Berry Phase

Georg Manten (georg@manten.biz) 17th May 2017

1 Berry Phase

1.1 Introduction

We consider the general Hamiltonian

$$H\left(x^a;\lambda^i\right)$$

x^a : degrees of freedom of the system / things evolving dynamically
λ^i : parameters of the Hamiltonian, which are externally adjusted

First, we pick some values for λ, and then after placing the system in some energy eigenstate $|\psi\rangle$, which we choose for simplicity to be the ground state, we slowly vary λ. Therefore, the Hamiltonian changes and also the ground state $|\psi\left(\lambda\left(t\right)\right)\rangle$.

We make use of the **adiabatic theorem**, which says, that if we place a system in a non-degenerate energy eigenstate and vary parameters sufficiently slowly, the system will stick to this energy eigenstate and will not be excited to any higher or lower energystate.

Hereby, it is important how fast you change the parameters, which depends on the gap between the actual state and the nearest other state.
A very tricky case is **level-crossing**, where another case becomes degenerate with the one you are in, after seperating again, it is hard to tell in which linear combination of states the system is.

If we now vary the parameters slowly and perform a closed path in the space of parameters with the assumption that we do not pass a point with level-crossing, we would like to know, which point we are in afterwards.

Due to the adiabatic theorem, we are still in the ground state, and the only uncertainty is the phase

$$|\psi\rangle \longrightarrow e^{i\gamma}|\psi\rangle \tag{1}$$

This phase could have physical consequence, since we could start with two states and vary just one of them, and afterwards, $e^{i\gamma}$ has an effect if we interfere both.
There are two contributions to the phase, the dynamic one $e^{-i\frac{Et}{\hbar}}$, which is there for every energy eigenstate, even if we do not change the parameters, and the other one is the **Berry phase**.

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1.2 Computing the Berry Phase

The evolution of states is given by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\left|\psi\right\rangle}{\partial t}=H\left(\lambda\left(t\right)\right)\left|\psi\right\rangle \tag{2}$$

As a first step, we introduce a ground state with some arbitrary but fixed choice of phase $\left|n\left(\lambda\right)\right\rangle$ for every parameter λ. Therefore we can write the ground state as

$$\left|\psi\left(t\right)\right\rangle=U\left(t\right)\left|n\left(\lambda\left(t\right)\right)\right\rangle \tag{3}$$

with $U\left(t\right)$ a time-dependent phase. If we pick $\left|n\left(\lambda\left(t=0\right)\right)\right\rangle=\left|\psi\left(t=0\right)\right\rangle$ then we have $U\left(t=0\right)=1$.

There is always the dynamic contribution $e^{-i\int dtE_0(t)/\hbar}$, which we can ignore by setting the ground state energy $E_0\left(t\right)=0$. For the extra contribution, we plug in our adiabatic ansatz (3) in (2) and take the overlap with $\left\langle\psi\right|$:

$$\left\langle\psi\middle|\dot{\psi}\right\rangle=\dot{U}U^{\star}+\left\langle n|\dot{n}\right\rangle=0$$

where we have used $H\left(\lambda\right)\left|n\left(\lambda\right)\right\rangle=0$ to get zero on the right side of the equation. We get:

$$U^{\star}\dot{U}=-\left\langle n|\dot{n}\right\rangle=-\left\langle n\right|\frac{\partial}{\partial\lambda^{i}}\left|n\right\rangle\dot{\lambda}^{i} \tag{4}$$

Here we define the **Berry connection**

$$\mathcal{A}_{i}\left(\lambda\right)=-i\left\langle n\right|\frac{\partial}{\partial\lambda^{i}}\left|n\right\rangle \tag{5}$$

so we get the differential equation

$$\dot{U}=-i\mathcal{A}_{i}\dot{\lambda}^{i}U$$

which has the solution

$$U\left(t\right)=\exp\left(-i\int\mathcal{A}_{i}\left(\lambda\right)\dot{\lambda}^{i}dt\right)$$

Therefore, after integrating over a closed curve C, we get:

$$e^{i\gamma}=\exp\left(-i\oint_{C}\mathcal{A}_{i}\left(\lambda\right)d\lambda^{i}\right) \tag{6}$$

This is the **Berry phase**.

1.3 The Berry Connection

Since the Berry connection looks like a gauge potential in electromagnetism, we will investigate in this direction:
In the relativistic electromagnetism, the gauge potential is given by $A_\mu(x)$ with $\mu = 0, 1, 2, 3$ and x are the coordinates from the Minkowski spacetime. The gauge transformation is given by

$$A_\mu \longrightarrow A'_\mu = A_\mu + \partial_\mu \omega \tag{7}$$

for an arbitrary function $\omega(x)$. The field strength tensor is given by

$$F_{\mu\nu} = \frac{\partial A_\mu}{\partial x^\nu} - \frac{\partial A_\nu}{\partial x^\mu} \tag{8}$$

and is invariant under gauge transformations.
Now we compare this to $\mathcal{A}_i$.
In our case, we can think of changing $x \longrightarrow \lambda^i$ for $i = 1, \ldots, d$ which turns $\mathcal{A}_i$ into a one-form.
Since we could pick a different choice of reference state, we get

$$|n'(\lambda)\rangle = e^{i\omega(\lambda)} |n(\lambda)\rangle$$

For an aribitrary function $\omega(\lambda)$, we get as the new Berry connection the following expression

$$\mathcal{A}_i^{prime} = -i \langle n'| \frac{\partial}{\partial \lambda^i} |n'\rangle = \mathcal{A}_i + \frac{\partial \omega}{\partial \lambda^i} \tag{9}$$

which looks quite similar to our gauge transformation above.
Therefore, we can calculate the gauge invariant field strength tensor (or curvature 2-form)

$$\mathcal{F}_{ij}(\lambda) = \frac{\partial \mathcal{A}_i}{\partial \lambda^j} - \frac{\partial \mathcal{A}_j}{\partial \lambda^i}$$

with the help of $\Omega = d\mathcal{A} + \mathcal{A} \wedge \mathcal{A}$ and the fact that the $\mathcal{A}_i$'s commute in this case.
In the present context, we want to investigate more to actually calculate the Berry Phase. Since $\oint \partial_i \omega d\lambda^i = 0$, the Berry phase is invariant of the transformation, and with Stokes Theorem we get

$$e^{i\gamma} = \exp\left(-i \oint_C \mathcal{A}_i(\lambda)\, d\lambda^i\right) = \exp\left(-i \int_S \mathcal{F}_{ij} dS^{ij}\right) \tag{10}$$

where S is the two-dimensional surface bound by the path C.

1.4 A Spin in a Magnetic Field

As an example, we consider a spin in a magnetic field $\vec{B}$. The Hamiltonian

$$H = -\vec{B}\vec{\sigma} + B$$

$\vec{\sigma}$: Pauli matrix vector
$B = \|\vec{B}\|$.

We get two eigenvalues 0 and $2B$ and therefore two eigenstates, the ground state $|\downarrow\rangle$ and the excited state $|\uparrow\rangle$ with

$$H|\downarrow\rangle = 0 \text{ and } H|\uparrow\rangle = 2B|\uparrow\rangle$$

If we now take $\lambda^i \equiv \vec{B}$ and given $\vec{B}$ in polar coordinates

$$\vec{B} = \begin{pmatrix} B\sin(\theta)\cos(\phi) \\ B\sin(\theta)\sin(\phi) \\ B\cos(\theta) \end{pmatrix}$$

with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$ we get

$$H = -B \begin{pmatrix} \cos(\theta) - 1 & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & -\cos(\theta) - 1 \end{pmatrix}$$

and the normalised eigenstates

$$|\downarrow\rangle = \begin{pmatrix} e^{-i\phi}\sin(\theta/2) \\ -\cos(-\theta/2) \end{pmatrix} \text{ and } |\uparrow\rangle = \begin{pmatrix} e^{-i\phi}\cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}$$

We can now compute the Berry phase (and do not take $\theta = \pi$ so that ϕ is well-defined) and start with

$$\mathcal{A}_\theta = -i\langle\downarrow|\frac{\partial}{\partial\theta}|\downarrow\rangle = 0 \text{ and } \mathcal{A}_\phi = -i\langle\downarrow|\frac{\partial}{\partial\phi}|\downarrow\rangle = -\sin^2\left(\frac{\theta}{2}\right)$$

For this result, we get

$$\mathcal{F}_{\theta\phi} = \frac{\partial\mathcal{A}_\phi}{\partial\theta} - \frac{\partial\mathcal{A}_\theta}{\partial\phi} = -\sin(\theta)$$

as the only entry of the antisymmetric tensor. Transforming this into cartesian coordinates gives us

$$\mathcal{F}_{ij}\left(\vec{B}\right) = -\epsilon_{ijk}\frac{B^k}{2\|\vec{B}\|^3}$$

which looks like a magnetic monopole at $\vec{B} = 0$, but in the space of magnetic fields. In the origin, the field strength tensor gets singular and the two energy levels coincide. The magnetic pole has charge $g = -\frac{1}{2}$, since we get

$$\int_{S^2} \mathcal{F}_{ij} dS^{ij} = 4\pi g = -2\pi \tag{11}$$

for any two-sphere S^2, since $\mathcal{F}_{\theta\phi}$ does not depend on the radius. With this we can compute the Berry phase as long as the path C does not cross the origin. Suppose the area S surrounded by C has the solid angle Ω.
Then we get:

$$e^{i\gamma} = \exp\left(-i\int_S \mathcal{F}_{ij}dS^{ij}\right) = \exp\left(\frac{i\Omega}{2}\right) \tag{12}$$

One could also calculate the integral over $S' = S^2 - S$ with the angle $\Omega' = 4\pi - \Omega$ and get

$$e^{i\gamma'} = \exp\left(-i\int_{S'} \mathcal{F}_{ij}dS^{ij}\right) = \exp\left(\frac{-i\,(4\pi - \Omega)}{2}\right) = e^{i\gamma} \tag{13}$$

This requires that $2g \in \mathbb{Z}$.

1.5 Particles Moving Around a Flux Tube

As assumed in electromagnetism, the gauge potential A_μ is an unphysical quantity. In this section we will discuss a set-up where the gauge potential appears in the Hamiltonian, invariant under gauge tranformations.
Consider the situation shown in the picture:

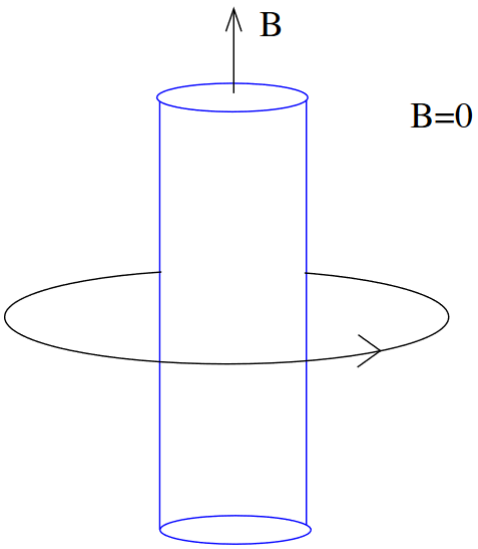

Figure 1: A particle moving around a solenoid

The magnetic flux, with A the area of the solenoid, is $\Phi = BA$. While the magnetic field is zero, the vector potential is not and this follows with Stokes Theorem:

$$\oint \vec{A} \cdot d\vec{r} = \int \vec{B} \cdot d\vec{S} = \Phi$$

Solving this, we get

$$A_\phi = \frac{\Phi}{2\pi r}$$

Consider now a quantum particle, which lies on a ring of radius r outside the cylinder with angle $\phi \in [0, 2\pi)$ and has the Hamiltonian

$$\frac{1}{2m}\left(p_\phi + eA_\phi\right)^2 = \frac{1}{2mr^2}\left(-i\hbar\frac{\partial}{\partial\phi} + \frac{e\Phi}{2\pi}\right)^2$$

since its only degree of freedom is the angle $\phi \in [0, 2\pi)$.
The energy eigenstates are simply

$$\phi = \frac{1}{\sqrt{2\pi r}} e^{in\phi} \quad n \in \mathbb{Z}$$

with $n \in \mathbb{Z}$ because it has to be periodic. The energy eigenvalues are

$$E_n = \frac{\hbar^2}{2mr^2}\left(n + \frac{\Phi}{\Phi_0}\right) \quad n \in \mathbb{Z}$$

with $\Phi_0 = \frac{2\pi\hbar}{e}$. Note, that if Φ is a multiple of Φ_0, then the spectrum is unaffected by the solenoid and if not, the spectrum gets shifted.
The spectrum looks like this:

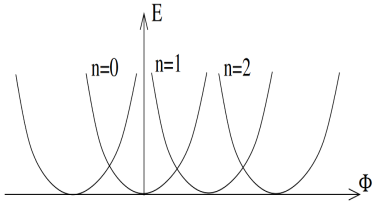

Figure 2: Energy spectrum of a particle moving around a solenoid

Now, the following situation can occur: We start with a turned off solenoid in the particle's ground state and then slowly increase the flux. By the adiabatic theorem, the particle stays in the ground state, but after some time, we reach $\Phi = \Phi_0$ and is now in the state, we just called the $n = 1$-state.
This effect is called **spectral flow**.

1.6 The Aharonov-Bohm Effect

Now we consider a similar situation, where the magnetic field is localised to a region like the solenoid, but this time, our particle is inside a small box. We just include a potential $V(\vec{x})$ into the Hamiltonian in order to trap the particle with an infinitely high potential outside the box.
Small in this case means, that the gauge potential is constant inside the box. If we start by placing the center of the box at $\vec{x} = \vec{X}$, the Hamiltonian is given by

$$H = \frac{1}{2m}\left(-i\hbar\vec{\nabla} + e\vec{A}(X)\right)^2 + V\left(\vec{x} - \vec{X}\right)$$

After starting with the center of the box at $\vec{x} = \vec{X}_0$ and gauge so that $\vec{A}\left(\vec{X}_0\right) = 0$ we get the particle in the box with the ground state $\psi\left(\vec{x} - \vec{X}_0\right)$ localised around $\vec{x} = \vec{X}_0$. As we now slowly move the box, we have the potential $\vec{A}\left(\vec{x} - \vec{X}\right)$ in the Hamiltonian and the solution for the SGE

$$\psi\left(\vec{x} - \vec{X}\right) = \exp\left(-\frac{ie}{\hbar}\int_{\vec{x}=\vec{X}_0}^{\vec{x}=\vec{X}} \vec{A}(\vec{x}) \cdot d\vec{x}\right)\psi\left(\vec{x} - \vec{X}_0\right)$$

If we now make a loop C with the box, we get:

$$\psi\left(\vec{x} - \vec{X}_0\right) \rightarrow e^{i\gamma}\psi\left(\vec{x} - \vec{X}_0\right) \; ; \; e^{i\gamma} = \exp\left(-\frac{ie}{\hbar}\oint_C \vec{A}(\vec{x}) \cdot d\vec{x}\right) \tag{14}$$

where in this case, our Berry connection is a real electromagnetic potential given by

$$\vec{\mathcal{A}}\left(\vec{X}\right) = \frac{e}{\hbar}\vec{A}\left(\vec{x} = \vec{X}\right)$$

The electron has charge $q = -e$. In the general case, where a particle with charge q travels around an area with flux Φ, we get the **Aharonov-Bohm phase**

$$e^{iq\Phi/\hbar}$$

There is an experiment showing the Aharonov-Bohm effect:

It is a variant of the double split experiment, with the addition, that between the slits, there is a solenoid hidden on the other side of the wall with flux Φ. The wave-function never touches the magnetic field $\vec{B}$,but induces a phase difference $e^{i\gamma}$ between the two possible ways a particle could take. The phase difference can then be seen in the interference pattern on the screen. It stay the same, if Φ is a multiple of Φ_0, and changes in the other cases.

1.7 Non-Abelian Berry Connection

We now talk about the case where the ground state is N-times degenerate and remains like this for all values of λ. As before, we place the system in one of the N states

and vary the parameters along a closed path, but now, since the adiabatic theorem only tells us that the system stays in a particular energy eigenstate, the system is somewhere in the N-dimensional subspace and we have to compute a unitary matrix $U \subset U(N)$ instead of just a phase.

We therefore assume $E = 0$ as before to get rid of the dynamic phase as before and the time-dependent SGE is

$$i\frac{\partial |\psi\rangle}{\partial t} = H(\lambda(t))|\psi\rangle = 0 \tag{15}$$

But this time, we introduce an N-dimensional basis of the ground states

$$|n^a(\lambda)\rangle \quad a = 1, \ldots, N$$

and get

$$|\psi_a(t)\rangle = U_{ab}|n_b(\lambda(t))\rangle$$

As before, after plugging this into the SGE we get

$$\left|\dot{\psi_a}\right\rangle = \dot{U_{ab}}|n_b\rangle + U_{ab}|\dot{n_b}\rangle = 0$$

and from there

$$U^\dagger_{ac}\dot{U_{ab}} = -\langle n_b|\dot{n_c}\rangle = -\langle n_b|\frac{\partial}{\partial\lambda^i}|n_c\rangle\dot{\lambda^i}$$

This leads us to the **non-Abelian Berry connection**

$$(\mathcal{A}_i)_{ab} = -i\langle n_b|\frac{\partial}{\partial\lambda^i}|n_a\rangle$$

which can be later be seen as an element of the Lie algebra $u(N)$.
Since we could have picked another choice of basis vectors at each point, we would have

$$|n'_a(\lambda)\rangle = \Omega_{ab}|n_b(\lambda)\rangle$$

with $\Omega(\lambda) \subset U(N)$ a unitary rotation. As a berry connection we get

$$\mathcal{A}'_i = \Omega\mathcal{A}_i\Omega^\dagger + i\frac{\partial\Omega}{\partial\lambda^i}\Omega^\dagger \tag{16}$$

We can now construct the **field strength**

$$\mathcal{F}_{ij} = \frac{\partial\mathcal{A}_i}{\partial\lambda^j} - \frac{\partial\mathcal{A}_j}{\partial\lambda^i} - i[\mathcal{A}_i, \mathcal{A}_j]$$

which is not a gauge-invariant quantity, since it transforms like this:

$$\mathcal{F}'_{ij} = \Omega \mathcal{F}_{ij} \Omega^{\dagger}$$

One could take the trace of this to get one, but we will anyways compute the Berry phase.
Since the $\mathcal{A}_i(\lambda)$ does not have to commute for different values of λ, we have to solution

$$U = \mathcal{P} \exp\left(-i \oint \mathcal{A}_i d\lambda^i\right)$$

where $\mathcal{P}$ means "path ordered": here, if we expand the matrix exponential, we order the products so that $\mathcal{A}_i(\lambda)$ are later in the path are placed to the right. This matrix is called the **Berry holonomy**.

References

[1] David Tong (ed.): The Quantum Hall Effect. TIFR Infosys Lectures, Cambridge, 2016.