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**Some weird small things looking for
counteradiabatic elements**

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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.

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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*, functions as lower case and operators with *hat*.

Introduction

Let's have some fun with geometry!

1. Mathematical introduction

The modern approach to the closed system dynamics is using differential geometry formalism. Before we get to the quantum mechanics itself, let's 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

$$\gamma : \mathbb{R} \xrightarrow{\text{open}} I \rightarrow \mathcal{M} \quad \xi \mapsto \gamma(\xi).$$

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

$$f : \mathcal{M} \rightarrow U \xrightarrow{\text{open}} \mathbb{R} \quad x \mapsto f(x).$$

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

$$\begin{aligned} \gamma_1(0) &= \gamma_2(0) \equiv P \\ \frac{d}{dt}x^i(\gamma_1(t))\Big|_{t=0} &= \frac{d}{dt}x^i(\gamma_2(t))\Big|_{t=0}. \end{aligned}$$

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 cotangent 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 $\mathcal{T}_q^p\mathcal{M}$.

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

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

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

$$\mathbf{v} : \mathcal{F}(\mathcal{M}) \rightarrow \mathbb{R} \quad f \mapsto \mathbf{v}[f] \equiv \frac{df(\gamma(\xi))}{d\xi}\Big|_P \equiv \partial_\xi\Big|_P f. \tag{1.2}$$

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

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

The directionnal derivative will be denoted

$$\nabla_v$$

¹ The direction itself is usually denoted as

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

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 $\mathbf{e}_i \equiv \partial/\partial x^i$ we will denote

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

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 *fiber bundle*.

Definition 1. *Structure $(\mathcal{E}, \mathcal{B}, \pi, \mathcal{F})$, for topological spaces \mathcal{E} (total space), \mathcal{B} (base space), \mathcal{F} (fibre) and a continuous surjection $\pi : \mathcal{E} \rightarrow \mathcal{B}$ satisfying a local triviality² is called a Fiber bundle (projection map). In addition, the \mathcal{B} is assumed to be connected³ 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*

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

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, $\pi : \mathcal{E} \rightarrow \mathcal{B}$ must be open map. The meaning of

$$\begin{array}{ccc} \pi^{-1}(U) & \xrightarrow{\varphi} & U \times F \\ \pi \downarrow & \nearrow \text{proj}_1 & \\ U & & \end{array}$$

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 Section

Section is a function

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

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

²local triviality

³cannot be represented as a union of two disjoint sets

1.3 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

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

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

$$\phi^* : \mathcal{FN} \rightarrow \mathcal{FM} \quad \tilde{f} \mapsto f = (\phi^* \tilde{f})(x) \equiv \phi^* \tilde{f}(x) = \tilde{f}(\phi x).$$

Push-forward of a vector is defined as

$$\phi_* : \mathbb{T}_x \mathcal{M} \rightarrow \mathbb{T}_{\phi x} \mathcal{N} \quad \phi_* \frac{D\gamma(\xi)}{d\xi} \Big|_x = \frac{D\phi\gamma(\xi)}{d\xi} \Big|_x$$

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

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

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

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

and push-forward of covectors

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

1.4 Flow

1.5 Covariant derivative and parallel transport

[probably not needed](#)

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

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

Affine connection can be expressed as

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

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

$$\frac{Da^\mu}{dx^\nu} = a^\mu_{,\nu} - \Gamma_{\alpha\beta}^\mu x^\alpha a^\beta \tag{1.8}$$

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

$$\frac{D\alpha_\mu}{dx^\nu} = \alpha_{\mu,\nu} - \Gamma_{\mu\beta}^\alpha x^\beta \alpha_\alpha \tag{1.9}$$

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

$$\frac{Dv^\mu}{d\xi} = 0 \tag{1.10}$$

vanishes along γ .

1.6 Parallel transport on fiber bundles

this is what we need

1.7 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

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

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

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

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

$$A \wedge B \equiv \frac{(p+q)!}{p!q!} A^{[i_1 \dots i_p} \otimes B^{i_{p+1} \dots i_{p+q}]} \quad (1.12)$$

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.

Assume parameter $\lambda \in \mathbb{R}^n$ controlling some Hamiltonian $\hat{H}(\lambda)$, which is bounded from below and the spectrum is discrete for the first $f > 1$ energies, where f depends on considered excitation level and will be clear later on. From this we can construct fiber bundle, such that at every point of base manifold $\lambda \in \mathbb{R}^n$, we construct fiber consisting of all possible states of $\hat{H}(\lambda)$, thus the fiber structure, defined in section 1.1, is

$$\left(\mathcal{H}_{full} := \bigcup_{\lambda} \mathcal{H}(\lambda), \mathcal{U} \subset \textcolor{red}{open} \mathbb{R}^n, \pi, \mathcal{H}(\lambda) := \bigcup_{states} |\psi(\lambda)\rangle \right).$$

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

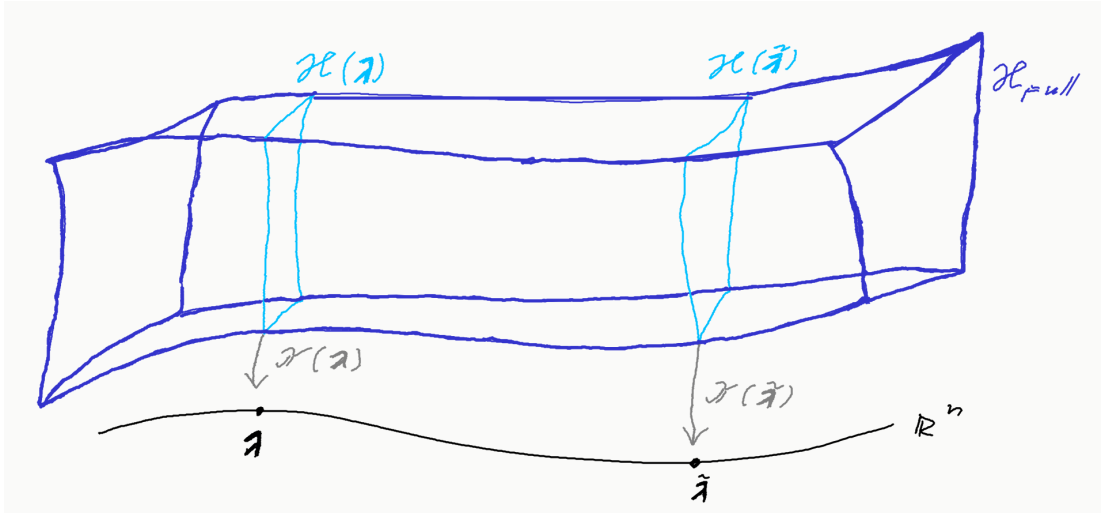


Figure 2.1: Fiber bundle over \mathbb{R}^n with Hilbert spaces $\mathcal{H}(\lambda)$ as individual fibres.

In quantum mechanics physical observables are not related to the space of *bare states* \mathcal{H}_{full} , but the *space of rays*, defined as $\mathcal{PH} := \mathcal{H}_{full}/U(1)$. 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 displayed for any λ on fig. 2.2

Because we are interested only in discrete part of spectrum¹, it will further on be referred to only as *spectrum*.

The states of the system evolves according to the Schrödinger equation

$$i\hbar d_t |\psi(\lambda(t))\rangle = \hat{H}(\lambda(t)) |\psi(\lambda(t))\rangle, \quad (2.1)$$

which for eigenstates reads as energy Schrödinger equation

$$\hat{H}(\lambda(t)) |n(\lambda(t))\rangle = E_n(\lambda(t)) |n(\lambda(t))\rangle. \quad (2.2)$$

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

Figure 2.4: some trip around C, draw angle

2.1 Transporting states

As was pointed out in introduction of this chapter, \mathcal{H}_{full} can be decomposed to different state manifolds \mathcal{M}_s , as displayed on figure 2.5.

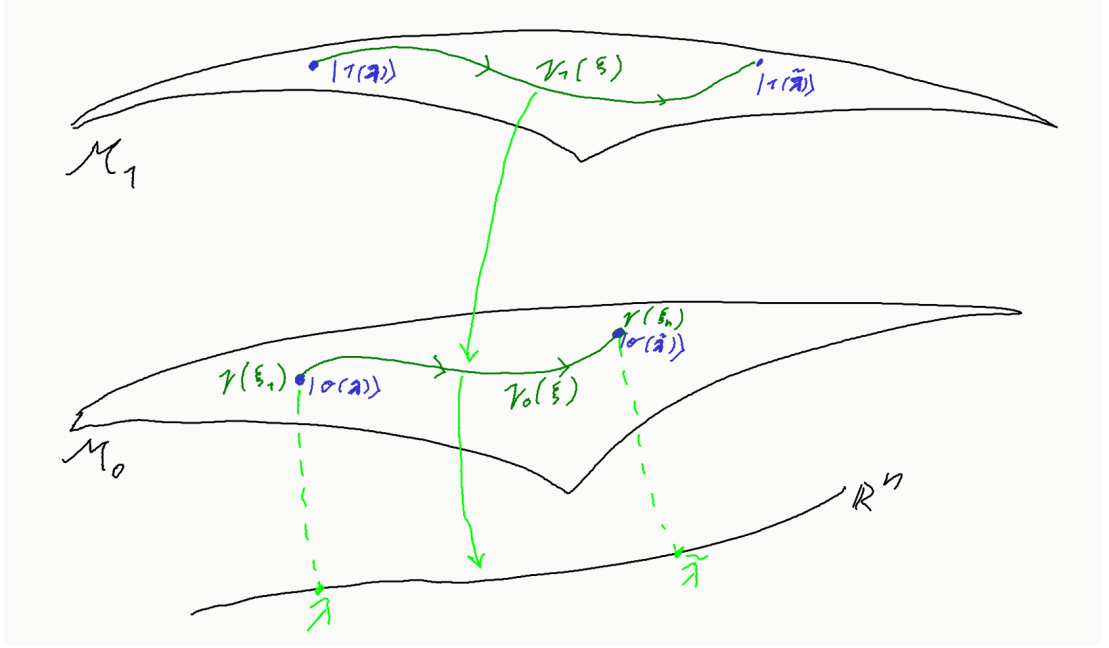


Figure 2.5: Geometrical intuition to transport on fiber manifold sections \mathcal{M}_i .

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

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

The first exponential, the *dynamical phase*, is well known solution to energy Schrödinger equation 2.2 with $\boldsymbol{\lambda} = \text{const.}$ 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 $\gamma_s(\boldsymbol{\lambda}(t))$ and for some closed curve on \mathcal{M}

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

we generally get $\text{par}_C |\psi(\boldsymbol{\lambda})\rangle \neq |\psi(\boldsymbol{\lambda})\rangle$. This property is sometimes more generally called an *anholonomy* and should be defined properly.

Definition 2 (Anholonomy). *Geometrical phenomenon, which causes some variable $V(\gamma(p))$ not to return to it's original value while varying it's parameter p around some closed curve $\gamma(p)$.*

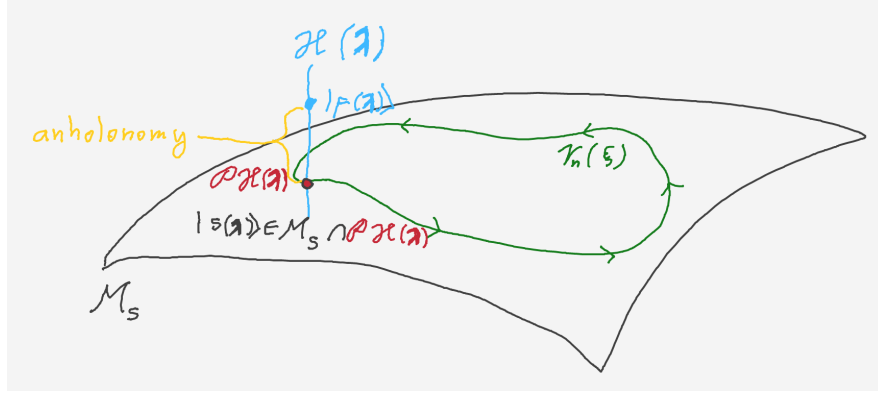


Figure 2.6: Parallel transporting around some closed curve C with anholonomy represented by angle α .

The geometric intuition of anholonomy can be seen on fig. 2.6.

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

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

Substituting general solution 2.3 to eq. 2.1 yields

$$d_t \gamma(t) = i \langle n(\lambda(t)) | \nabla_\lambda n(\lambda(t)) \rangle \cdot d_t \lambda(t). \quad (2.5)$$

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

$$\gamma_n(C) = i \oint_C \langle n(\lambda) | \nabla_\lambda n(\lambda) \rangle \cdot d\lambda. \quad (2.6)$$

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 this expression lies in $\partial_\lambda n(\lambda)$, which locally requires knowledge of single-valued basis $\{|n\rangle\}_n$. This can be avoided in 3-dimensions using Stokes's theorem for S as the surface with boundary $\partial S = C$

$$\begin{aligned} \gamma_n(C) &= -\text{Im} \iint_C dS \cdot \nabla \times \langle n(\lambda) | \nabla n(\lambda) \rangle \\ &= -\text{Im} \iint_C dS \cdot \langle \nabla n(\lambda) | \times | \nabla n(\lambda) \rangle \\ &= -\text{Im} \iint_C dS \cdot \sum_{m \neq n} \langle \nabla n(\lambda) | m(\lambda) \rangle \times \langle m(\lambda) | \nabla n(\lambda) \rangle \\ &= -\iint_C dS \cdot V_n(\lambda) \end{aligned} \quad (2.7)$$

for

$$V_n(\lambda) = \text{Im} \frac{\langle n(\lambda) | \nabla_\lambda \hat{H}(\lambda) | m(\lambda) \rangle \times \langle m(\lambda) | \nabla_\lambda \hat{H}(\lambda) | n(\lambda) \rangle}{(E_m(\lambda) - E_n(\lambda))^2} \quad (2.8)$$

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

if we differentiate the Schrödinger equation 2.2, with any derivative ∇ , we get

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

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

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

defining vector potential of $V_n(\boldsymbol{\lambda})$. In addition, it extends our definition from single valued basis to any solution of 2.2.

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],

$$\gamma_n(C) = - \iint_C dS \cdot \text{Im} \frac{\langle n(\boldsymbol{\lambda}) | d\hat{H}(\boldsymbol{\lambda}) | m(\boldsymbol{\lambda}) \rangle \wedge \langle m(\boldsymbol{\lambda}) | d\hat{H}(\boldsymbol{\lambda}) | n(\boldsymbol{\lambda}) \rangle}{(E_m(\boldsymbol{\lambda}) - E_n(\boldsymbol{\lambda}))^2}. \tag{2.11}$$

Definition 3 (Adiabaticity). *Slow change 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. For more see Theorem 1.*

2.2 Metric and geometric tensor

Only this chapter is for ground state only. From now on we will use natural units, so $\hbar = 1$.

Now we need to find some reasonable way to measure distance on \mathcal{M} . This is needed to be *gauge dependent*, meaning the change in phase factor ϕ of some state $|i(\boldsymbol{\lambda})\rangle \in \mathbb{T}_{\boldsymbol{\lambda}}\mathcal{M}$ induces the change

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

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

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

sometimes referred to as the *fidelity*. 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 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}*

$$ds^2 \equiv 1 - f^2 = 1 - |\langle i(\boldsymbol{\lambda} + d\boldsymbol{\lambda}) | i(\boldsymbol{\lambda}) \rangle|^2. \tag{2.14}$$

We can easily check, that the axioms of metric 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: $s(|\psi\rangle, |\psi_2\rangle) < s(|\psi\rangle, |\psi_1\rangle) + s(|\psi_1\rangle, |\psi_2\rangle)$ for any $|\psi_1\rangle$.

Using $ds^2 = g_{\mu\nu}d\lambda^\mu d\lambda^\nu + \mathcal{O}(\lambda^3)$, we get the metric tensor

$$g_{\mu\nu}^{(i)}(\boldsymbol{\lambda}) = \Re(\langle\partial_{\lambda^\mu}i(\boldsymbol{\lambda})|\partial_{\lambda^\nu}i(\boldsymbol{\lambda})\rangle - \langle\partial_{\lambda^\mu}i(\boldsymbol{\lambda})|i(\boldsymbol{\lambda})\rangle\langle i(\boldsymbol{\lambda})|\partial_{\lambda^\nu}i(\boldsymbol{\lambda})\rangle). \quad (2.15)$$

Let's have an initial state described by Hamiltonian $\mathcal{H}_i(\boldsymbol{\lambda})$ in eigenstate $|i(\boldsymbol{\lambda})\rangle$, which undergoes change of parameters $\boldsymbol{\lambda} \rightarrow \boldsymbol{\lambda} + d\boldsymbol{\lambda}$ resulting in Hamiltonian \mathcal{H}_f with eigenstates $|f_n(\boldsymbol{\lambda} + d\boldsymbol{\lambda})\rangle$, $n \in \{1, \dots, \dim(\mathcal{H}_f)\}$. Probability amplitude of going to some specific excited state is

$$\begin{aligned} a_n &= \langle f_n(\boldsymbol{\lambda} + d\boldsymbol{\lambda})|i(\boldsymbol{\lambda})\rangle \approx d\lambda^\mu \langle \partial_\mu f_n(\boldsymbol{\lambda})|i(\boldsymbol{\lambda})\rangle \\ &= -d\lambda^\mu \langle f_n(\boldsymbol{\lambda})|\partial_\mu i(\boldsymbol{\lambda})\rangle. \end{aligned} \quad (2.16)$$

If we introduce the *gauge potential*, a.k.a *calibration potential*, as²

$$\hat{\mathcal{A}}_\mu \equiv i\partial_\mu, \quad (2.17)$$

the probability amplitude can be expressed as

$$a_n = \sum_\mu i \langle f_n(\boldsymbol{\lambda})|\hat{\mathcal{A}}_\mu|i(\boldsymbol{\lambda})\rangle d\lambda^\mu, \quad (2.18)$$

which has meaning of matrix elements of the gauge potential. Probability of the excitation i.e. transition to any state $n > 0$ from ground state is then

$$\begin{aligned} \sum_{n \neq 0} |a_n|^2 &= \sum_{f_n \neq 0} d\lambda^\mu d\lambda^\nu \langle i|\hat{\mathcal{A}}_\mu|f_n\rangle \langle f_n|\hat{\mathcal{A}}_\nu|i\rangle + \mathcal{O}(|d\lambda|^3) \\ &= d\lambda^\mu d\lambda^\nu \langle i|\hat{\mathcal{A}}_\mu \hat{\mathcal{A}}_\nu|i\rangle_c \equiv d\lambda^\mu d\lambda^\nu \chi_{\mu\nu} + \mathcal{O}(|d\lambda|^3), \end{aligned} \quad (2.19)$$

where we defined *connected correlation function*, or *covariance*

$$\langle i|\hat{\mathcal{A}}_\mu \hat{\mathcal{A}}_\nu|i\rangle_c \equiv \langle i|\hat{\mathcal{A}}_\mu \hat{\mathcal{A}}_\nu|i\rangle - \langle i|\hat{\mathcal{A}}_\mu|i\rangle \langle i|\hat{\mathcal{A}}_\nu|i\rangle \quad (2.20)$$

and the *geometric tensor*³, which can also be defined directly as

$$\chi_{\mu\nu} \equiv \langle \partial_\mu i|\partial_\nu i\rangle_c = \langle \partial_\mu i|\partial_\nu i\rangle - \langle \partial_\mu i|i\rangle \langle i|\partial_\nu i\rangle. \quad (2.21)$$

Because χ is Hermitian ($\chi_{\mu\nu} = \chi_{\nu\mu}^*$), only the symmetric part adds up to the distance between states

$$ds^2 = g_{\mu\nu}d\lambda^\mu d\lambda^\nu = \chi_{\mu\nu}d\lambda^\mu d\lambda^\nu. \quad (2.22)$$

and only the symmetric part determines the distance between the states. Therefore it's practical to decompose it as

$$\chi_{\mu\nu} \equiv g_{\mu\nu} - i\frac{1}{2}\nu_{\mu\nu}, \quad (2.23)$$

²in SI units, the gauge potential is $\hat{\mathcal{A}}_\mu \equiv i\hbar\partial_\mu$

³sometimes defined directly as the expression in eq. 2.20

where the *Fubini-Study tensor*, as it's called, is

$$g_{\mu\nu} = \frac{\chi_{\mu\nu} + \chi_{\nu\mu}}{2} = \Re \langle \partial_\mu i | \partial_\nu i \rangle_c = \Re \sum_{i \neq j} \frac{\langle i | \frac{\partial \mathcal{H}}{\partial \lambda^\mu} | j \rangle \langle j | \frac{\partial \mathcal{H}}{\partial \lambda^\nu} | i \rangle}{(E_i - E_j)^2}, \quad (2.24)$$

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

$$\nu_{\mu\nu} = i(\chi_{\mu\nu} - \chi_{\nu\mu}) = \text{Im} \langle i | [\overleftarrow{\partial}_\nu, \partial_\mu] | i \rangle_c = -2\text{Im} \sum_{i \neq j} \frac{\langle i | \frac{\partial \mathcal{H}}{\partial \lambda^\mu} | j \rangle \langle j | \frac{\partial \mathcal{H}}{\partial \lambda^\nu} | i \rangle}{(E_i - E_j)^2}, \quad (2.25)$$

where $\overleftarrow{\partial}_\nu$ affects the covector on the left. Because $g_{\mu\nu}$ is positive semidefinite, as we already proved, it really can be used as metric tensor.

The Fubini-Study tensor can be seen as the Pull-back of the full Hilbert space metric to \mathcal{M} .

2.3 Gauge potentials

Adiabatic transformation is such a transformation from \mathcal{M} to \mathcal{M} , which does not excite the system. Generally it can be achieved by two ways – infinitely slow transformation of states, or adding some *counterdiabatic 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 and adiabatic potentials as affine connection. To understand it more, let's first consider classical system and then move to the quantum mechanics.

move elsewhere: 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.

2.3.1 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.

$$\{q^i, p_j\} = \delta_j^i, \quad (2.26)$$

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

$$\{A, B\} \equiv \frac{\partial A}{\partial q^j} \frac{\partial B}{\partial p_j} - \frac{\partial B}{\partial q^j} \frac{\partial A}{\partial p_j}, \quad (2.27)$$

we will examine continuous canonical transformations generated by gauge potential \mathcal{A}_λ

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

$$p_j(\lambda + \delta\lambda) = p_j(\lambda) - \frac{\partial \mathcal{A}_\lambda, \mathbf{p}, \mathbf{q}}{\partial q^j} \delta\lambda \Rightarrow \frac{\partial p_j}{\partial \lambda} = -\frac{\partial \mathcal{A}_\lambda}{\partial q^j} = \{\mathcal{A}_\lambda, p_j\}. \quad (2.29)$$

Substituting this to eq. 2.26, we get

$$\{q^j(\lambda + \delta\lambda), p_j(\lambda + \delta\lambda)\} = \delta_j^i + \mathcal{O}(\delta\lambda^2). \quad (2.30)$$

Equations 2.28, 2.29 are identical to the Hamilton equations

$$\begin{aligned} \dot{q}^j &= -\{\mathcal{H}, q^j\} = \frac{\partial \mathcal{H}}{\partial p_j} \\ \dot{p}_j &= -\{\mathcal{H}, p_j\} = -\frac{\partial \mathcal{H}}{\partial q^j}, \end{aligned} \quad (2.31)$$

if $\mathcal{A}_t = -\mathcal{H}$. Because the Hamiltonian is generator of the movement in the phase space (\mathbf{q}, \mathbf{p}) , we can interpret \mathcal{A}_t as the generators of the movement on \mathcal{M} . Specially if we chose $\lambda = X^i$, we get $\mathcal{A}_{X^i} = p_i$.

2.3.2 Quantum gauge potential

[Kolodrubetz et al., 2017][kap. 2.2] The role of Poisson brackets in quantum mechanics is taken by commutators, canonical transformations are called *unitary transformations* and calibrational 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 on \mathcal{M} defined by eigenstates $\{|m(\boldsymbol{\lambda})\rangle\}_m$. Let the initial state be $|\psi\rangle \equiv |\psi(0)\rangle$ and define unitary transformation

$$\hat{U}(\lambda)^+ : |\psi\rangle \rightarrow |\tilde{\psi}(\lambda)\rangle, \quad (2.32)$$

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

$$i\hbar\partial_\lambda\hat{U}(\lambda) = \hat{H}(\lambda)\hat{U}(\lambda) \quad (2.33)$$

for any point on γ . The wavefunction $|\psi\rangle$ in S can be decomposed using Schmidt decomposition⁴, as

$$|\psi\rangle = \sum_{m,n} \psi_n \hat{U}_{nm}^* |m(\boldsymbol{\lambda})\rangle = \sum_m \overbrace{\tilde{\psi}_m(\boldsymbol{\lambda})}^{\langle m(\boldsymbol{\lambda})|\psi\rangle} |m(\boldsymbol{\lambda})\rangle. \quad (2.34)$$

We can define adiabatic potentials analogically to the classical case as

$$i\hbar\partial_\lambda |\tilde{\psi}(\boldsymbol{\lambda})\rangle = i\hbar\partial_\lambda \left(\hat{U}^+(\boldsymbol{\lambda}) |\psi\rangle \right) = \underbrace{i\hbar \left(\partial_\lambda \hat{U}^+(\boldsymbol{\lambda}) \right) \hat{U}(\boldsymbol{\lambda})}_{-\tilde{\mathcal{A}}_\lambda} |\tilde{\psi}(\boldsymbol{\lambda})\rangle, \quad (2.35)$$

which can be transformed to non-tilde system as

$$\begin{aligned} \hat{\mathcal{A}}_\lambda &= \hat{U}(\boldsymbol{\lambda}) \tilde{\mathcal{A}}_\lambda \hat{U}^+(\boldsymbol{\lambda}) = -i\hbar \left(\hat{U}(\boldsymbol{\lambda}) \partial_\lambda \hat{U}^+(\boldsymbol{\lambda}) \right) = \\ &= -i\hbar \left(\partial_\lambda \underbrace{(U^+(\boldsymbol{\lambda}) U(\boldsymbol{\lambda}))}_{\mathbb{1}} - \partial_\lambda (U(\boldsymbol{\lambda})) U^+(\boldsymbol{\lambda}) \right) = i\hbar \left(\partial_\lambda U(\boldsymbol{\lambda}) \right) U^+(\boldsymbol{\lambda}). \end{aligned} \quad (2.36)$$

⁴The 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.

Thus we get equations for adiabatic potentials

$$\hat{\mathcal{A}}_\lambda = i\hbar(\partial_\lambda U(\boldsymbol{\lambda}))U^+(\boldsymbol{\lambda}) \quad (2.37)$$

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

These potenciales are Hermitean (omitting reference to $\boldsymbol{\lambda}$ in brackets)

$$\tilde{\tilde{\mathcal{A}}}_\lambda^+ = i\hbar U^+ \partial_\lambda \hat{U} = -i\hbar \partial_\lambda \hat{U}^+ \hat{U} = \tilde{\tilde{\mathcal{A}}}_\lambda, \quad (2.39)$$

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

$$\langle n | \tilde{\tilde{\mathcal{A}}}_\lambda | m \rangle = i\hbar \langle n | \hat{U}^+ \partial_\lambda \hat{U} | m \rangle = i\hbar \langle \tilde{n}(\lambda) | \partial_\lambda | \tilde{m}(\lambda) \rangle. \quad (2.40)$$

and because

$$\langle \tilde{n}(\lambda) | \hat{\mathcal{A}}_\lambda | \tilde{m}(\lambda) \rangle = \langle n | \tilde{\tilde{\mathcal{A}}}_\lambda | m \rangle, \quad (2.41)$$

we get

$$\mathcal{A}_\lambda = i\hbar \partial_\lambda. \quad (2.42)$$

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.

According to eq. 2.3, \hat{U} can be explicitly chosen as

$$\hat{U}(t) = \sum_n \exp\left(\frac{i}{\hbar} E_n(\tau) d\tau - \int_0^t \langle n(\tau) | \partial_\tau n(\tau) \rangle d\tau\right) |n(t)\rangle \langle n(0)|. \quad (2.43)$$

This was not needed for the derivation of the adiabatic element, but gives us explicit formula for.....

2.4 Berry phase and curvature

Next we define the *Berry connection*

$$A_\mu \equiv \langle i | \hat{\mathcal{A}}_\mu | i \rangle, \quad (2.44)$$

which empowers us to write

$$\nu_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \quad (2.45)$$

and *Berry phase* ⁵

$$\phi_B \equiv - \oint_C A_\mu d\lambda^\mu = \int_S \nu_{\mu\nu} d\lambda^\mu \wedge d\lambda^\nu, \quad (2.48)$$

⁵ The reasonability of this definition can be seen, if we assume the ground state of a free particle $\langle \mathbf{x} | i(\boldsymbol{\lambda}) \rangle = i(\mathbf{x}, \boldsymbol{\lambda}) = |i(\mathbf{x})| e^{i\phi(\boldsymbol{\lambda})}$, then the Berry connection is

$$A_\mu = - \int d\mathbf{x} |i(\mathbf{x}, \boldsymbol{\lambda})|^2 \partial_\mu \phi(\boldsymbol{\lambda}) = -\partial_\mu \phi(\boldsymbol{\lambda}) \quad (2.46)$$

and Berry phase

$$\phi_B = \oint_C \partial_\mu \phi d\lambda^\mu, \quad (2.47)$$

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 $\phi_B = 2\pi$

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

Wave-functions are elements of the tangent bundle $\mathcal{T} \in \mathcal{M}$, the gauge potentials are affine connections defining the parallel transport. Covariant derivative is

$$D_\mu = \partial_\mu + i\hat{\mathcal{A}}_\mu, \quad (2.49)$$

which yields $D_\mu |\psi_n\rangle = 0$ for every eigenstate, which justifies our initial claim, that the transport of eigenvalues is parallel. Applied on any state, we need to use definition 2.37, which generally gives non-zero covariant derivative.

2.5 Adiabatic transformations

In this chapter, we will be dealing with the system described by finite-dimensional Hamiltonian $\hat{H}(\boldsymbol{\lambda})$ which drives the system according to Schrödinger equation from some initial state $|n(\boldsymbol{\lambda}(0))\rangle$ to $|n(\boldsymbol{\lambda}(t))\rangle$. Again we reduce dimension of \mathcal{M} from the \mathbb{R}^n to 1 using parametrization $\gamma(\lambda)$, so we get $\hat{H} = \hat{H}(\lambda)$, thus only transporting the system along some prescribed way.

2.5.1 Adiabatic potential

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 $\mathcal{H}(\boldsymbol{\lambda} + d\boldsymbol{\lambda})$, we get

$$[\hat{H}(\boldsymbol{\lambda}), \hat{H}(\boldsymbol{\lambda} + d\boldsymbol{\lambda})] = 0, \quad (2.50)$$

meaning Hamiltonian commutes with it's canonically transformed version.⁶

2.5.2 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*

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

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

$$||\psi(t) - \psi_{ad}(t)|| \approx o\left(\frac{1}{T}\right) \quad (2.51)$$

for adiabatic state

$$|\psi_{ad}\rangle = e^{\theta_n(t)} e^{\gamma_n(t)} |\psi(t)\rangle, \quad (2.52)$$

⁶This can be easily reformulated to the world of classical physics, where the commutator is replaced by Poisson bracket.

where we define nongeometrical phase induced by energy transitions,

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

and geometrical phase, also called Berry phase

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

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 eigenstates⁷ The transition amplitude between states for adiabatic change is

$$0 = \langle m | \hat{H} | n \rangle \quad \text{pro } n \neq m. \quad (2.53)$$

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

$$\begin{aligned} 0 &= \langle \partial_\lambda m | \hat{H} | n \rangle + \langle m | \partial_\lambda \hat{H} | n \rangle + \langle m | \hat{H} | \partial_\lambda n \rangle \\ &= E_n \langle \partial_\lambda m | n \rangle + E_m \langle m | \partial_\lambda n \rangle + \langle m | \partial_\lambda \hat{H} | n \rangle \\ &= (E_m - E_n) \underbrace{\langle m | \partial_\lambda n \rangle}_{-\frac{i}{\hbar} \langle m | \hat{\mathcal{A}}_\lambda | n \rangle} + \langle m | \partial_\lambda \hat{H} | n \rangle, \end{aligned} \quad (2.54)$$

where \hat{H} , $|n\rangle$, $|m\rangle$ and E_n are functions of λ .

In matrix form, we can rewrite this equation as

$$i\hbar \partial_\lambda \hat{H} = [\hat{\mathcal{A}}_\lambda, \hat{H}] - i\hbar \hat{M}_\lambda \quad \text{for } \hat{M}_\lambda \equiv - \sum_n \frac{\partial E_n(\lambda)}{\partial \lambda} |n(\lambda)\rangle \langle n(\lambda)|. \quad (2.55)$$

\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

$$[\hat{H}, i\hbar \partial_\lambda \hat{H} - [\hat{\mathcal{A}}_\lambda, \hat{H}]] = 0. \quad (2.56)$$

This can be used as the definition for *counterdiabatic potential* $\hat{\mathcal{A}}_\lambda$. The strength of this equation lies in the fact, that it finds counterdiabatic potential without the need of Hamiltonian diagonalisation.

2.6 Counterdiabatic driving

[Kolodrubetz et al., 2017][page 15–17] Again consider two bases consisting of eigenstates of Hamiltonian $\hat{H} = \hat{H}(\lambda(t))$. $B(t)$ for external observer and $\tilde{B}(t)$ for frame actively transformed by Hamiltonian (moving frame), in which $\tilde{\hat{H}}(t)$ is diagonal. Transforming vectors in Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(\lambda(t)) |\psi(t)\rangle \quad (2.57)$$

⁷In the case of energy level crossing, the eigenstates are not unified, because transition between them is not adiabatical.

to moving frame using unitary operator for time varying Hamiltonian (compare to eq. 2.32

$$\hat{U}(\lambda(t)) : |\tilde{\psi}(\lambda(t))\rangle \rightarrow |\psi(t)\rangle. \quad (2.58)$$

and using *dot* notation for time derivative, we get

$$i\hbar \frac{d}{dt}(\hat{U} |\tilde{\psi}\rangle) = \hat{H} \hat{U} |\tilde{\psi}\rangle \quad (2.59)$$

$$i\hbar \dot{\lambda} \partial_{\lambda} \hat{U} |\tilde{\psi}\rangle + i\hbar \hat{U} \frac{d}{dt} |\tilde{\psi}\rangle = \hat{H} \hat{U} |\tilde{\psi}\rangle. \quad (2.60)$$

This can be rewritten using adiabatic potential from eq. 2.42) as

$$i\hbar \frac{d}{dt} |\tilde{\psi}\rangle = \left[\hat{U}^+ \hat{H} \hat{U} - \dot{\lambda} \tilde{\mathcal{A}}_{\lambda} \right] |\tilde{\psi}\rangle = \left[\tilde{\hat{H}} - \dot{\lambda} \tilde{\mathcal{A}}_{\lambda} \right] |\tilde{\psi}\rangle = \tilde{\hat{H}}_m |\tilde{\psi}\rangle. \quad (2.61)$$

Hamiltonian in moving frame is $\tilde{\hat{H}}(t) = \hat{U}^+(\lambda(t)) \hat{H}(\lambda(t)) \hat{U}(\lambda(t))$ and the term $-\dot{\lambda} \tilde{\mathcal{A}}_{\lambda}$ is called *Galilean*. To Hamiltonian in moving frame $\tilde{\hat{H}}_m = \tilde{\hat{H}} - \dot{\lambda} \tilde{\mathcal{A}}_{\lambda}$ we can add *counterdiabatic element* $\dot{\lambda} \tilde{\mathcal{A}}_{\lambda}$ and the only remaining element is $\tilde{\hat{H}}$, which does not excite the system.

2.7 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 knowledge of exact adiabatic potential would allow to maintain the system in the ground state thus not exciting it, as the 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*

$$E_n - E_m \propto \exp\left(\frac{S}{2}\right). \quad (2.62)$$

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.

$$\langle m | \hat{\mathcal{A}}_{\lambda} | n \rangle = i\hbar \frac{\langle m | \partial_{\lambda} \hat{H} | n \rangle}{E_m - E_n} \propto \exp(-a). \quad (2.63)$$

Fortunately in the limit "number of particles" $\rightarrow \infty$ the expression in eq. 2.63 converges.

2.7.1 Variational methods

Conclusion

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A. Attachments

A.1 First Attachment