Westfälische-Wilhelms-Universität

Seminar zur Theorie der Atome, Kerne
und kondensierten Materie

Adiabatic Approximation and Berry Phase with regard to the Derivation

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1 Adiabatic Approximation

1.1 Motivation

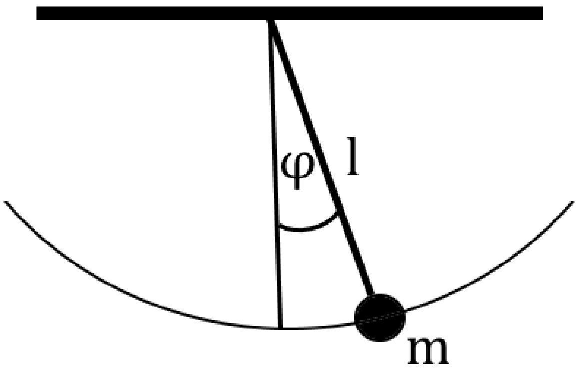


Figure 1: Mathematical pendulum with the mass m, the length l and the deflection φ

To give a short motivation let us have a look at the mathematical pendulum (c.f. Figure 1) with the mass m, the length l and the deflection φ. The differential equation is given by

$$\varphi(t) + \frac{g}{l}\varphi(t) = 0 \tag{1.1}$$

where g is the acceleration of gravity. Solving this equation leads us to the period T with

$$T = 2\pi\sqrt{\frac{l}{g}}\,. \tag{1.2}$$

If we move the pendulum from a location A to a location B we can consider two ways doing this. If the pendulum is moved fast it will execute a complicated oscillation not easy to be described. But if the motion is slow enough, the pendulum remains in its oscillation. This motion is a good example for an adiabatic process which means that the conditions respectively the environment are changed slowly.

Oscillation is also well known in quantum mechanics systems. A good example is the potential well (c.f. Figure 2(a)). In our case we have

$$V(x) = \begin{cases} 0 & \text{when } 0 < x < a \\ \infty & \text{else} \end{cases} \tag{1.3}$$

With the continuity condition we find the first eigenfunction

$$\psi_A(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)\,. \tag{1.4}$$

Now we alter the environment by moving the right border from a to $2a$. In the case of a fast motion we get superposition of the eigenfunctions ψ_n of the new potential well (c.f. Figure 2(b))

$$V(x) = \begin{cases} 0 & \text{when } 0 < x < 2a \\ \infty & \text{else} \end{cases} \tag{1.5}$$

$$\Psi_E(x) = \sum_n c_n \psi_n \tag{1.6}$$

$$= \begin{cases} \psi_A(x) & \text{when } 0 < x < a \\ 0 & \text{else} \end{cases} \tag{1.7}$$

where

$$\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi n x}{2a}\right) . \tag{1.8}$$

We can now calculate the linear coefficients:

$$c_n = \langle\, \psi_n | \Psi_E \rangle = \frac{\sqrt{2}}{a} \int_0^a \sin\left(\frac{\pi}{a} x\right) \sin\left(\frac{\pi n}{2a} x\right) dx \tag{1.9}$$

$$= \frac{4\sqrt{2}\sin\left(\frac{\pi n}{2}\right)}{4\pi - \pi n^2} \tag{1.10}$$

We see that as in the case of the mathematical pendulum we get a complicated oscillation.
If we move the right border slowly enough, i.e. in steps with a width of $da = \frac{a}{N}$ we will find the remaining of the system in its first eigenstate (c.f. Figure 2(c)):

$$\Psi_E(x) = \sum_n c_n \psi_n \tag{1.11}$$

$$= \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a} x\right) \tag{1.12}$$

Calculating the linear coefficients c_n in the same way as in Equation (1.9) results in

$$c_n = \begin{cases} \sim 1 - (da)^2 & \text{when } n = 1 \\ \sim (da)^2 & \text{else} \end{cases} \tag{1.13}$$

In particular we have for a large number of steps N

$$c_n \approx \begin{cases} 1 & \text{when } n = 1 \\ 0 & \text{else} \end{cases} \tag{1.14}$$

where the eigenfunctions are given by

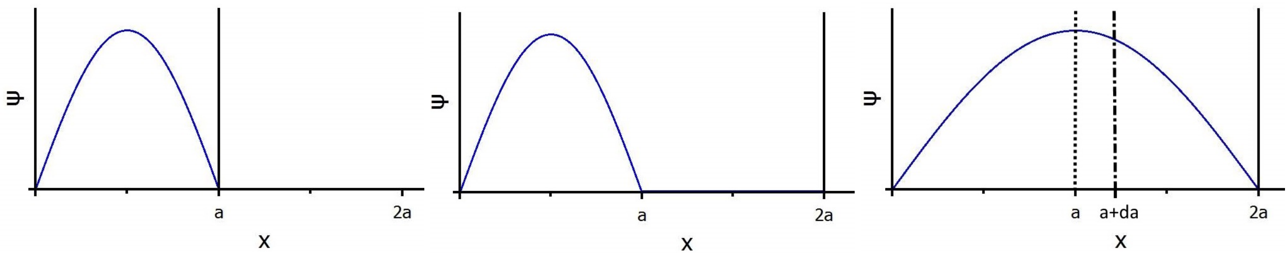
$$\psi_n(x) = \sqrt{\frac{2}{a + da}} \sin\left(\frac{\pi n x}{a + da}\right) . \tag{1.15}$$

As we have seen the system remains in its n-th eigenstate if the motion is done slowly. This is exactly what the adiabatic theorem says: If the environment of a system is changed slowly enough, and if at the beginning the system is in its n-th eigenstate, it stays in its n-th eigenstate at any instant.
One can ask now: What does *slowly* mean? Therefore we define an inner time scale T_i and an outer time scale T_o. The condition "slowly" is now given by

$$T_o \gg T_i\, . \tag{1.16}$$

In case of the mathematical pendulum the inner time scale is the period of the pendulum and the outer time scale is the time needed to move the pendulum from a location A to a location B.
For a quantum mechanic system we have

$$T_\mathrm{o} \gg T_\mathrm{i} = \frac{2\pi\hbar}{E_\mathrm{ab}} \tag{1.17}$$



(a) Wave function in its initial state (b) Wave function after a fast change (c) Wave function after a slow change

Figure 2: Potential well

where

$$E_{\mathrm{ab}} = |E_{\mathrm{a}} - E_{\mathrm{b}}| \tag{1.18}$$

where E_a is the initial energy and E_b the final energy.

1.2 Derivation of the Adiabatic Theorem

Due to the fact our Hamiltonian is time-dependent since we alter the environment with the time we have the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \tag{1.19}$$

and the eigenvalue equation

$$H(t)\psi_n(t) = E_n(t)\psi_n(t) \tag{1.20}$$

where the solutions are represented by a linear combination of the eigenfunction ψ_n:

$$\Psi(t) = \sum_n c_n(t)\psi_n(t)e^{i\theta_n(t)} \tag{1.21}$$

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt' \tag{1.22}$$

As a first step we apply Equation (1.21) to Equation (1.19) and get

$$i\hbar\sum_n \left[\dot{c}_n\psi_n + c_n\dot{\psi}_n + ic_n\psi_n\dot{\theta}_n\right]e^{i\theta_n} = \sum_n .c_n(H\psi_n)e^{i\theta_n} \tag{1.23}$$

Using Equation (1.22) and (1.20) we find

$$\sum_n \dot{c}_n\psi_n e^{i\theta_n} = -\sum_n c_n\dot{\psi}_n e^{i\theta_n}\,. \tag{1.24}$$

Now we multiply the equation from the left side with ψ_m, and with $\langle\psi_m|\psi_n\rangle = \delta_{mn}$ we obtain

$$\sum_n \dot{c}_n\delta_{mn}e^{i\theta_n} = -\sum_n c_n\langle\psi_m|\dot{\psi}_n\rangle e^{i\theta_n} \tag{1.25}$$

what leads us to

$$\dot{c}_m(t) = -\sum_n c_n\langle\psi_m|\dot{\psi}_n\rangle e^{i(\theta_n-\theta_m)}\,. \tag{1.26}$$

Starting from Equation (1.20) we have with the derivation with respect to time:

$$\dot{H}\psi_n + H\dot{\psi}_n = \dot{E}_n\psi_n + E_n\dot{\psi}_n \tag{1.27}$$

Multiplying with ψ_m we obtain:

$$\langle\psi_m|\dot{H}|\psi_n\rangle + \langle\psi_m|H|\dot{\psi}_n\rangle = \dot{E}_n\delta_{mn} + E_n\langle\psi_m|\dot{\psi}_n\rangle \tag{1.28}$$

Since we know the Hamiltonian is Hermitian and we claim $m \neq n$ we get:

$$\langle\psi_m|\dot{H}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\dot{\psi}_n\rangle \tag{1.29}$$

Combined with Equation (1.26) we arrive at:

$$\dot{c}_m(t) = -c_m\langle\psi_m|\dot{\psi}_m\rangle - \sum_{n\neq m} c_n \frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m} \cdot \exp\left(-\frac{i}{\hbar}\int_0^t E_n(t') - E_m(t')dt'\right) \tag{1.30}$$

The case of degeneracy is beyond the scope of this paper and has to be treated separately.
The result above is exact and we have not done any approximation yet. Since we deal with an adiabatic process the environment changes only slowly and hence the Hamiltonian H also changes slowly. For that reason the time derivation of the Hamiltonian is almost zero and we can neglect the second expression so that differential equation is obtained:

$$\dot{c}_m(t) = -c_m\langle\psi_m|\dot{\psi}_m\rangle \tag{1.31}$$

The solution is:

$$c_m(t) = c_m(0)e^{i\gamma_m(t)} \tag{1.32}$$

where $\gamma(t)$ is the so-called geometrical phase given by

$$\gamma_m(t) = i\int_0^t \langle\psi_m(t')|\frac{\partial}{\partial t'}\psi_m(t')\rangle dt' \,. \tag{1.33}$$

At this point it is easy to prove that $\gamma(t)$ is imaginary what it should be since the argument of the exponential function has to be imaginary. On the one hand we have:

$$\frac{d}{dt}\langle\psi_m|\psi_m\rangle = 0 \tag{1.34}$$

On the other hand we can make use of the product rule and get:

$$\frac{d}{dt}\langle\psi_m|\psi_m\rangle = \langle\psi_m|\dot{\psi}_m\rangle + \langle\dot{\psi}_m|\psi_m\rangle \tag{1.35}$$

$$= \langle\psi_m|\dot{\psi}_m\rangle + \langle\psi_m|\dot{\psi}_m\rangle^* \tag{1.36}$$

$$= 2\mathrm{Re}(\langle\psi_m|\dot{\psi}_m\rangle) \tag{1.37}$$

It is implied here that the real part of $\gamma_n(t)$ is zero.
From Equation (1.32) we can deduce that the evolution coefficients c_m are constant apart from the phase factor. Considering the special case that, at the beginning, our system is in the n-th eigenstate we get $c_m(0) = 0$, and $c_n(0) = 1$ and with Equation (1.21):

$$\Psi(t) = e^{i(\theta_n(t)+\gamma_n(t))}\psi_n(t) \tag{1.38}$$

This equation implies the retention in the n-th eigenstate and thus, at this point, the Adiabatic Theorem is proven.
As we can see the exponential function depends on two phases: The dynamical phase $\theta_n(t)$ and the geometrical phase $\gamma_n(t)$.

2 Berry Phase

2.1 Nonholonomic System

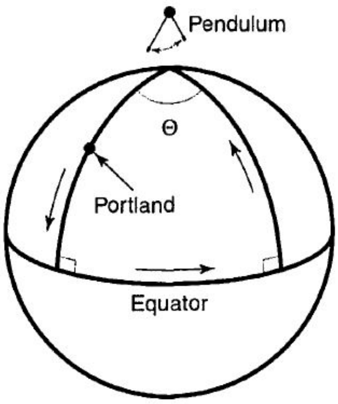


Figure 3: Image of the Pendel positioned at the North Pole

Now let us have a look at a pendulum at the North Pole with its vibration oriented towards Portland (c.f. Figure 3). If we move the pendulum along the longitude through Portland to the Equator, from there along the Equator to an arbitrary longitude and then up to the North Pole we will find that the Pendulum is at the same place as it was at the beginning. But apparently it has a new plane of vibration enclosing an angle Ω with its old plane of vibration.
Ω is donated the solid angle being the three dimensional obverse of the angle in a plane. For an arbitrary surface it can be calculated with

$$\Omega = \int \sin(\theta) d\theta d\varphi \,. \tag{2.1}$$

This pendulum is an example for a nonholonomic system, i.e system that – if it is carried along a closed path – does return to its old state.

2.2 Derivation of the Berry Phase

In 1.2 we have inferred the equation

$$\Psi(t) = e^{i(\theta_n(t)+\gamma_n(t))}\psi_n(t) \tag{2.2}$$

As we have seen the phase factor consists of the dynamical phase and the geometrical phase. The first phase is without any importance for us so that in the following we will pay more attention to the geometrical phase

$$\gamma_m(t) = i \int_0^t \langle \psi_m | \frac{\partial}{\partial t'} \psi_m \rangle dt' \,. \tag{2.3}$$

In this expression we find the derivation of the wave function with respect to the time. Since ψ depends on the parameter R, and R is altered over the time, we can, due to the chain, replace $\frac{\partial \psi}{\partial t}$ rule with $\frac{\partial \psi_n}{\partial R} \frac{dR}{dt}$, so that we get

$$\gamma_m(t) = i \int_0^t \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle \frac{dR}{dt'} dt' \tag{2.4}$$

$$= i \int_{R_A}^{R_E} \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle dR \,. \tag{2.5}$$

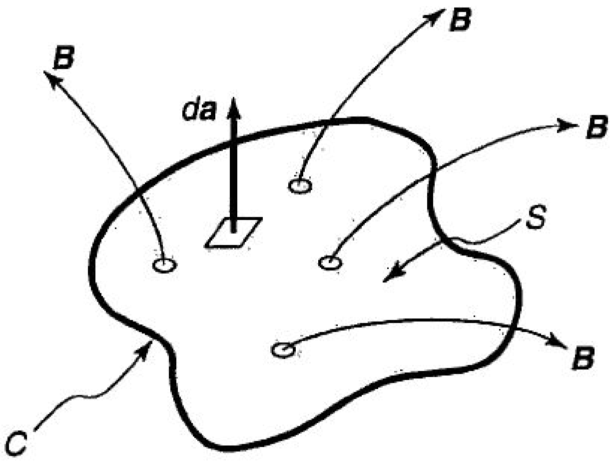


Figure 4: The flux Φ caused by a magnetic field $\vec{B}$ through a surface S [1]

For example R could be the width of the potential well.
Now let the initial point R_A and the final point R_E be the same:

$$\gamma_n(t) = i \oint_C \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle dR \tag{2.6}$$

This line integral is obviously zero. But if we now assume that not only one parameter but n parameters are varied so that $R = \vec{R} = (R_1, \dots R_n)$, our derivation with respect to R is changed to $\nabla \psi$, and we get the so-called Berry Phase

$$\gamma_n(t) = i \oint_C \langle \psi_n | \nabla \psi_n \rangle d\vec{R} \tag{2.7}$$

$$= i \oint_C \langle n | \nabla n \rangle d\vec{R} \qquad (\langle \psi_n | = \langle n |) \tag{2.8}$$

named after the physicist Michael Berry who presented his studies about this in his paper "Quantal phase factors accompanying adiabatic changes" in 1983. In particular is this expression (2.8) generally not equal zero.

2.3 Berry Potential and Berry Curvature

At first let us recapitulate Stokes' Theorem. We consider a surface S bounded by the curve C and the magnetic field $\vec{B}$ (c.f. Figure 4). We can now calculate the flux Φ through the surface:

$$\Phi = \int_S \vec{B}\, d\vec{a} \tag{2.9}$$

Since we know $\vec{B} = \nabla \times \vec{A}$, where $\vec{A}$ is the vector potential, we can say:

$$\Phi = \int_S \nabla \times \vec{A}\, d\vec{a} \tag{2.10}$$

Due to Stokes' Theorem this expression is equal to an integral over the curve where the rotation of $\vec{A}$ disappears. We find

$$\Phi = \oint_C \vec{A}\, d\vec{r}. \tag{2.11}$$

Starting from Equation (2.8) we obtain

$$\gamma_n(t) = \oint_C i \langle n | \nabla n \rangle d\vec{R} = \int \nabla \times i \langle n | \nabla n \rangle\, d\vec{a} = \int \vec{V}_n\, d\vec{a} \tag{2.12}$$

where $i\langle n|\nabla n\rangle$ is named similarly to the example above the Berry potential $\vec{A}$. Its rotation is called the Berry curvature $\vec{V}_n$ at which we want to have a closer look.

$$V_n = i\,\nabla \times \langle n|\nabla n\rangle \tag{2.13}$$

Using theorems of the vector analysis one can show

$$V_n = i\langle \nabla n| \times |\nabla n\rangle\,. \tag{2.14}$$

If we now apply the identity $\mathbb{1} = \sum |m\rangle\langle m|$ we get

$$V_n = \sum_{m\neq n} i\langle \nabla n|m\rangle \times \langle m|\nabla n\rangle\,. \tag{2.15}$$

We can neglect the case of $m = n$, because if $m = n$, $\langle m|\nabla n\rangle$ is imaginary and in particular multiplied with itself real and as we have shown in 1.2, the real part has no influence on the dynamical phase. With

$$\langle m|\nabla n\rangle = \frac{\langle m|\nabla H|n\rangle}{E_n - E_m} \tag{2.16}$$

being similar to Equation (1.29) we achieve our finale expression for the Berry curvature:

$$V_n = i\sum_{m\neq n} \frac{\langle n|\nabla H|m\rangle \times \langle m|\nabla H|n\rangle}{(E_n - E_m)^2}$$

2.4 Summary

- According to the Adiabatic Theorem a system in the n-th eigenstate remains in the n-th eigenstate if the environment is changed slowly enough
- If the Hamiltonian is slowly altered and returns to its original state we can deduce from the Adiabatic Theorem that the system remains in its original state but a phase factor called Berry Phase is added
- The Berry Phase does not depend on the time needed to change the environment alongside a circuit (as long as it is slow enough) but only on the path taken
- The Berry Phase is measurable and can be made visible by experiments involving interference as for example the Aharanov-Bohm effect

References

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