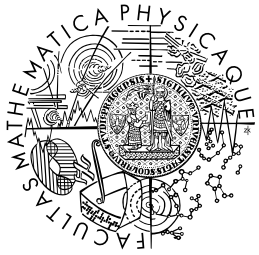

FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

MASTER THESIS

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Some funny small things looking for counterdiabatic elements

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Study programme: Theoretical physics

Study branch: hmmmmm

Prague 2022

I declare that I carried out this master thesis independently, and only with the cited sources, literature and other professional sources. It has not been used to obtain another or the same degree.

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Dedication.

Title: Some funny small things looking for counterdiabatic elements

Author: Jan Střeleček

Institute:

Supervisor:

Abstract: Abstract.

Keywords: key words

Contents

Some notes to the notation

Symbol	Meaning	Defining formula
$\mathcal{A}$	Gauge (calibrational) potential	$\mathcal{A}_\mu = i\hbar\partial_\mu$

Mathematical spaces will be denoted *mathcal* and operators with *hat*.

Introduction

1. Mathematical introduction

The modern approach to the closed system dynamics is using differential geometry formalism. Before we get to the quantum mechanics itself, lets define the formalism and recapitulate some definitions of this branch of mathematics. More detailed notes can be found for example in [Fecko, 2006].

Let's have a manifold $\mathcal{M}$ and curves

$$\gamma : \mathbb{R} \overset{open}{\supset} I \to \mathcal{M} \qquad \xi \mapsto \gamma(\xi).$$

The space of functions is $\mathcal{F}(\mathcal{M}) \equiv \{f : \mathcal{M} \to \mathbb{R}\}$, where

$$f : \mathcal{M} \to U \overset{open}{\subset} \mathbb{R} \qquad x \mapsto f(x).$$

To define *vectors* on $\mathcal{M}$, we need to make sense of the *direction*. It is defined using curves satisfying

$$\gamma_1(0) = \gamma_2(0) \equiv P$$
$$\frac{\mathrm{d}}{\mathrm{d}t} x^i(\gamma_1(t))\Big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t} x^i(\gamma_2(t))\Big|_{t=0}.$$

Taking the equivalence class created by those two rules, sometimes noted as $[\gamma] = v$, we have element of the tangent space to $\mathcal{M}$. We will use standard notation for the tangent space to $\mathcal{M}$ in some point xP as $\mathbb{T}_P\mathcal{M}$ and contangent space as $\mathbb{T}^*_P\mathcal{M}$. Unifying all those spaces over all x we get tangent and cotangent bundle, $\mathcal{T}\mathcal{M}$ and $\mathcal{T}^*\mathcal{M}$ respective. To generalize this notation to higher tensors, we denote $\mathbb{T}_P\mathcal{M} \in \mathcal{T}^1\mathcal{M}$, $\mathbb{T}^*_P\mathcal{M} \in \mathcal{T}_1\mathcal{M}$, thus the space of $p-$times contravariant and $q-$times covariant tensors is denoted $\mathcal{T}^p_q\mathcal{M}$.

Using the congruence of the curves on $\mathcal{M}$, the expression

$$\frac{\mathrm{d}}{\mathrm{d}\xi} f \circ \gamma(\xi)\Big|_{\xi=0} \tag{1.1}$$

has a good meaning and we can define the *derivative* in some $P \in \mathcal{M}$ as

$$\boldsymbol{v} : \mathcal{F}(\mathcal{M}) \to \mathbb{R} \qquad f \mapsto \boldsymbol{v}[f] \equiv \frac{\mathrm{d}f(\gamma(\xi))}{\mathrm{d}\xi}\Big|_P \equiv \partial_\xi\Big|_P f. \tag{1.2}$$

It holds, that $\boldsymbol{v} \in \mathbb{T}_P\mathcal{M}$ and can be expressed as the *derivative in direction*,[1] which can be understood in coordinates as

$$\boldsymbol{v}[f] = \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{v}} f \circ \gamma(\xi)\Big|_{\xi=0} = v^\mu \frac{\mathrm{d}}{\mathrm{d}x^\mu} f(\boldsymbol{x})\Big|_P. \tag{1.4}$$

The directionnal derivative will be denoted

$$\nabla_v$$

[1] The direction itself is usually denoted as

$$\frac{\mathrm{D}}{\mathrm{d}\boldsymbol{\alpha}}\gamma(\xi), \tag{1.3}$$

where the big D notation is used to point out that it's not a classical derivative, but it maps curves to some entirely new space of directions.

and in basis $\boldsymbol{e}_i \equiv \partial/\partial x^i$ we will denote

$$\nabla = (\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z).$$

To get some physical application, we need to define one strong structure on manifolds – differentiable metric tensor $g_{\mu\nu} \in \mathcal{T}_2^0\mathcal{M}$ – so the covariant derivatives and parallel transport are well-defined everywhere.

1.1 Fiber bundle

We already know tangent and cotangent spaces. Thinking of manifold $\mathcal{M}$ as a fiber, for which at any point x we create new manifold $\mathbb{T}_x\mathcal{M}$, we and unifying all those tangent spaces, we get so-called *vector bundle*.

Definition 1. *Structure* $(\mathcal{E}, \mathcal{B}, \pi, \mathcal{F})$*, for topological spaces* $\mathcal{E}$ *(*total space*),* $\mathcal{B}$ *(*base space*),* F *(*fibre*) and a continuous surjection* $\pi : \mathcal{E} \to \mathcal{B}$ *satisfying a local triviality*[2] *is called a* Fiber bundle *(*projection map*). In addition, the* $\mathcal{B}$ *is assumed to be connected*[3] *and for every* $x \in \mathcal{B}$*, there is an open neighborhood* $\mathcal{U} \subset \mathcal{B}$ *(*trivializing neighborhood*) such that there exists a homeomorphism from* $\mathcal{U}$ *to so-called* product space

$$\phi : \pi^{-1}(\mathcal{U}) \to \mathcal{U} \times \mathcal{F},$$

such that $\pi^{-1}\pi(\mathcal{U}) = \mathcal{U}$*.*

The above mappings can be more clear from figure 1.1. Because projections of products are open maps, $\pi : \mathcal{E} \to \mathcal{B}$ must be open map. The meaning of

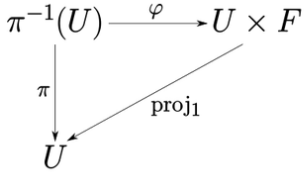

Figure 1.1: Mappings needed for the bundle definition.

definition is, that manifolds at every point $x \in \mathcal{F}$ are all locally diffeomorphic to each other.

1.2 Vector Bundle

Conversely, given a fiber bundle (E, X, π, Rk) with a GL(k) cocycle acting in the standard way on the fiber Rk, there is associated a vector bundle. This is sometimes taken as the definition of a vector bundle

[2] local triviality

[3] can't be represented as a union of two disjoint sets

1.2.1 Connection on vector bundles

[Loring, 20017][chap. 10.1] Connection maps vector from tangent space to base manifold $\mathcal{X}$ with some element from total space $\mathcal{E}$ to total space

$$\Gamma : \mathcal{X} \times \mathcal{E} \to \mathcal{E}$$

such, that

- $\Gamma_X s$ is $\mathcal{F}-$linear in X and $\mathbb{R}-$linear in s
- Leibniz rule for $f \in \mathcal{C}^\infty$ is satisfied: $\Gamma_X(fs) = (Xf)s + f\Gamma_X s$

1.2.2 Metric on vector bundles

Map

$$g_{\mu\nu} : \mathcal{B} \times \mathcal{B} \to \mathbb{R}$$

1.3 Section

Section is a function

$$f : \mathcal{B} \to \mathcal{F},$$

such that $\pi(f(x)) = x$ for $\forall x \in \mathcal{B}$. This defines new manifold cutting throw $\mathcal{E}$.

Sectioning of fiber bundles creates vector spaces

1.4 Pull-back and push forward

Push-forward and pull-back are used to transport vectors and covectors between manifolds. Let's have two manifolds $\mathcal{M}$, $\mathcal{N}$, a smooth mapping ϕ and functions $f, \tilde{f}$ such that

$$\begin{aligned} \phi &: \mathcal{M} \to \mathcal{N} \qquad x \mapsto \phi x \\ \tilde{f} &: \mathcal{N} \to \mathbb{R} \end{aligned}$$

Pull-back of the function then defines a new function $f : \mathcal{M} \to \mathbb{R}$ as

$$\phi^* : \mathcal{F}\mathcal{N} \to \mathcal{F}\mathcal{M} \qquad \tilde{f} \mapsto f = (\phi^* \tilde{f})(x) \equiv \phi^* \tilde{f}(x) = \tilde{f}(\phi x).$$

Push-forward of a vector is defined as

$$\phi_* : \mathbb{T}_x\mathcal{M} \to \mathbb{T}_{\phi x}\mathcal{N} \qquad \phi_* \frac{\mathrm{D}\gamma(\xi)}{\mathrm{d}\xi}\bigg|_x = \frac{\mathrm{D}\phi\gamma(\xi)}{\mathrm{d}\xi}\bigg|_x$$

and *pull-back of a covector* $\tilde{\alpha} \in \mathbb{T}_{\phi x}\mathcal{N}$ is

$$\phi^* : \mathbb{T}_{\phi x}\mathcal{N} \to \mathbb{T}_x\mathcal{M} \qquad (\phi^* \tilde{\alpha})_\mu v^\mu\Big|_x = \tilde{\alpha}_\mu (\phi_* \boldsymbol{v})^\mu\Big|_{\phi x}.$$

If ϕ has a smooth inversion, i.e. it is a dippheomorphism, we can define pull-back of vectors as

$$\phi^* = \phi_*^{-1} \tag{1.5}$$

and push-forward of covectors

$$\phi_* = (\phi^{-1})^* \tag{1.6}$$

1.5 Flow

1.6 Covariant derivative and parallel transport

this section is probably not needed

Covariant derivative is generally... Metric covariant derivative is...

Parallel transport of vector $\boldsymbol{v} \in \mathbb{T}_p\mathcal{M}$ will be denoted $\mathrm{par}_\gamma \boldsymbol{v} \in \mathbb{T}$

Affine connection can be expressed as

$$\Gamma^\alpha_{\mu\nu} = \frac{1}{2} g^{\alpha\beta} \left(g_{\beta\mu,\nu} + g_{\nu\beta,\mu} - g_{\mu\nu,\beta} \right), \tag{1.7}$$

where we used comma notation for the coordinate derivative. The covariant derivative of $\boldsymbol{a} \in \mathbb{T}_P\mathcal{M}$ is then defined

$$\frac{\mathrm{D}a^\mu}{\mathrm{d}x^\nu} = a^\mu_{,\nu} - \Gamma^\mu_{\alpha\beta} x^\alpha a^\beta \tag{1.8}$$

and for $\boldsymbol{\alpha} \in \mathbb{T}^*_P\mathcal{M}$ it is

$$\frac{\mathrm{D}\alpha_\mu}{\mathrm{d}x^\nu} = \alpha_{\mu,\nu} - \Gamma^\alpha_{\mu\beta} x^\beta \alpha_\alpha \tag{1.9}$$

The vector $v \in \mathbb{T}_P\mathcal{M}$ is said to be parallel transported along curve $\gamma(\lambda)$, if it's covariant derivative

$$\frac{\mathrm{D}v^\mu}{\mathrm{d}\xi} = 0 \tag{1.10}$$

vanishes along γ.

1.7 Parallel transport on vector bundles

this is what we need Parallel transport of vector V along curve γ will be denoted

$$\mathrm{par}_\gamma V.$$

It is

1.8 Antisymmetric tensors and wedge product

p-form $A \in \mathcal{T}_p\mathcal{M}$ is called *antisymmetric*, if changing the order of the indices has impact only on the sign, symbolically

$$A_{i_1 \dots i_p} = \mathrm{sign}(\sigma) A_{i_{\sigma_1} \dots i_{\sigma_p}},$$

where σ is some permutation. *Antisymmetrisation* is defined as a normalized sum over all permutation

$$A^{[i_1 \dots i_p]} \equiv \frac{1}{p!} \sum_\sigma A^{[i_{\sigma_1} \dots i_{\sigma_p}]}. \tag{1.11}$$

The *wedge product* of $A \in \mathcal{T}_p\mathcal{M}$ and $B \in \mathcal{T}_q\mathcal{M}$ is antisymmetrisation of the tensor product in the sense

$$A \wedge B \equiv \frac{(p+q)!}{p!q!} A^{[i_1 \dots i_p} \otimes B^{i_1 \dots i_q]} \tag{1.12}$$

2. Physical introduction

Most parts of this chapter are inspired by [Kolodrubetz et al., 2017] and original notes [Berry, 1984], [Berry, 1989], [Berry, 2009] Now we will assign some physical background to the structure defined in the first chapter. We will see, that the whole space structure is quite complicated, because it's of fiber structure, where every fiber is another fiber bundle. Luckily what we will be using later on are only some much easier Riemannian submanifolds.

Assume parameter $\boldsymbol{\lambda} \in \mathcal{U} \subset \mathbb{R}^n$ controlling some Hamiltonian $\hat{H}(\boldsymbol{\lambda})$, which is bounded from below and the spectrum is discrete for the first $k > 1$ energies, will be clear later on. From this we can construct fiber bundle, such that at every point of base manifold $\boldsymbol{\lambda} \in \mathcal{U}$, we construct fiber spanning all possible states of $\hat{H}(\boldsymbol{\lambda})$, thus the fiber structure can be according to section 1.1 written as

$$\left(\mathcal{H}_{full} \coloneqq \bigcup_{\boldsymbol{\lambda}} \mathcal{H}(\boldsymbol{\lambda}), \mathcal{U} \subset \mathbb{R}^n, \pi, \mathcal{H}(\boldsymbol{\lambda}) \coloneqq \bigcup_{states} |\psi(\boldsymbol{\lambda})\rangle\right).$$

The projection is defined as $\pi(\boldsymbol{\lambda}) : |\psi(\boldsymbol{\lambda})\rangle \mapsto \boldsymbol{\lambda}$ and $\mathcal{H}(\boldsymbol{\lambda})$ is Hilbert space for all pure states of $\hat{H}(\boldsymbol{\lambda})$. Geometric intuition is displayed in fig. 2.1

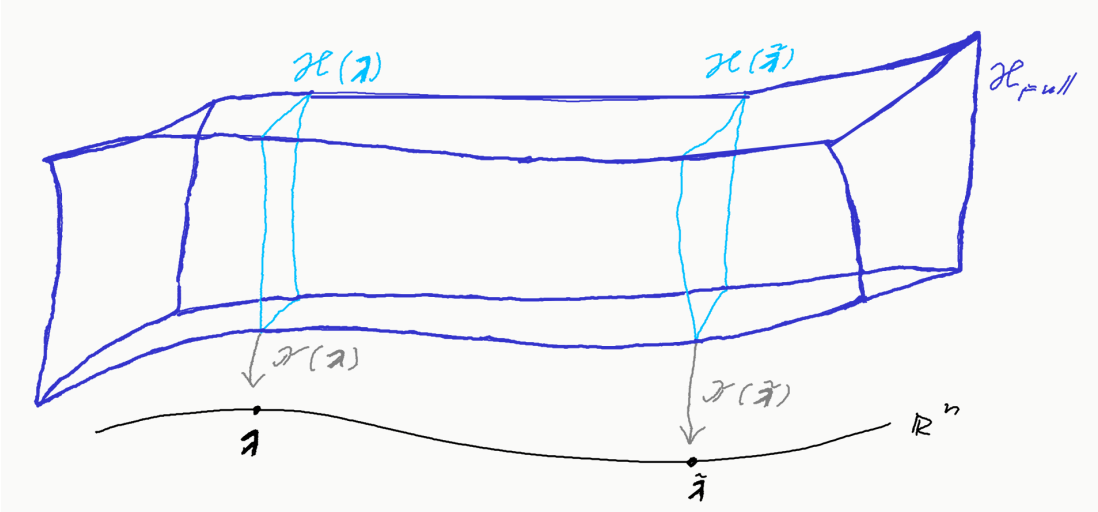

Figure 2.1: Fiber bundle over $\mathbb{R}^n$ with Hilbert spaces $\mathcal{H}(\boldsymbol{\lambda})$ as individual fibers.

Because we are interested only in discrete part of spectrum[1], it will further on be referred to only as *spectrum*.

The states of the system evolve according to the Schrödinger equation

$$i\hbar \mathrm{d}_t |\psi(\boldsymbol{\lambda}(t))\rangle = \hat{H}(\lambda) |\psi(\boldsymbol{\lambda}(t))\rangle , \tag{2.1}$$

which for eigenstates of instantaneous Hamiltonian reads as energy Schrödinger equation

$$\hat{H}(\lambda) |s(\lambda)\rangle = E_s(\lambda) |s(\lambda)\rangle . \tag{2.2}$$

For every $\mathcal{H}(\boldsymbol{\lambda})$ the first k energies can be sorted from the lowest to create discrete set $\sigma(\hat{H}(\boldsymbol{\lambda})) \equiv \{E_0, \ldots, E_k\}$. Clearly, there exists a bijection between all fibers

[1]Spectrum of the operator consists of discrete spectrum, calculable as eigenvalue problem, continuous and residual spectrum.

$\mathcal{H}(\boldsymbol{\lambda})$, thus we can define *section* $\sec_s$, mapping eigenstate corresponding to energy E_s to base manifold

$$\sec_s : |o(\boldsymbol{\lambda})\rangle \mapsto \mathcal{U} \subset \mathbb{R}^n,$$

which is also bijection. For $\forall s \in \{0, k\}$ we can create according to sec. 1.3 new *energy manifolds*

$$\mathcal{M}_s \subset \mathcal{M},$$

with special importance of the *ground state manifold* $\mathcal{M}_0$, which will be used later on for adiabatic transports of ground states. Geometrical intuition is drawn on fig. 2.2. Because those manifolds were created by sectioning, they are considered to be vector spaces in a geometrical sense. This was expected, because they contain quantum states.

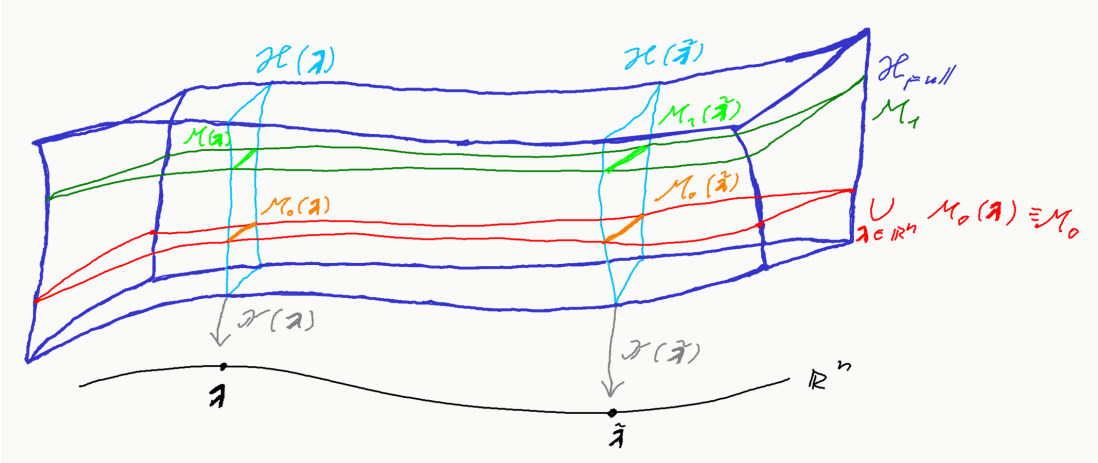

Figure 2.2: Geometrical intuition to transport on fiber manifold sections $\mathcal{M}_i$.

All Hilbert spaces above are considered to be spaces of *bare states* $\mathcal{H}$. In quantum mechanics, physical observables are related to the *space of rays*, defined as $\mathcal{PH} \coloneqq \mathcal{H}/U(1)$, where elements of $U(1)$ are unitary transformations $e^{i\phi}$ for $\phi \in \mathbb{R}$ defining gauge symmetry between quantum states. The geometrical intuition is drawn for any $\boldsymbol{\lambda}$ on fig. 2.3.

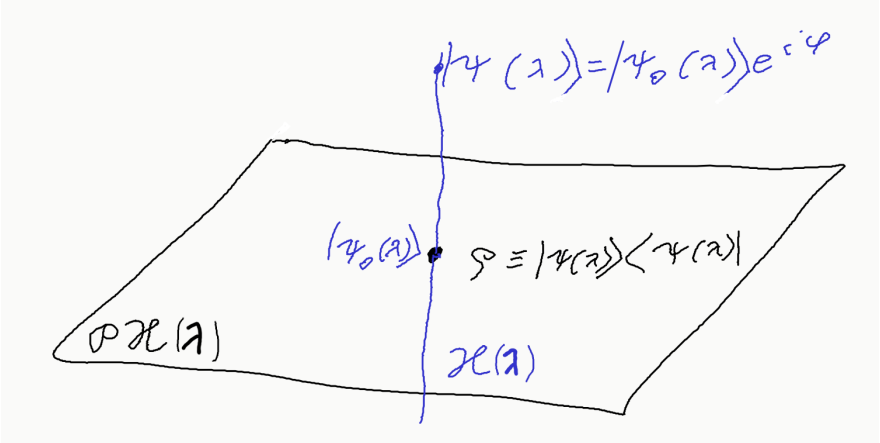

Figure 2.3: Space of bare states and its projection to space of rays $\mathcal{PH}(\boldsymbol{\lambda}) \coloneqq \mathcal{H}(\boldsymbol{\lambda}/U(1)$.

This means, that energy manifolds $\mathcal{M}_s$, generated by bare states, are again of fiber structure, defined as

$$\left(\mathcal{H}, \mathcal{P}\mathcal{H}, \pi_{rays}, \{e^{i\phi}\,|\psi\rangle \;\text{ for } \phi \in \mathbb{R}\}\right),$$

where π_{rays} is just rule setting phase ϕ to zero. Because ll $\mathcal{M}_s$ are compact and connected, they are diffeomorphic to each other.

2.1 Transporting states

Let's now focus on decomposition of $\mathcal{H}_{full}$ to different state manifolds $\mathcal{M}_s$, as displayed on figure 2.4.

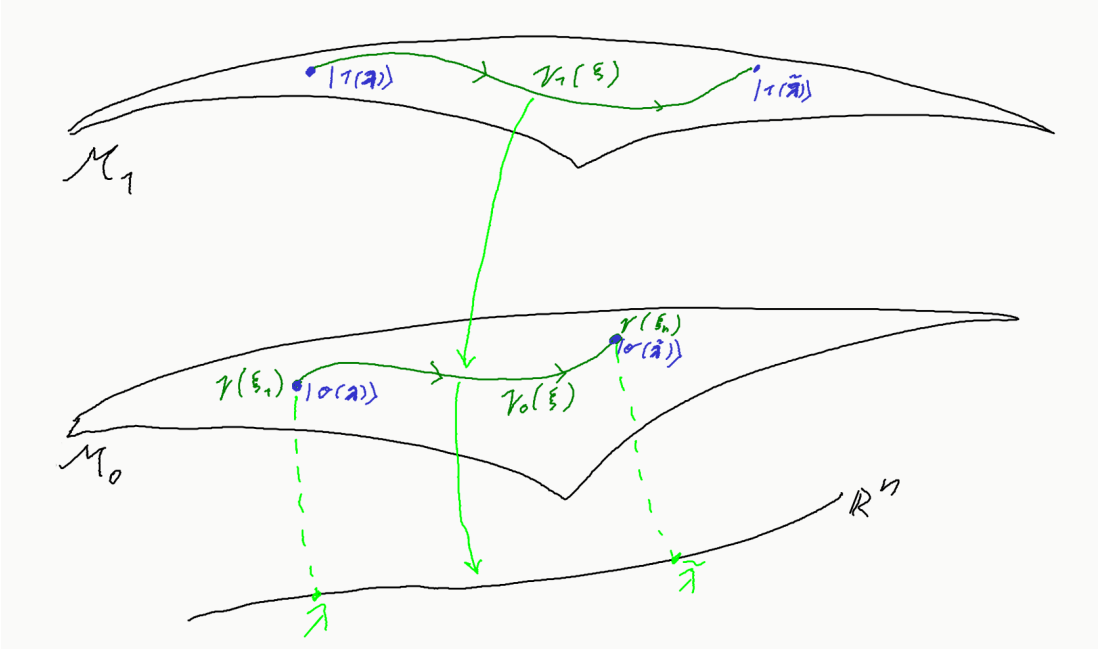

Figure 2.4: Geometrical intuition to transport on fiber manifold sections $\mathcal{M}_s$.

Changing state from eigenstate $|s(\boldsymbol{\lambda})\rangle$ to any pure state $|\psi(\tilde{\boldsymbol{\lambda}})\rangle$, during some time period, is unitary transformation and can be thought of as *parallel transport on fiber bundle* between two vectors. Assuming the transport goes along curve $\{\gamma_s(\xi)|\xi \in [\xi_1, \xi_2] \subset \mathbb{R}\} \subset \mathcal{M}_s$ This can be written as

$$|\psi(t)\rangle \equiv \mathrm{par}_{\gamma_s}\,|s(\lambda)\rangle = \exp\left(-\frac{i}{\hbar}\int_0^t E_s(\tau)\mathrm{d}\tau\right)\exp(i\gamma_s(\xi))\,|s(\lambda)\rangle\,. \tag{2.3}$$

The first exponential, the *dynamical phase*, is well known solution to energy Schrödinger equation 2.2 with $\boldsymbol{\lambda} = const$ and depends only on time and energy of states during the transport. The second exponential is called *geometrical phase*. This phase is generally non-integrable, meaning it cannot be written simply as $\gamma_s(\lambda)$ and for some closed curve on $\mathcal{M}$

$$C = \{\boldsymbol{\lambda}(\xi)|\xi \in [0, \Xi], \text{ such that } \boldsymbol{\lambda}(0) = \boldsymbol{\lambda}(\Xi)\} \tag{2.4}$$

we generally get $\mathrm{par}_C\,|\psi(\boldsymbol{\lambda})\rangle \neq |\psi(\boldsymbol{\lambda})\rangle$. This property is sometimes more generally called an *anholonomy* and geometric intuition can be seen on fig. 2.5.

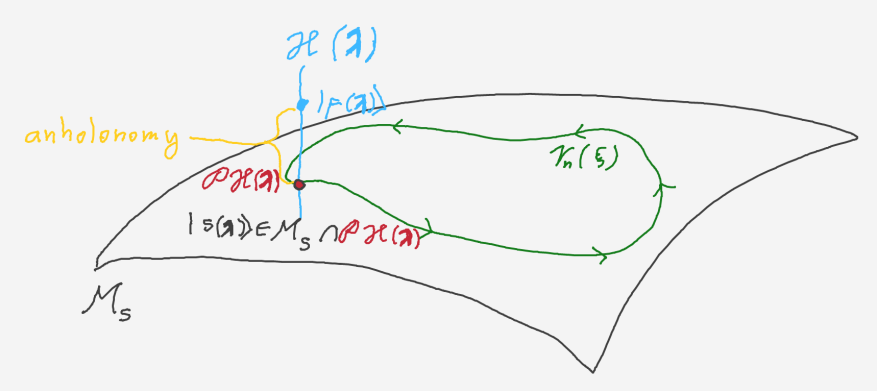

Figure 2.5: Parallel transporting around some closed curve C with anholonomy drawn in yellow.

For quantum states, the anholonomy can be measured as a non-zero angle between $|V\rangle$ and $\mathrm{par}_C |V\rangle$, meaning

$$\langle V|\mathrm{par}_C|V\rangle \neq 0.$$

Substituting general solution 2.3 to eq. 2.1 yields (see [Berry, 1984])

$$\mathrm{d}_t\gamma(\lambda) = i\,\langle s(\lambda)|\partial_\mu s(\lambda)\rangle\,\mathrm{d}_t\lambda^\mu(\lambda). \tag{2.5}$$

Integrating this equation around some closed curve C and assuming the dynamical phase to be zero, thus not exciting the system, we get

$$\gamma_n(C) = i\oint_C \langle s(\boldsymbol{\lambda})|\partial_\mu s(\boldsymbol{\lambda})\rangle\,\mathrm{d}\lambda^\mu. \tag{2.6}$$

We see, that the geometric phase does not depend on energy or time, only on the sequence of Hamiltonians, which means it depends only on the path itself.

The problem of expressions above lies in $\partial_{\boldsymbol{\lambda}} s(\boldsymbol{\lambda})$, which locally requires knowledge of single-valued basis $\{|0\rangle, \ldots, |k\rangle\}$. This can be avoided in 3-dimensions using Stokes's theorem for S as the surface with boundary $\partial S = C$, for coordinate gradient ∇

$$\begin{aligned}
\gamma_s(C) &= -\mathrm{Im}\iint_C \mathrm{d}S\cdot\nabla\times\langle s(\boldsymbol{\lambda})|\nabla n(\boldsymbol{\lambda})\rangle \\
&= -\mathrm{Im}\iint_C \mathrm{d}S\cdot\langle\nabla s(\boldsymbol{\lambda})|\times|\nabla s(\boldsymbol{\lambda})\rangle \\
&= -\mathrm{Im}\iint_C \mathrm{d}S\cdot\sum_{m\neq s}\langle\nabla s(\boldsymbol{\lambda})|m(\boldsymbol{\lambda})\rangle\times\langle m(\boldsymbol{\lambda})|\nabla s(\boldsymbol{\lambda})\rangle \\
&= -\iint_C \mathrm{d}S\cdot V_s(\boldsymbol{\lambda})
\end{aligned} \tag{2.7}$$

for

$$V_s(\boldsymbol{\lambda}) = \mathrm{Im}\frac{\langle s(\boldsymbol{\lambda})\nabla_{\boldsymbol{\lambda}}\hat{H}(\boldsymbol{\lambda})|m(\boldsymbol{\lambda})\rangle\times\langle m(\boldsymbol{\lambda})|\nabla_{\boldsymbol{\lambda}}\hat{H}(\boldsymbol{\lambda})|s(\boldsymbol{\lambda})\rangle}{(E_m(\boldsymbol{\lambda})-E_s(\boldsymbol{\lambda}))^2} \tag{2.8}$$

where the element of summation $m = s$ in third step of derivation is real, therefore has no influence on γ_s and can be omitted. The last equivalence holds, because

if we differentiate the Schrödinger equation 2.2, we get for any $|s\rangle, |m\rangle \in \mathcal{M}$

$$\begin{aligned} \nabla\hat{H}\,|s(\boldsymbol{\lambda})\rangle + \hat{H}\,|\nabla s(\boldsymbol{\lambda})\rangle &= E_s\,|\nabla s(\boldsymbol{\lambda})\rangle \\ \langle m(\boldsymbol{\lambda})|\nabla\hat{H}|s(\boldsymbol{\lambda})\rangle + \langle m(\boldsymbol{\lambda})|E_m|\nabla s(\boldsymbol{\lambda})\rangle &= \langle m(\boldsymbol{\lambda})|\nabla\hat{H}|s(\boldsymbol{\lambda})\rangle \\ \langle m(\boldsymbol{\lambda})|\nabla s(\boldsymbol{\lambda})\rangle &= \frac{\langle m(\boldsymbol{\lambda})|\nabla\hat{H}|s(\boldsymbol{\lambda})\rangle}{E_m(\boldsymbol{\lambda}) - E_s(\boldsymbol{\lambda})}, \qquad s \neq m, \end{aligned} \tag{2.9}$$

where we used $|\nabla s\rangle \equiv \nabla\,|s\rangle$. Comparing the first expression in eq. 2.7 with its last one and extending it to real numbers, we get

$$V_s(\boldsymbol{\lambda}) = \nabla \times \langle s(\boldsymbol{\lambda})|\nabla m(\boldsymbol{\lambda})\rangle\,, \tag{2.10}$$

defining vector potential of $V_s(\boldsymbol{\lambda})$. In addition, it extends our definition from single valued basis to any solution of 2.2, thus instead of ground state manifold, we can use any $\mathcal{M}_s$.

As was mentioned, the above procedure from eq. 2.6 was performed only for three-dimensional space. Proper generalization to n-dimensional space would yield, see [Berry, 1984],

$$\gamma_s(C) = -\iint_C \mathrm{d}S \cdot \mathrm{Im}\frac{\langle s(\boldsymbol{\lambda})\mathrm{d}\hat{H}(\boldsymbol{\lambda})|m(\boldsymbol{\lambda})\rangle \wedge \langle m(\boldsymbol{\lambda})|\mathrm{d}\hat{H}(\boldsymbol{\lambda})|s(\boldsymbol{\lambda})\rangle}{(E_m(\boldsymbol{\lambda}) - E_s(\boldsymbol{\lambda}))^2}, \tag{2.11}$$

which will not be needed in this thesis.

2.2 Metric and geometric tensor

As a playground for this chapter, we will choose the ground state manifold $\mathcal{M}_0$, but it can be easily generalized to any energy states manifold $\mathcal{M}_s$. From now on we will use natural units, so $\hbar = 1$.

Let's first look at $\mathcal{P}\mathcal{M}_s$, which is needed to be *gauge independent*. Gauge dependence in quantum mechanics means, that the change in phase factor ϕ of some state $|o(\boldsymbol{\lambda})\rangle \in \mathbb{T}_{\boldsymbol{\lambda}}\mathcal{M}$ induces the change

$$|o(\boldsymbol{\lambda})\rangle \mapsto e^{i\phi(\boldsymbol{\lambda})}\,|o(\boldsymbol{\lambda})\rangle \implies \langle o(\boldsymbol{\lambda})|\nabla o(\boldsymbol{\lambda})\rangle \mapsto \langle o(\boldsymbol{\lambda})|\nabla o(\boldsymbol{\lambda})\rangle + i\nabla\phi(\boldsymbol{\lambda}) \tag{2.12}$$

For $\phi(\boldsymbol{\lambda}) \in \mathcal{C}^2$ we see from eq. 2.10, that gauge independent choice would be for infinitesimal change for example

$$f = \langle o(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})|o(\boldsymbol{\lambda})\rangle\,, \tag{2.13}$$

sometimes referred to as the *fidelity of a ground state*[2]. We can see it's physical meaning imagining *quantum quench* (rapid change of some Hamiltonian parameters), in which case f^2 is the probability that system will remain in the new

[2]Generalization for any mixed state is for two density matrices σ, ρ as

$$f \coloneqq \left(\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)$$

ground state. $1 - f^2$ is therefore probability of exciting the system during this quench, which leads to the definition of *distance on* $\mathcal{M}_0$[3]

$$\mathrm{d}s^2 \equiv 1 - f^2 = 1 - |\langle o(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})|o(\boldsymbol{\lambda})\rangle|^2 . \tag{2.14}$$

We can easily check, that the axioms of metric defined using distance as bilinear form s between elements $|\psi\rangle\,,\ |\phi\rangle \in \mathcal{M}_0$ are for closed systems satisfied:

- identity of indiscernibles $s(|\psi\rangle\,, e^{i\alpha}\,|\psi\rangle) = 0 \Leftrightarrow |\psi\rangle = |\phi\rangle$, $\alpha \in \mathbb{R}$,
- symmetry for any two states $|\psi\rangle$, $|\phi\rangle$ is implied by $|\,\langle\psi|\phi\rangle\,| = |\,\langle\phi|\psi\rangle\,|$
- triangle inequality: $s(|\psi\rangle\,, |\psi_2\rangle) < s(|\psi\rangle\,, |\psi\rangle_1) + s(|\psi_1\rangle\,, |\psi_2\rangle)$ for any $|\psi_1\rangle$.

Because $1 - f^2 > 0$, the first term of Taylor expansion is zero, thus we have for metric tensor

$$\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}\lambda^\mu\mathrm{d}\lambda^\nu + \mathcal{O}(\lambda^3). \tag{2.15}$$

Let's define the metric on the space of states $\mathcal{M}_0$ and then see, how it corresponds to fidelity. This metric is called the *Geometric tensor*, and can be expressed as

$$\chi_{\mu\nu} \coloneqq \langle\partial_\mu o|\partial_\nu o\rangle_c \equiv \langle\partial_\mu o|\partial_\nu o\rangle - \langle\partial_\mu o|o\rangle\,\langle o|\partial_\nu o\rangle\,, \tag{2.16}$$

where shortened notation $\partial_\nu \coloneqq \frac{\partial}{\partial\lambda^\nu}$ was used. Because χ is Hermitian ($\chi_{\mu\nu} = \chi^*_{\nu\mu}$), only the symmetric part determines the distance between states

$$\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}\lambda^\mu\mathrm{d}\lambda^\nu = \chi_{\mu\nu}\mathrm{d}\lambda^\mu\mathrm{d}\lambda^\nu, \tag{2.17}$$

therefore it is practical to decompose it as

$$\chi_{\mu\nu} \equiv g_{\mu\nu} - i\frac{1}{2}\nu_{\mu\nu}, \tag{2.18}$$

where the *Fubini-Study tensor*[4], as it's called, is metric on $\mathcal{PM}_0$ and can be expressed as

$$g_{\mu\nu} = \frac{\chi_{\mu\nu} + \chi_{\nu\mu}}{2} = \Re\,\langle\partial_\mu o|\partial_\nu o\rangle_c = \Re\sum_{o\neq j}\frac{\langle o|\frac{\partial\mathcal{H}}{\partial\lambda^\mu}|j\rangle\,\langle j|\frac{\partial\mathcal{H}}{\partial\lambda^\nu}|o\rangle}{(E_o - E_j)^2}, \tag{2.19}$$

and the *curvature tensor* a.k.a. *Berry curvature* is

$$\nu_{\mu\nu} = i(\chi_{\mu\nu} - \chi_{\nu\mu}) = \mathrm{Im}\,\langle o|[\overleftarrow{\partial}_\nu, \partial_\mu]|o\rangle_c = -2\mathrm{Im}\sum_{o\neq j}\frac{\langle o|\frac{\partial\mathcal{H}}{\partial\lambda^\mu}|j\rangle\,\langle j|\frac{\partial\mathcal{H}}{\partial\lambda^\nu}|o\rangle}{(E_o - E_j)^2}, \tag{2.20}$$

where $\overleftarrow{\partial}_\nu$ affects the covector on the left.

[3] d notation is in differential geometry assumed to be an exterior differential. On functions, it acts as $\mathrm{d} : \mathcal{FM} \to \mathcal{T}_1\mathcal{M}$ and intuitively corresponds to total differential from functional analysis.

[4] In some literature, this is called Geometric tensor

2.3 Derivation of the geometric tensor

To prove the correspondence of geometric tensor, described by eq. 2.16, to distance on $\mathcal{M}_0$, see eq. 2.14, we start with eigenstate $|o(\boldsymbol{\lambda})\rangle \in \mathcal{M}_0 \cap \mathcal{H}(\boldsymbol{\lambda})$. Changing parameters $\boldsymbol{\lambda}$ to $\boldsymbol{\lambda} + \delta\boldsymbol{\lambda}$ results in Hamiltonian $\hat{H}_f$ with eigenstates $|s(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})\rangle \in \mathcal{M}_s \cap \mathcal{H}(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})$, meaning it can be excited. Probability amplitude of going to such state is

$$\begin{aligned} a_s &= \langle s(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})|o(\boldsymbol{\lambda})\rangle \approx \delta\lambda^\mu \langle \partial_\mu s(\boldsymbol{\lambda})|o(\boldsymbol{\lambda})\rangle \\ &= -\delta\lambda^\mu \langle s(\boldsymbol{\lambda})|\partial_\mu|o(\boldsymbol{\lambda})\rangle . \end{aligned} \tag{2.21}$$

If we introduce the *gauge potential*, aka *calibration potential*, as[5]

$$\widehat{\mathcal{A}}_\mu \equiv i\partial_\mu, \tag{2.22}$$

the probability amplitude can be expressed as

$$a = i \langle s(\boldsymbol{\lambda})|\widehat{\mathcal{A}}_\mu|o(\boldsymbol{\lambda})\rangle \, \delta\lambda^\mu, \tag{2.23}$$

which has meaning of matrix elements of the gauge potential. Probability of the excitation i.e. transition to any state $s > 0$ from ground state is then (omitting the $\boldsymbol{\lambda}$ dependence in notation)

$$\begin{aligned} \sum_{s\neq 0} |a_s|^2 &= \sum_{s\neq 0} \delta\lambda^\mu \delta\lambda^\nu \langle o|\widehat{\mathcal{A}}_\mu|s\rangle \langle s|\widehat{\mathcal{A}}_\nu|o\rangle + \mathcal{O}(|\delta\lambda^3|) \\ &= \delta\lambda^\mu \delta\lambda^\nu \langle o|\widehat{\mathcal{A}}_\mu \widehat{\mathcal{A}}_\nu|o\rangle_c =: \delta\lambda^\mu \delta\lambda^\nu \chi_{\mu\nu} + \mathcal{O}(|\delta\lambda^3|), \end{aligned} \tag{2.24}$$

where last term defines the geometric tensor.

[5] In SI units, the gauge potential is $\widehat{\mathcal{A}}_\mu \equiv i\hbar\partial_\mu$

2.4 Gauge potentials

Adiabatic transformation is such a transformation from $\mathcal{M}$ to $\mathcal{M}$, which does not excite the system, meaning the fidelity $f = 1$. Generally it can be achieved by two ways – infinitely slow transformation of states, or adding some *counter-diabatic elements* to the Hamiltonian to counter the excitation.

In case of adiabatic gauge potential we choose the basis for $\mathcal{M}$ as eigenstates of the Hamiltonian of the full system $\mathcal{H}$. Adiabatic transformation can be understood as parallel transport on fiber bundle and adiabatic potentials its defining affine connection. To understand more the physical meaning, let's first consider classical system and then move to the quantum mechanics.

2.4.1 Classical gauge potential

In the Hamiltonian classical mechanics, we assume the manifold $\mathcal{M}$ to be an accessible part of the phase space using the Hamiltonian $\mathcal{H} = \mathcal{H}(p_i, q_i)$, where momentum p_i and position q_i are assumed to form the orthogonal basis of the phase space, i.e.

$$\{q^i, p_j\} = \delta^i_j, \tag{2.25}$$

which also defines *calibrational freedom* in their choice. *Canonical transformations* then by definition preserve this formula. Using the *Poisson bracket*, defined as

$$\{A, B\} \equiv \frac{\partial A}{\partial q^j}\frac{\partial B}{\partial p_j} - \frac{\partial B}{\partial q^j}\frac{\partial A}{\partial p_j}, \tag{2.26}$$

we will examine continuous canonical transformations generated by gauge potential $\mathcal{A}_\lambda$

$$q^j(\lambda + \delta\lambda) = q^j(\lambda) - \frac{\partial \mathcal{A}_\lambda(\boldsymbol{p}, \boldsymbol{q})}{\partial p_j}\delta\lambda \;\Rightarrow\; \frac{\partial q^j}{\partial \lambda} = -\frac{\partial \mathcal{A}_\lambda}{\partial p_j} = \{\mathcal{A}_\lambda, q^j\} \tag{2.27}$$

$$p_j(\lambda + \delta\lambda) = p_j(\lambda) - \frac{\partial \mathcal{A}_\lambda(\boldsymbol{p}, \boldsymbol{q})}{\partial q^j}\delta\lambda \;\Rightarrow\; \frac{\partial p_j}{\partial \lambda} = -\frac{\partial \mathcal{A}_\lambda}{\partial q^j} = \{\mathcal{A}_\lambda, p_j\}. \tag{2.28}$$

Substituting this to eq. 2.25, we get

$$\{q^j(\lambda + \delta\lambda), p_j(\lambda + \delta\lambda)\} = \delta^i_j + \mathcal{O}(\delta\lambda^2). \tag{2.29}$$

Equations 2.27,2.28 are identical to the Hamilton equations

$$\begin{aligned} \dot{q}^j &= -\{\mathcal{H}, q^j\} = \frac{\partial \mathcal{H}}{\partial p_j} \\ \dot{p}_j &= -\{\mathcal{H}, p_j\} = -\frac{\partial \mathcal{H}}{\partial q^j}, \end{aligned} \tag{2.30}$$

if λ is time parameter and $\mathcal{A}_t = -\mathcal{H}$. Because the Hamiltonian is generator of the movement in the phase space $(\boldsymbol{q}, \boldsymbol{p})$, we can interpret $\mathcal{A}_t$ as the generators of the movement on $\mathcal{M}$. Other specific choice might be $\lambda = X^i$, which gives us the momentum components $\mathcal{A}_{X^i} = p_i$.

2.4.2 Quantum gauge potential

[Kolodrubetz et al., 2017][chap. 2.2] The role of Poison brackets in quantum mechanics is taken by commutators, canonical transformations are called *unitary transformations* and calibration freedom is hidden in the choice of basis. We can write the unitary transformation $\hat{U}$ between initial system S and the transformed $\tilde{S}$ along some path $\gamma(\lambda)$ on $\mathcal{M} \equiv \cup_{\boldsymbol{\lambda}}\{|m(\boldsymbol{\lambda})\rangle\}$. Let the initial state be $|\psi\rangle \equiv |\psi(0)\rangle$ and define unitary transformation

$$\hat{U}(\lambda)^+ |\psi\rangle = |\tilde{\psi}(\lambda)\rangle\,, \tag{2.31}$$

where scalar parameter λ is assumed to be changing along the path $\gamma(\lambda)$, corresponding to situation on fig. 2.4. This satisfies

$$i\hbar\partial_t\hat{U}(\lambda) = \hat{H}(\lambda)\hat{U}(\lambda) \tag{2.32}$$

for any point on γ, along which the partial derivative is taken. The wave function $|\psi\rangle$ in S can be decomposed using Schmidt decomposition[6], as

$$|\psi\rangle = \sum_{m,n}\psi_n\hat{U}^*_{nm}|m(\boldsymbol{\lambda})\rangle = \sum_m \overbrace{\tilde{\psi}_m(\boldsymbol{\lambda})}^{\langle m(\boldsymbol{\lambda})|\psi\rangle}|m(\boldsymbol{\lambda})\rangle\,. \tag{2.33}$$

We can define adiabatic potentials analogically to the classical case as

$$i\hbar\partial_t|\tilde{\psi}(\boldsymbol{\lambda})\rangle = i\hbar\partial_t\left(\hat{U}^+(\boldsymbol{\lambda})|\psi\rangle\right) = \underbrace{i\hbar\left(\partial_t\hat{U}^+(\boldsymbol{\lambda})\right)\hat{U}(\boldsymbol{\lambda})}_{-\tilde{\hat{\mathcal{A}}}_\lambda}|\tilde{\psi}(\boldsymbol{\lambda})\rangle\,, \tag{2.34}$$

where we defined the adiabatic potential $\tilde{\hat{\mathcal{A}}}_\lambda$, which can be transformed to non-tilde system as

$$\begin{aligned}\widehat{\mathcal{A}}_\lambda &= \hat{U}(\boldsymbol{\lambda})\tilde{\hat{\mathcal{A}}}_\lambda\hat{U}^+(\boldsymbol{\lambda}) = -i\hbar\Big(\hat{U}(\boldsymbol{\lambda})\partial_t\hat{U}^+(\boldsymbol{\lambda})\Big) = \\ &= -i\hbar\Big(\partial_t(\underbrace{U^+(\boldsymbol{\lambda})U(\boldsymbol{\lambda})}_{\mathbb{1}}) - \partial_t(U(\boldsymbol{\lambda}))U^+(\boldsymbol{\lambda})\Big) = i\hbar\Big(\partial_t U(\boldsymbol{\lambda}))U^+(\boldsymbol{\lambda}).\end{aligned} \tag{2.35}$$

Thus we get equations for adiabatic potentials

$$\widehat{\mathcal{A}}_\lambda = i\hbar\Big(\partial_t U(\boldsymbol{\lambda}))U^+(\boldsymbol{\lambda}) \tag{2.36}$$

$$\tilde{\hat{\mathcal{A}}}_\lambda = -i\hbar\left(\partial_t\hat{U}^+(\boldsymbol{\lambda})\right)\hat{U}(\boldsymbol{\lambda}) \tag{2.37}$$

These potencials are Hermitean

$$\tilde{\hat{\mathcal{A}}}_\lambda{}^+ = i\hbar U(\boldsymbol{\lambda})^+\partial_t\hat{U}(\boldsymbol{\lambda}) = -i\hbar\partial_t\hat{U}(\boldsymbol{\lambda})^+\hat{U}(\boldsymbol{\lambda}) = \tilde{\hat{\mathcal{A}}}_\lambda, \tag{2.38}$$

analogically holds for $\widehat{\mathcal{A}}_\lambda$ and using the eigenbasis of $\hat{H}$, the matrix elements are

$$\langle n(\mathbf{0})|\,\tilde{\hat{\mathcal{A}}}_\lambda\,|m(\mathbf{0})\rangle = i\hbar\,\langle n(\mathbf{0})|\,\hat{U}(\boldsymbol{\lambda})^+\partial_t\hat{U}(\boldsymbol{\lambda})\,|m(\mathbf{0})\rangle = i\hbar\,\langle\tilde{n}(\boldsymbol{\lambda})|\,\partial_t\,|\tilde{m}(\boldsymbol{\lambda})\rangle\,. \tag{2.39}$$

[6]The Schmidt decomposition can be performed in finite dimension, or if the Hamiltonian is compact, which is not automatic in quantum mechanics. What's more, the Hamiltonian is usually not even bounded. Anyway, for simple systems with bounded energy we can assume so.

and because

$$\langle \tilde{n}(\boldsymbol{\lambda})| \, \widehat{\mathcal{A}}_\lambda \, |\tilde{m}(\boldsymbol{\lambda})\rangle = \langle n(\mathbf{0})| \, \widehat{\tilde{\mathcal{A}}}_\lambda \, |m(\mathbf{0})\rangle \,, \tag{2.40}$$

we get

$$\widehat{\mathcal{A}}_\lambda = i\hbar\partial_t. \tag{2.41}$$

It's good to point out, that we were applying tilde operators to non-tilde states et vice versa. This can be justified only if we consider $\mathcal{M}$ big enough to contain all necessary states, which can be achieved during the transformation.

If we now consider the parametrization with time $\lambda \coloneqq t$, $\hat{U}$ can be explicitly expressed according to eq. 2.3 as

$$\hat{U}(\lambda) = \sum_n \exp\left(\frac{i}{\hbar}E_n(\tau)\mathrm{d}\tau - \int_0^t \langle s(\tau)|\partial_\tau n(\tau)\rangle \, \mathrm{d}\tau\right) |s(\lambda)\rangle \langle s(0)| \,. \tag{2.42}$$

2.5 Berry phase and curvature

Let's now consider only the ground state manifold, because it will be used later on. Thought every step can be easily generalized to any state manifold $\mathcal{M}_m$.

On the ground state manifold $\mathcal{M}_0 \equiv \cup_{\boldsymbol{\lambda}}\{|o(\boldsymbol{\lambda})\rangle\}$, the *Berry connection* is defined as

$$A_\mu(\boldsymbol{\lambda}) \equiv \langle o(\boldsymbol{\lambda})|\widehat{\mathcal{A}}_\mu|o(\boldsymbol{\lambda})\rangle \,, \tag{2.43}$$

which uses the decomposition of $\boldsymbol{\lambda}$ to some basis, thus it empowers us to take derivatives in any direction in the base manifold $\mathbb{R}^n$ and thus the geometric tensor can be written as

$$\chi_{\mu\nu}(\boldsymbol{\lambda}) = \partial_\mu A_\nu(\boldsymbol{\lambda}) - \partial_\nu A_\mu(\boldsymbol{\lambda}) \tag{2.44}$$

and the *Berry phase*[7] as the integral of a connection along some closed curve $\mathcal{C}$

$$\phi_B \equiv -\oint_{\mathcal{C}} A_\mu(\boldsymbol{\lambda})\mathrm{d}\lambda^\mu = \int_{\mathcal{S}} \chi_{\mu\nu}(\boldsymbol{\lambda})\mathrm{d}\lambda^\mu \wedge \mathrm{d}\lambda^\nu, \tag{2.47}$$

where we used the Stokes theorem for some area $\mathcal{S}$ with boundary $\partial\mathcal{S} = \mathcal{C}$.

The gauge potentials can then be understood as affine connections defining the parallel transport. Covariant derivative is thus

$$D_\mu = \partial_\mu + i\widehat{\mathcal{A}}_\mu, \tag{2.48}$$

which yields $D_\mu \, |\psi_n\rangle = 0$ for every eigenstate, which is the promissed claim, that the transport of eigenvalues on $\mathcal{M}_0$ is parallel. $\widehat{\mathcal{A}}_\mu$ is generally defined 2.36, which generally gives non-zero covariant derivative for states outside of $\mathcal{M}_0$.

[7] The reasonability of this definition can be seen, if we assume the ground state of a free particle $\langle \boldsymbol{x}|i(\boldsymbol{\lambda})\rangle = i(\boldsymbol{x},\boldsymbol{\lambda}) = |i(\boldsymbol{x})|e^{i\phi(\boldsymbol{\lambda})}$, then the Berry connection is

$$A_\mu = -\int \mathrm{d}\boldsymbol{x}|i(\boldsymbol{x},\boldsymbol{\lambda})|^2\partial_\mu\phi(\boldsymbol{\lambda}) = -\partial_\mu\phi(\boldsymbol{\lambda}) \tag{2.45}$$

and Berry phase

$$\phi_B = \oint_{\mathcal{C}} \partial_\mu\phi\mathrm{d}\lambda^\mu, \tag{2.46}$$

which represents total phase accumulated by the wave function. It is really the analogy for Berry phase in classical mechanics, which for example in the case Foucault pendulum on one trip around the Sun makes $\phi_B = 2\pi$

2.6 Adiabatic transformations

In this chapter, we will be dealing with the system described by the finite-dimensional Hamiltonian $\hat{H}(\boldsymbol{\lambda})$ which drives the system according to Schrödinger equation from some initial state $|s(\boldsymbol{\lambda}\rangle$ to $|s(\tilde{\boldsymbol{\lambda}})\rangle$ along some path. Again we reduce the dimension from $\mathbb{R}^n$ to 1 prescribing the curve $\gamma(\lambda)$ parametrized by time t, so we get $\hat{H} = \hat{H}(\lambda)$.

Important knowledge about symmetries of the system is encoded in canonical transformations, or in quantum mechanics more commonly referred to as *unitary transformations*. In our case, the generators of such canonical transformations are adiabatic potentials. In case of the Hamiltonian $\mathcal{H}(\boldsymbol{\lambda})$ and it's adiabatic transformation $\mathcal{H}(\boldsymbol{\lambda} + \mathrm{d}\boldsymbol{\lambda})$, we get

$$[\hat{H}(\boldsymbol{\lambda}), \hat{H}(\boldsymbol{\lambda} + \delta\boldsymbol{\lambda})] = 0, \tag{2.49}$$

meaning Hamiltonian commutes with it's canonically transformed version.[8] Before going throw the details of adiabatic transformations, let's define its meaning properly.

Definition 2 (Adibaticity)**.** *Slow change of parameters driving Hamiltonian in a sense, that it does not excite the system and allows the system to return to the same energetic state after circulation around any closed path on the manifold with fidelity $f = 1$. For more see Theorem 1.*

2.6.1 Adiabatic transformation

[Kolodrubetz et al., 2017][chap. 2.3] As was mentioned in the introduction to this chapter, one way to change the system parameters without exciting it is to change the driving parameter slowly enough. The meaning of the word "slow" clears up next theorem.

Theorem 1 (Adiabatic theorem)**.** *For Hamiltonian $\hat{H}$ varying in the time range T, the solution of the Schrödinger equation*

$$\hat{H}(\lambda)\,|\psi_n(\lambda)\rangle = E_n(\lambda)\,|\psi_n(\lambda)\rangle$$

with initial condition in x-representation $\langle x|\psi(t=0\rangle = \psi_n(x,0)$ can be approximated as

$$||\psi(\lambda) - \psi_{ad}(\lambda)|| \approx o\left(\frac{1}{T}\right) \tag{2.50}$$

for adiabatic state

$$|\psi_{ad}\rangle = e^{\theta_n(\lambda)} e^{\gamma_n(\lambda)}\,|\psi(\lambda)\rangle\,, \tag{2.51}$$

where we define nongeometrical phase *induced by energy transitions,*

$$\theta_n(\lambda) \equiv -\frac{1}{\hbar}\int_0^t E_n(\tau)\mathrm{d}\tau$$

and geometrical phase*, also called* Berry phase

$$\gamma_n(\lambda) \equiv \int_0^t \underbrace{i\,\langle\psi_n(\tau)|\partial_t\psi_n(\tau)\rangle}_{\nu_n(\tau)}\,\mathrm{d}\tau.$$

[8] This can be easily reformulated to the world of classical physics, where the commutator is replaced by Poisson bracket.

Proof. TBD (na wiki je)

□

Assume differentiable and non-singular Hamiltonian $\hat{H}(\boldsymbol{\lambda})$ with degenerate basis $\{|m, \boldsymbol{\lambda}\rangle\}_m$ called the *adiabatic basis*. This is generally the family of adiabatically connected eigenstates[9] The transition amplitude between states for adiabatic change is

$$0 = \langle m(\boldsymbol{\lambda})| \hat{H} |n(\tilde{\boldsymbol{\lambda}})\rangle \quad \text{for } n \neq m, \forall \boldsymbol{\lambda}, \forall \tilde{\boldsymbol{\lambda}}. \tag{2.52}$$

This can be driven along some curve $\gamma(\lambda)$, i.e. differentiated by ∂_t:

$$\begin{aligned} 0 &= \langle \partial_t m(\boldsymbol{\lambda})| \hat{H}(\tilde{\boldsymbol{\lambda}}) |n(\tilde{\boldsymbol{\lambda}})\rangle + \langle m(\boldsymbol{\lambda})| \overbrace{\partial_t \hat{H}(\tilde{\boldsymbol{\lambda}})}^{\approx \partial_t \hat{H}(\boldsymbol{\lambda})} |n(\tilde{\boldsymbol{\lambda}})\rangle + \langle m(\boldsymbol{\lambda})| \hat{H}(\tilde{\boldsymbol{\lambda}}) |\partial_t n(\tilde{\boldsymbol{\lambda}})\rangle \\ &= E_n(\lambda) \langle \partial_t m(\boldsymbol{\lambda}) | n(\tilde{\boldsymbol{\lambda}})\rangle + E_m(\lambda) \langle m(\boldsymbol{\lambda}) | \partial_t n(\tilde{\boldsymbol{\lambda}})\rangle + \langle m(\boldsymbol{\lambda})| \partial_t \hat{H}(\tilde{\boldsymbol{\lambda}}) |n(\tilde{\boldsymbol{\lambda}})\rangle \\ &= (E_m(\lambda) - E_n(\lambda)) \underbrace{\langle m | \partial_t(\tilde{\boldsymbol{\lambda}})\rangle}_{-\frac{i}{\hbar}\langle m|\widehat{\mathcal{A}}_t|n(\tilde{\boldsymbol{\lambda}})\rangle} + \langle m|\partial_t \hat{H}|n(\tilde{\boldsymbol{\lambda}})\rangle \,. \end{aligned} \tag{2.53}$$

In matrix form, we can rewrite this equation as

$$i\hbar\partial_t \hat{H} = [\widehat{\mathcal{A}}_t, \hat{H}] - i\hbar \hat{M}_t \qquad \text{for } \hat{M}_t \equiv -\sum_n \frac{\partial E_n(\lambda)}{\partial t} |n(\lambda)\rangle \langle n(\lambda)| \,. \tag{2.54}$$

$\hat{M}$ is diagonal in energetic basis and it's elements has meaning of *generalized force*, which correspond to corresponding energetic states. We can easily see that $[\hat{H}, \hat{M}] = 0$, implying

$$[\hat{H}, i\hbar\partial_t \hat{H} - [\widehat{\mathcal{A}}_t, \hat{H}]] = 0. \tag{2.55}$$

This can be used as the definition for *counter-diabatic potential* $\widehat{\mathcal{A}}_t$. The strength of this equation lies in the fact, that it finds counter-diabatic potential without the need of Hamiltonian diagonalization.

2.7 Counter-diabatic driving

[Kolodrubetz et al., 2017][page 15–17] The main idea of a counter-diabatic driving is, that any excitation of the system can be countered by adding so called *counter-diabatic potential* to the Hamiltonian. Consider again any eigenstate $|\psi(t)\rangle$ of the Hamiltonian $\hat{H} = \hat{H}(\lambda)$ driven along the curve $\gamma(\lambda(t))$ on $\mathcal{M}_0$ depending on time t, during which the fidelity $f \neq 0$. Because the system is not measured during the trip, it can't be stated if or if not it was excited, but the main goal here is to make fidelity zero, which is iff (is it equivalence, or just implication?) $\tilde{\hat{H}}$ is diagonal. For diagonalizable Hamiltonian, there exist such transformation (same as eq. 2.31)

$$\hat{U}(\lambda)^+ : |\psi(\lambda)\rangle \to |\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\rangle \,, \tag{2.56}$$

[9] In the case of energy level crossing, the eigenstates are not unified, because transition between them is not adiabatical.

for which the fidelity will be zero. Such a transformation does not have to be unique, but we can choose any one of them. This can be seen more clearly from direct transformation of the Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(\lambda)\right\rangle = \hat{H}(\lambda)\left|\psi(\lambda)\right\rangle \tag{2.57}$$

to the transformed frame using unitary operator for time varying Hamiltonian

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\hat{U}(\tilde{\boldsymbol{\lambda}})\left|\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\right\rangle) = \hat{H}(\lambda)\hat{U}(\tilde{\boldsymbol{\lambda}})\left|\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\right\rangle \tag{2.58}$$

$$i\hbar\frac{\mathrm{d}\lambda}{\mathrm{d}t}\partial_\lambda\hat{U}(\tilde{\boldsymbol{\lambda}})\left|\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\right\rangle + i\hbar\hat{U}(\tilde{\boldsymbol{\lambda}})\frac{\mathrm{d}}{\mathrm{d}t}\left|\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\right\rangle = \hat{H}(\lambda)\hat{U}(\tilde{\boldsymbol{\lambda}})\left|\tilde{\psi}(\tilde{\boldsymbol{\lambda}})\right\rangle. \tag{2.59}$$

This can be rewritten using adiabatic potential from eq. 2.41, using *dot* notation for time derivatives and omitting the points in which the objects are evaluated, as

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\tilde{\psi}\right\rangle = \left[\hat{U}^{+}\hat{H}\hat{U} - \dot{\lambda}\tilde{\hat{\mathcal{A}}}_\lambda\right]\left|\tilde{\psi}\right\rangle = \left[\tilde{\hat{H}} - \dot{\lambda}\tilde{\hat{\mathcal{A}}}_\lambda\right]\left|\tilde{\psi}\right\rangle = \tilde{\hat{H}}_m\left|\tilde{\psi}\right\rangle, \tag{2.60}$$

where the term $-\dot{\lambda}\tilde{\hat{\mathcal{A}}}_\lambda$ is called *Galilean*.

From this can be seen, that the Hamiltonian can be transformed as $\tilde{\hat{H}}(\boldsymbol{\lambda}) = \hat{U}^{+}(\lambda)\hat{H}(\lambda)\hat{U}(\lambda)$ and to the Hamiltonian in transformed frame $\hat{H}_m = \hat{H} - \dot{\lambda}\hat{\mathcal{A}}_\lambda$ we can add *counter-diabatic element* $\dot{\lambda}\hat{\mathcal{A}}_\lambda$ and the only remaining element is $\hat{H}$, which does not excite the system ($f = 0$). Intuition for transformations using original Hamiltonian vs. transformed one can be seen on fig. 2.6. It is good to point out, that the eigenstates on this figure belong to the space $\mathcal{PM}$, but the paths itself need to be considered in the whole $\mathcal{M}$, which can be seen as the phase change described by equation 2.42.

Figure 2.6: Comparison between transport by Hamiltonian $\hat{H}$ (blue path $\gamma(\lambda)$ and the one with counter-diabatic potential added (pink path $\gamma(\tilde{\lambda})$), which has zero fidelity. The nonzero fidelity area for path $\gamma(\lambda)$ is marked green and initial and final states $|\psi(\lambda_i)\rangle$, resp. $|\psi(\lambda_f)\rangle$ are marked purple.

2.8 Approximations of adiabatic potentials

Adiabatic potentials can be calculated from the principal of minimal action, which leads to variational method.

If the difference between eigenstates of $\hat{H}$ is small, or generalized force between some states is zero, the computation of the adiabatic potential is numerically unstable. The knoledge of exact adiabatic potential would allow to maintain the system in the ground state thus not exciting it, as th Eigenstate thermalization hypotheses states.

Hypotheses 1 (Eigenstate thermalization hypotheses)**.** *For the difference between eigenstates of $\hat{H}$ and extensive thermodynamic entropy S, it holds that*

$$E_n - E_m \propto \exp\left(\frac{S}{2}\right). \tag{2.61}$$

If the states are close, better approximation would be $E_n - E_m \propto \exp(S)$. For matrix elements it holds, that they vanish exponentially with the characteristic scale of the system a, i.e.

$$\langle m|\,\widehat{\mathcal{A}}_\lambda\,|n\rangle = i\hbar\frac{\langle m|\partial_t\hat{H}|n\rangle}{E_m - E_n} \propto \exp(-a). \tag{2.62}$$

Fortunatelly in the limit "number of particles" $\to \infty$ the expression in eq. 2.62 converges.

2.8.1 Variational methods

In the case of simple systems, the adiabatic potentials can be found analytically, but for more complicated Hamiltonians we will be forced to use approximations, or some perturbational and variational methods.

Conclusion

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List of Figures

A. Attachments

A.1 First Attachment