Z^2} =: \pm R \ , \tag{2.4}$$

with eigenfunctions, for $E = R$ ($\psi = (\psi_1, \psi_2)$)

$$(H_2 - E\mathbb{1})\psi = 0 \implies (Z - R)\psi_1 + (X + \mathrm{i}Y)\psi_2 = 0 \implies \psi_1 = \frac{X + \mathrm{i}Y}{R - Z}\psi_2 \ ; \tag{2.5}$$

imposing $|\psi|^2 = 1$, we have

$$1 = |\psi_2|^2 \left( \frac{X^2 + Y^2 + R^2 + Z^2 - 2RZ}{(R - Z)^2} \right) = |\psi_2|^2 \frac{2R}{R - Z} \ , \tag{2.6}$$

so, up to an arbitrary phase (i.e. an analogous of gauge transform), we have

$$\psi_2 = \sqrt{\frac{R - Z}{2R}} = \sqrt{\frac{1}{2}(1 - \cos\theta)} = \sin\frac{\theta}{2} \ , \tag{2.7}$$

where we used spherical coordinates $\vec{R} = R(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ (and recall $\cos\theta = 1 - 2\sin^2(\theta/2)$). Similarly,

$$\psi_1 = \frac{X + \mathrm{i}Y}{R - Z}\sqrt{\frac{R - Z}{2R}} = \frac{\sin\theta \mathrm{e}^{\mathrm{i}\phi}}{\sqrt{2(1 - \cos\theta)}} = \cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi} \ . \tag{2.8}$$

For illustration purposes, let's consider two phase choices, $\chi = 0$ and $\chi = -\phi$; we then deal with the eigenfunctions

$$\psi_+ = \begin{pmatrix} \cos(\theta/2)\mathrm{e}^{\mathrm{i}\phi} \\ \sin\theta/2 \end{pmatrix} \ , \ \psi_- = \begin{pmatrix} \cos\theta/2 \\ \sin(\theta/2)\mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix} \ , \tag{2.9}$$

for the first and second phase choice respectively. The Berry connection then reads

$$\vec{\mathcal{A}}_\pm(\vec{R}) = \mathrm{i}\,\langle\psi_\pm|\boldsymbol{\nabla}_{\vec{R}}|\psi_\pm\rangle \ ; \tag{2.10}$$

in spherical coordinates,

$$\boldsymbol{\nabla}_{\vec{R}} = \hat{e}_R\frac{\partial}{\partial R} + \frac{\hat{e}_\theta}{R}\frac{\partial}{\partial\theta} + \frac{\hat{e}_\theta}{R\sin\theta}\frac{\partial}{\partial\phi} \ , \tag{2.11}$$

so

$$\boldsymbol{\nabla}_{\vec{R}}\psi_+ = \frac{\hat{e}_\theta}{2R}\begin{pmatrix} -\sin(\theta/2)\mathrm{e}^{\mathrm{i}\phi} \\ \cos\theta/2 \end{pmatrix} + \frac{\hat{e}_\phi \mathrm{i}\mathrm{e}^{\mathrm{i}\phi}\cos\theta/2}{R\sin\theta}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \ , \ \boldsymbol{\nabla}_{\vec{R}}\psi_- = \frac{\hat{e}_\theta}{2R}\begin{pmatrix} -\sin\theta/2 \\ \cos(\theta/2)\mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix} - \frac{\hat{e}_\phi \mathrm{i}\mathrm{e}^{-\mathrm{i}\phi}\sin\theta/2}{R\sin\theta}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \ . \tag{2.12}$$

The connection then reads

$$\mathcal{A}_\pm = -\hat{e}_\phi\frac{\pm 1 + \cos\theta}{2R\sin\theta} \ ; \tag{2.13}$$

notice that the two connections are related by

$$\boldsymbol{\nabla}\chi = \hat{e}_\phi\frac{1}{R\sin\theta} \ , \tag{2.14}$$

as it should.

## 3 A magnetic monopole?

We can compute the Berry curvature

$$\nabla \times \vec{\mathcal{A}}_\pm = \frac{\hat{e}_R}{R\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_{\pm,\phi}) = \frac{\hat{e}_R}{2R^2} \ , \tag{3.1}$$

with the connection of $\mathcal{A}$ as a vector potential of a "magnetic field in parameter space", we see that we obtain like a monopole sitting at the origin. Notice that the origin is the point of energy level crossing (since there the two energy levels are degenerate); due to this, one cannot apply our Berry phase computations on that part of the parameter space (which is a singularity). However, the mere presence of the singularity has effects outside the singularity itself, where the adiabatic theorem can be applied.

In particular, notice that Eq. (3.1) is the analogous of a magnetic monopole in parameter space, and it is independent from the gauge choice.

This magnetic monopole sitting at the center is what dictates the physics of the Berry phase in this system. To this magnetic monopole, we can assign the charge

$$4\pi g := \int_S \frac{\hat{e}_R}{2R^2}\cdot \mathrm{d}\vec{S} = 2\pi \implies \nabla\times\vec{\mathcal{A}}_\pm = g\frac{\hat{e}_R}{R^2} \ , \tag{3.2}$$

where $S$ is a sphere around the monopole, and $g = 1/2$.

We can connect the existence of this Berry magnetic monopole with a condition on the quantization of the Berry curvature flux, similar to how the presence of a electromagnetic magnetic monopole could explain the quantization of charge. In fact, from (1.3), by considering a path $C$ lying on the $X - Y$ plane, we have two (classes of) possible surface choices we can decide to do the computation with: one encircling the monopole from north, which we call $S_+$, one from south, which we call $S_-$; then

$$\int_{S_+} \frac{\hat{e}_R}{2R^2}\cdot \mathrm{d}\vec{S} = g\Omega \ , \tag{3.3}$$

where $\Omega$ is the solid angle corresponding to $S_+$, whereas

$$\int_{S_-} \frac{\hat{e}_R}{2R^2}\cdot \mathrm{d}\vec{S} = -g(4\pi-\Omega) \ , \tag{3.4}$$

where we took into account the different orientation of the surface. Notice that the two computations give the same phase factor modulo $2\pi$ only if $2g \in \mathbb{Z}$.

We can write this quantization condition (which ensures that physics does not depend on my choice of surface, as it should) as

$$\int_S \mathcal{F}_{ij}\,\mathrm{d}S_{ij} = 2\pi C \ , \tag{3.5}$$

where $C$ is called the Chern number, which labels different topological phases of the system.

## 4 Connections with Aharonov-Bohm flux

The previous discussion suggests a connection with the Aharonov-Bohm (AB) flux. We noticed that $\mathcal{A}_i(\vec{R})$ behaves as the vector potential $A_i(\vec{x})$. With the analogy $\mathcal{A}_i \to A_i$, $R_i \to x_i$, we have that the AB phase

$$\gamma \to \frac{q\Phi}{\hbar} = 2\pi\frac{\Phi}{\Phi_0} = 2\pi C \ ; \tag{4.1}$$

we see the Chern number entering here as well, which tells us that physics is unchanged if the AB flux is a multiple of $\Phi_0$.

## A The Dirac string

The attentive reader might have noticed that, in Eq. (3.1), there is associated a Dirac string. Notice in fact that $\mathcal{A}_+$ is singular for $\theta \to 0$; this corresponds to a branch cut in the positive $z$ axis. This, as you saw in the electromagnetic magnetic monopole lectures, can be called Dirac string. Instead, $\mathcal{A}_-$ is singular for $\theta \to \pi$; this corresponds to a branch cut in the negative $z$ axis. One can conclude that the orientation of the Dirac string is gauge dependent. This is not something harmful, since the Dirac string is not an observable.

We can euristically recover the magnetic field associated to the Dirac string (for more careful approaches, see [1810.13403]). Let's tentatively model the singularities arising in the curl computation as delta functions,

$$\nabla \times \vec{\mathcal{A}}_\pm = \frac{\hat{e}_R}{2R^2} + K\delta(X)\delta(Y)\Theta(\pm Z)\hat{Z} \ ; \tag{A.1}$$

The divergence of the previous gives

$$0 = 2\pi\delta(\vec{R}) + K\delta(X)\delta(Y)\hat{Z}\frac{\partial\Theta(\pm Z)}{\partial Z} = 2\pi\delta(\vec{R}) \pm K\delta(\vec{R}) \implies K = \mp 2\pi \ , \tag{A.2}$$

hence giving

$$\nabla \times \vec{\mathcal{A}}_\pm = \frac{\hat{e}_R}{2R^2} \mp 2\pi\delta(X)\delta(Y)\Theta(\pm Z)\hat{Z} \ . \tag{A.3}$$

Notice that the Dirac string makes such that the divergence of the curvature is zero everywhere, origin included. The effect of the Dirac string is unobservable granted that Eq. (3.5) holds (notice the strict parallelism with Dirac quantization argument and the Aharonov-Bohm effect; in fact, the string effect can be seen as the solenoid in Aharonov-Bohm, and if the AB flux is a multiple of $\Phi_0$, then the string is unobservable. This condition is easily seen to correspond to Eq. (3.5) in the context of Berry phase).