*”**Adiabatic theory** and **topological indices** in **molecular physics** and **solid state physics**”*

or

*“**Geometric and topological** aspects of **slow and fast coupled** dynamical systems in **quantum and classical** dynamics”.*

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Chapter 1

Introduction and Overview

The objective of these lectures is mainly to present a general framework for the description of dynamical systems containing a slow sub-dynamical system coupled with a faster sub-dynamical system, shortly called **slow-fast coupled systems**.

In the examples, we will mainly be concerned with nice examples in physics of such a situation, namely ***small molecules.***

We will describe the total dynamics in term of fiber space, where the slow motion takes place in the base space, whereas the fast motion takes place within the fibers.

This problematics can be considered in classical mechanics, or in (mixed description) Classical-Quantum mechanics, or in Quantum mechanics.

Using semi-classical rules, we will present the relations between the topological and geometrical properties respectively in these three possible descriptions.

In particular we will see the strong similarity between the semi-classical limit and the adiabatic limit.

The usefulness of using different descriptions will be clear for example, when we will see that topological characterization of fiber bundles within the mixed Classical-Quantum description (i.e. the Born-Oppenheimer description) gives a nice insight in the full exact quantum spectrum: the precise numbers of energy levels in each bands.

To summarize:

The subject of these lectures is:

Geometric and topological aspects of **slow and fast coupled** dynamical systems in **quantum and classical** dynamics.

In this introduction, we give some preliminary explanations to these three adjectives.

The author aknowledges the *Service of physique théorique of Saclay* for its kind hospitality during two months, and the M.A.S.I.E. group (Mechanics and Symmetry in Europe) for good scientific discussions and collaborations.

1.1 Fast and slow coupled systems in physics

We give here few examples of slow-fast mechanical coupled systems in physics.

1.1.1 Examples in the macroscopic world:

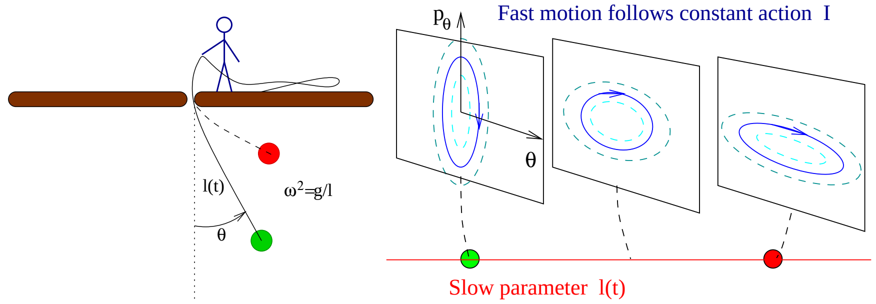
The ordinary Pendulum

with length $l(t)$ varying slowly. See figure.

The Classical adiabatic theorem says: The enclosed area in phase space $I = E(t)/\omega(t)$ is *approximatively conserved.*

One says that I is an **adiabatic invariant**.

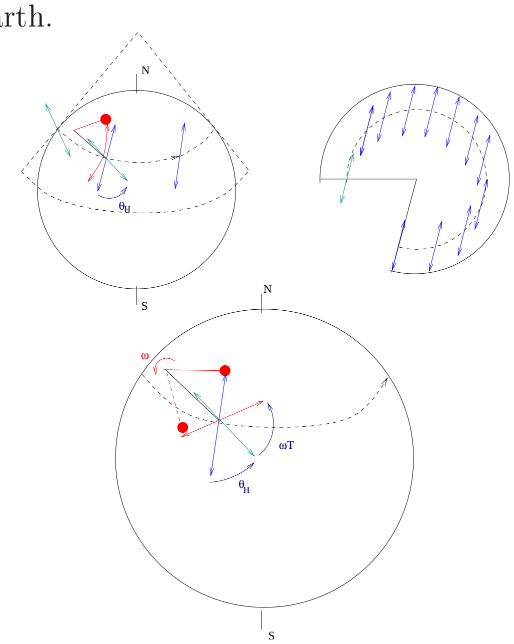
(More precisely, if $dl/dt \sim \varepsilon$, then $|I(t) - I(0)| < C\varepsilon$ for $t \in [0, T/\varepsilon]$).



We have say nothing about the angular position.

The Foucault pendulum:

The fast oscillations direction of the Foucault Pendulum follow **parallel transport** on the earth.



After one revolution, appearance of a **geometrical phase** (holonomy): the **Hannay angle**

$$\varphi_{Hannay} = \iint_{hemisphere} d\Omega = 2\pi \left(1 - \sin\left(latitude\right)\right)$$

For a *rotating* pendulum, the phase shift is **a dynamical phase + geometrical phase:**

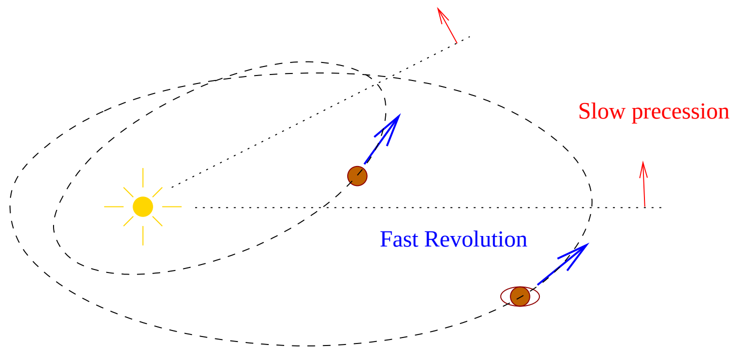
$$\Delta\varphi = \omega T + \varphi_{Hannay}$$

(This is a general relation).

<u>Revolution and Precession of planets</u>

This is the first historical application of the averaging method by Lagrange, Laplace, Gauss. They observed the absence of secularity in the variations of the major axes a of orbits.

In other terms, a is a adiabatic invariant.



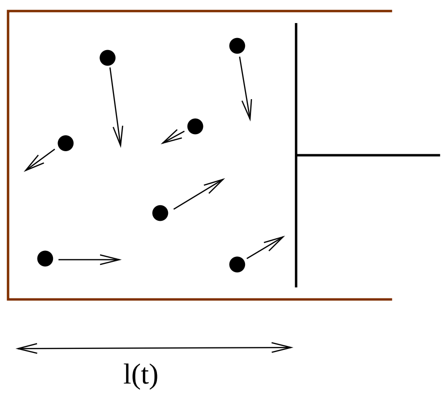
<u>Statistical systems.</u>

Ergodicity on energy surface, gives conservation of phase space volume:

$\mathcal{V}(E) = Vol\left\{(q,p),\ H(q,p) \leq E\right\}$,

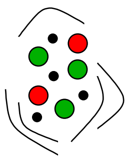
and then gives **entropy conservation** $S(E) = k \log \mathcal{V}(E)$.

(This gives important results in statistical physics).



Biological systems
Fast dynamics: the reproduction cycle of a predator-prey system.
Slow dynamics: climate evolution, modified by the vegetable food consumption by the prey.

1.1.2 Examples in the microscopic (quantum) world



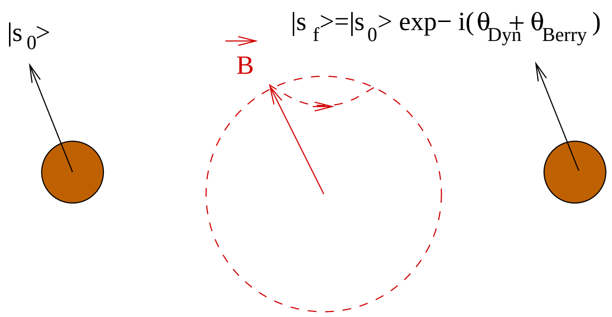
In these lectures we will consider mainly the following examples.

Small molecules,

are a very rich place to observe slow and fast coupled systems:
with **fast electrons** (typical period $\tau_e \simeq 10^{-15} \to 10^{-16} s.$),
slower vibrations of the nuclei ($\tau_v \simeq 10^{-14} \to 10^{-15} s.,$)
slower rotation of the molecule ($\tau_{rot} \simeq 10^{-10} \to 10^{-12} s.$).

Spin precession

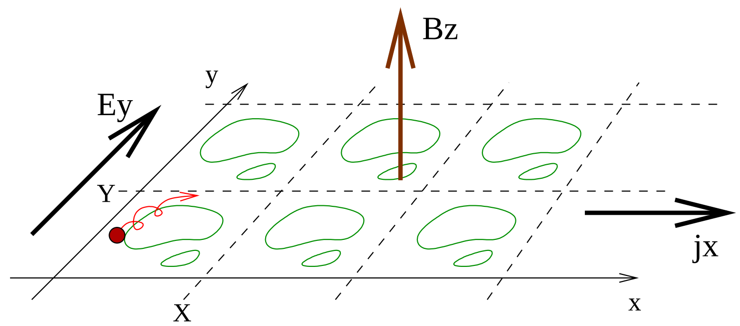
of a neutron in a slowly varying external magnetic field $\vec{B}(t)$.
The Quantum Adiabatic theorem tells: The spin state follows approximately the instantaneous eigenstate $|spin> \simeq |\pm_{\vec{B}}>$, up to a quantum phase.
After one period T of $\vec{B}(t)$, the final phase is $\theta_{Dynamical} = \omega T$ plus $\theta_{Berry} = \frac{1}{2}\iint_{hemisphere} d\Omega$.



__**Quantum Hall effect:**__

Bi-dimensional Electrons a ***strong Magnetic field***, in a periodic ***potential***, with a ***weak external electric field.***

- Fast Cyclotron motion on circles.
  - Slower precession of the circles.
  - Slower motion of quasi-momentum over the Brillouin zone.



In these lectures, we will consider only **conservative (i.e. Hamiltonian)** systems having a **finite number of degree of freedom.**

Remarks

From the above examples,

- <u>One can distinguish</u> __**two class of problems:**__
  - (A) "**Slow-Fast systems**": Fast system coupled with a slower system (reciprocal influences)
  - (B) "**Time adiabatic systems**": Fast system with slower external time-dependent parameters (uni-directional influences).

  Property: (B) is a special case of (A).

- The **coupling strength** between the fast and slow dynamics is **not necessary weak.**
  (non perturbative description).
  Interesting topological phenomena can then appear...

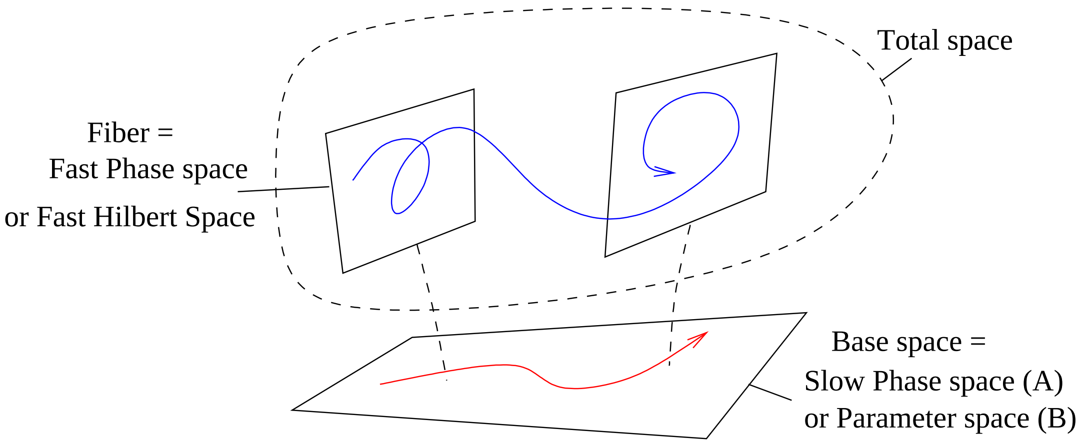
1.2 Geometrical and topological aspects

They concern **fiber bundles** with **connections** which naturally occur in the previous situations of slow and fast coupled systems.

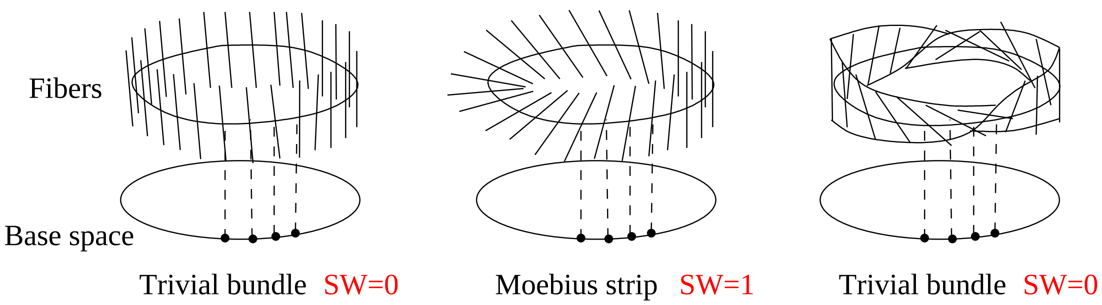
A **fiber bundle** is a continuous collection of isomorphic space.

Here the ***base space*** is the dynamical space of the slow sub-system, or the parameter space for Time-adiabatic systems.

The ***Fiber space*** is the dynamical space of the fast sub-system.



Note that from a global point of view, one can consider the **Topology of the bundle** related to possible twists of the fibers:



1.3 Classical versus Quantum models

In the above examples, the fast or slow motions can sometimes be consider in a quantum or classical description, independently. We recall some basic facts.

1.3.1 Expression of the dynamics for *a single system*

- The **classical dynamics** is express by ***Hamilton equation*** in ***Phase space*** $X = (q, p) \in P$ (dimension $2n$):

$$\frac{dq}{dt} = \frac{\partial H(q,p)}{\partial p}$$
$$\frac{dp}{dt} = -\frac{\partial H(q,p)}{\partial q}$$

- The **quantum dynamics** is expressed by ***Schrödinger equation*** in ***Hilbert space*** $\mathcal{H}$:

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

- **Semi-classical rules** relate the Classical and Quantum dynamics, in the limit "$\hbar$/action $\to 0$":

$$\begin{array}{rcl} \text{Phase space } P & \leftrightarrow & \text{Hilbert space } \mathcal{H} \\ \text{Hamiltonian } H & \leftrightarrow & \text{Hamiltonian } \hat{H} \end{array}$$

1.3.2 Hamiltonians for a slow-fast system

For a Slow-fast system (class A), there are then 4 possibilities of description:

Slow \ Fast	Classical in P_{Fast}	Quantum in $\mathcal{H}_{Fast}$
Classical in P_{Slow}	Function $H_{tot}(X_{slow}, X_{fast})$ (***Classical***)	Matrix Symbol $X_{slow} \to \hat{H}_{fast}(X_{slow})$ (***Semi-Quantum***)
Quantum in $\mathcal{H}_{Slow}$	No meaning (?)	$\hat{H}_{tot}$ in $\mathcal{H}_{slow} \otimes \mathcal{H}_{fast}$ (***Quantum***)

Remarks

- **Superposition property** in quantum dynamics:
  $\to$ ***One can not treat the influence of a quantum system on a classical system.***
  Then the Quantum-Classical description has no real dynamical meaning.
- The Semi-quantum description is the **Born-Oppenheimer approximation.**

1.3.3 Effective dynamics in fiber bundle

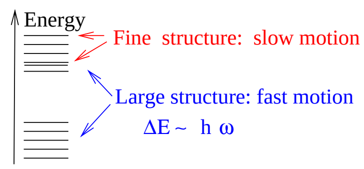
- **For a *Classical dynamics*, with *integrable* fast motion:**
  - The **fast motion in fibers** follows **tori with constant action**, and follows the (geometric) **Hannay connection plus a dynamical phase.**

  - The **slow motion on base space** is described (first order) by **averaging method**: $H_{effective}(X_{slow}) = \langle H_{tot}(X_{slow}, X_{fast})\rangle_{fast\,motion}$

- **For a *Semi-Quantum dynamics*, with *discrete* spectrum of $\hat{H}_{fast}(X_{slow})$:**

  - The **fast state in fibers** is an eigenstate $|\psi_n(X_{slow})\rangle$ of $\hat{H}_{fast}(X_{slow})$, with energy $E_n(X_{slow})$. Its follow the (geometric) **Berry connection plus a dynamical phase.**
  - The **slow motion on base space** is described (first order) by : $H_{effective}(X_{slow}) = \left\langle \psi_n(X_{slow})|\hat{H}_{fast}(X_{slow})|\psi_n(X_{slow})\right\rangle = E_n(X_{slow})$.

- ***Quantum dynamics*: *group of levels*** in the spectrum:



1.4 In the next chapters

- **Rigorous definitions of the different descriptions:**

  - *Classical* $H_{tot}(X_{fast}, X_{slow})$ on $P_{slow} \times P_{fast}$,
  - *Semi-Quantum* $\left(X_{slow} \to \hat{H}_{fast}(X_{slow})\right)$ on $P_{slow} \times \mathcal{H}_{fast}$,
  - *Quantum* $\hat{H}_{tot}$ on $\mathcal{H}_{slow} \otimes \mathcal{H}_{fast}$

- **Adiabatic theorems and Semi-classical Correspondences** between the three descriptions, at a **topological** and a **geometrical** level.

Slow \ Fast	Classical, Integrable in P_{Fast}	Quantum in $\mathcal{H}_{Fast}$
Classical in P_{Slow}	(***Classical***) *Topology of tori bundle* Hannay's connection	(***Semi-Quantum***) *Topology of eigenstates bundle* Berry's connection
Quantum in $\mathcal{H}_{Slow}$	No meaning (?)	(***Quantum***) *Number of states in group of levels* Density of states

- **Geometry of vector bundles,** Connections, curvature, (Semi-classical) Computation of topological Chern indices.

- **Remarks:**
  the ***Hannay connection*** needs integrability;
  the ***Berry connection*** is very general in Quantum mechanics.

Chapter 2

Berry's Connection and Berry's phase in quantum mechanics

2.1 Introduction

The purpose of this chapter is to present the **quantum dynamics in Hilbert space** from a **geometrical point of view**, initiated in physics by Berry in 1984: The Hilbert space is seen as a line bundle over its Projective space, with a natural connection, the Berry's connection. (In geometry, this is common since a longer time, and the Berry's connection is sometimes called the Chern's connection).

Here we will present this connection as a **Levi-Civita connection** which is the connection which defines parallel transport of tangent vectors on a surface embedded in $\mathbb{R}^3$.

This chapter contains more geometric informations than physics, and is to prepare the subsequent chapters.

Other important tools related to fiber bundles in physics will be presented in next chapters.

- The first section introduces the Levi-Civita connection on the sphere. This is an introduction to vector bundles from an intuitive point of view,

- The second section defines the Berry's connection and shows that any quantum evolution follows this natural connection plus a dynamical phase.

2.2 The Foucault pendulum and parallel transport in TS^2

References: [13][5].

Objective of this section: introduction to a vector bundle, the tangent bundle TS^2, with its connection.

We consider the sphere S^2 which is the earth surface, fixed in an inertial frame (actually the earth rotates in this frame, with period $T = 24$ hours). The attached point of the Foucault pendulum is forced to follows a path $\gamma(t)$ on the sphere, which is parallel to the equator.

In this section, we will also imagine any possible path $\gamma(t)$ on the sphere S^2.

2.2.1 The Levi-Civita Connection

We suppose small oscillations of the pendulum, and simplify the physical discussion by arguing that (from conservation of angular momentum along the local z axis) the oscillations try to maintain their direction in space $\mathbb{R}^3$, but are constrained to the tangent plane of the sphere. The result is that the oscillations follows the so-called **parallel transport** on the sphere, or **Levi-Civita connection** which we now define.

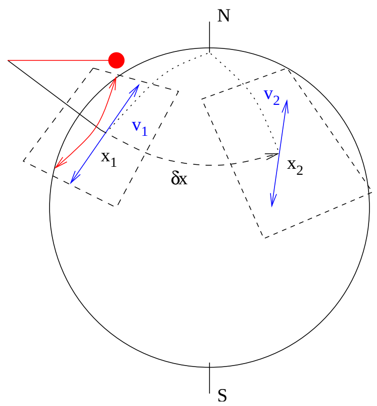


Figure 2.1: Foucault Pendulum

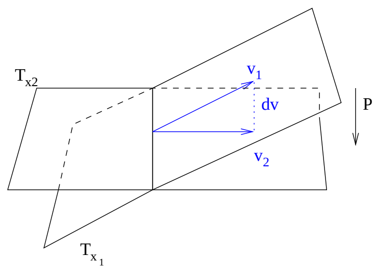


Figure 2.2: Levi-Civita Connection

For a given point $x \in S^2$, we note T_xS^2 the tangent plane. Over each point $x(t) = \gamma(t)$ of the path, we denote $v_x \in TS^2$ the tangent vector (which could be the velocity of the pendulum measured after each pendulum period). At a given point $x \in TS^2$, and for a small displacement δx on the path, there corresponds a small variation $dv = v_{x+\delta x} - v_x$.

Using the scalar product in $\mathbb{R}^3$, one defines the orthogonal projection P_x of vectors of $\mathbb{R}^3$ onto the tangent plane T_xS^2.

Then the continuous family of tangent vectors v_x is said to follow the **Levi-Civita connection** or **parallel transport** over the path γ if:

$$\underbrace{D_{\delta x} v}_{\substack{\uparrow \\ \text{Covariant Derivative}}} = P\,dv = 0$$

Property: **The Levi-Civita connection conserves the norm** of the transported vector.

Indeed: $d\,|v|^2 = d\,\langle v, v\rangle = 2\,\langle v, dv\rangle = 2\,\langle Pv, dv\rangle = 2\,\langle v, Pdv\rangle = 0.$

Remarks

- We have said that for physical reasons the Foucault pendulum follows this Levi-Civita connection. This is an exact result if γ is parallel to the equator, and can be shown using Coriolis forces in the pendulum frame [2].

- For any slowly varying path $\gamma(\varepsilon t) \in S^2$ with $\varepsilon \to 0$ (slow compared to the pendulum oscillations), the Foucault pendulum would follow approximatively the Levi-Civita connection, with an error less than ε on the time interval $t \in [0, 1/\varepsilon]$. This results from the **Classical Adiabatic theorem** [3][15], but non directly because this theorem needs a fast rotational motion of the pendulum around the z axis (see discussion in [11]).

- This connection is **geometric** in the sense that in that limit, the direction of the pendulum depends only on the geometry of the path γ on S^2.

2.2.2 Holonomy and curvature

Consider now any **closed path** γ on the sphere S^2. After one loop, one can compare the initial and final directions of the pendulum v_i,$v_f \in T_0S^2$. These two vectors have the same length, but they differ by an angle $h\,(\gamma)$, which depends only on the geometry of the path γ, and is called the **holonomy of the Connection on the path** γ.

From the second picture, one easily guess that $h(\gamma)$ is related to the surface enclosed by the so called curvature integral:

$$h\,(\gamma) = \theta = \Omega_S = \iint_S curvature = \iint_S \frac{d^2 s}{R^2} \quad : \text{holonomy } \in [0, 2\pi]$$

For the adiabatic pendulum the Holonomy is the **Hannay angle.** (See below for a more precise definition of the Hannay angle).

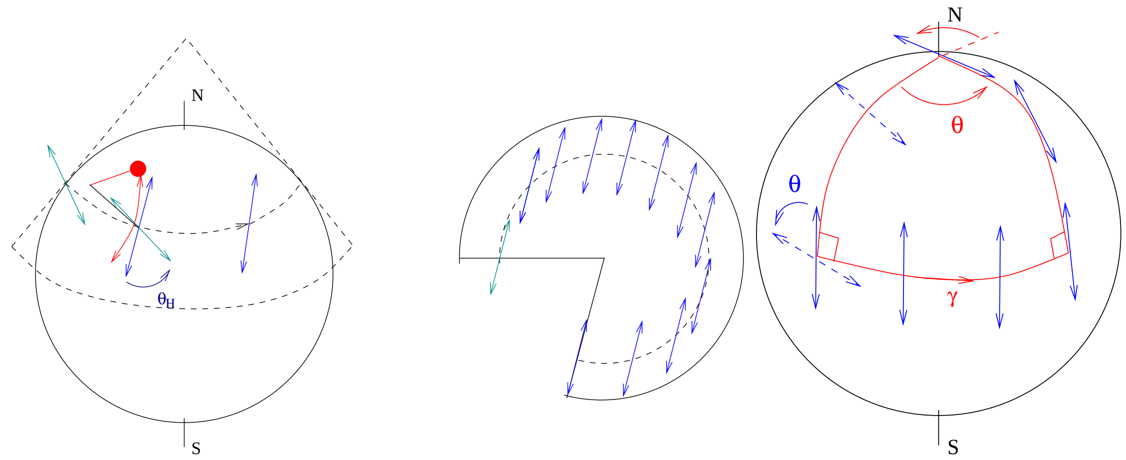


Figure 2.3: Holonomy

2.2.3 Fiber bundle description

Over each point $x \in S^2$ is attached a tangent plane T_xS^2. Each tangent plane T_xS^2 defines the **fiber** over the point x in **base space** S^2.

The collection of these fibers is called **the tangent bundle** TS^2. More precisely, TS^2 is **a real vector bundle of rank 2 over** S^2. In general, the rank of a vector bundle is the dimension of each fiber.

Two different tangent plane T_x and $T_{x'}$ are not identical, and there is no unique and natural way to identify them. If γ is a path which connect x and x', we have seen that T_x and $T_{x'}$ can be identified with the parallel transport (or Levi-Civita connection) in the fibers over the path γ. We insist that this connection has been defined from the scalar product in $\mathbb{R}^3$.

The whole set of fibers can have a global twist over the base space S^2 as in the well known example of the Moebius strip which is a real vector bundle of rank 1 over S^1.

Topology of a real vector bundle of rank 1 over S^1

The topology of such a bundle is characterized by an integer which represents the number of twists: **the Stiefel-Whitney index** $SW \in \mathbb{Z}_2 = \{0, 1\}$. (see [5][8]).

(This characterization is an intrinsic one: two bundles are isomorphic if there is a bijective mapping between them which respects the fibers. So the third example on the figure is trivial even if it can not be continuously deformed in $\mathbb{R}^3$ to the first example which is also trivial).

Topology of a complex vector bundle of rank 1 over S^2

Because each tangent plane T_xS^2 is oriented, one can identify T_xS^2 with the complex plane $\mathbb{C}$, and consider the bundle TS^2 as a complex vector bundle of rank 1 over S^2.

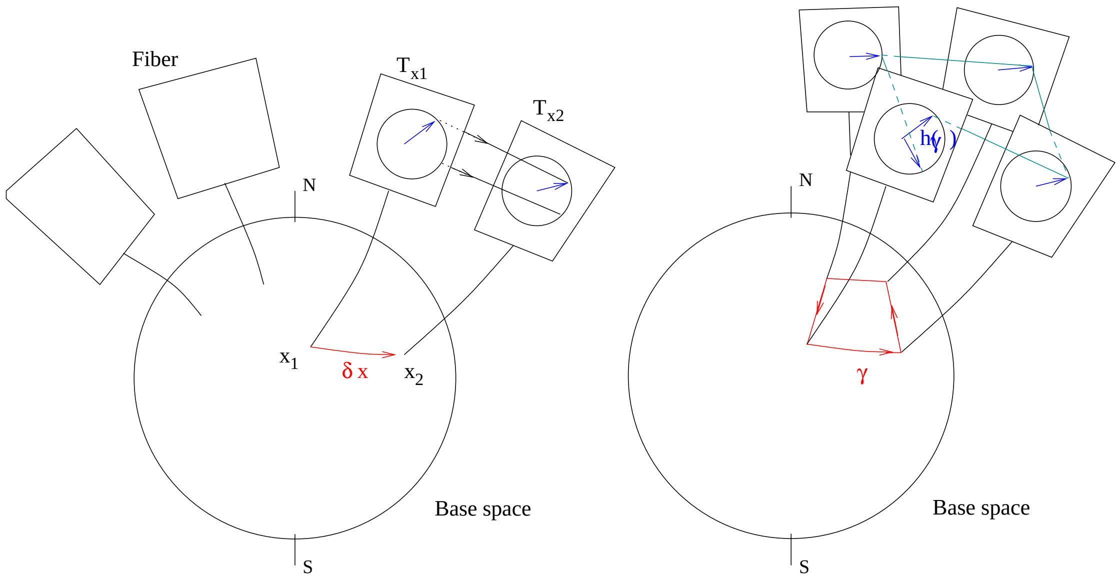


Figure 2.4: Vector bundle description

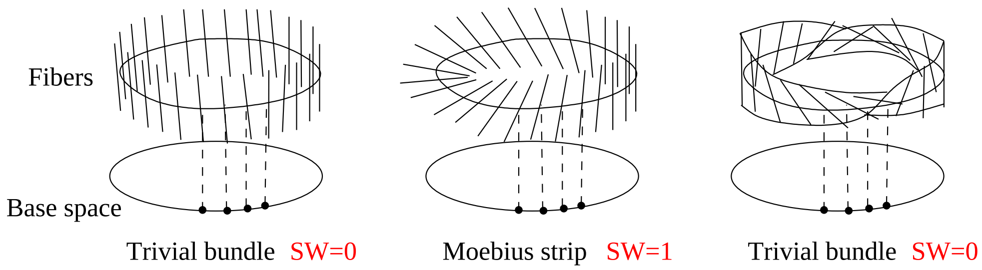


Figure 2.5: Real vector bundle of rank 1 over S^1.

As explained in the figure, the topology can be characterized by an integer $C \in \mathbb{Z}$ called the **Chern index**. (or first Chern class).

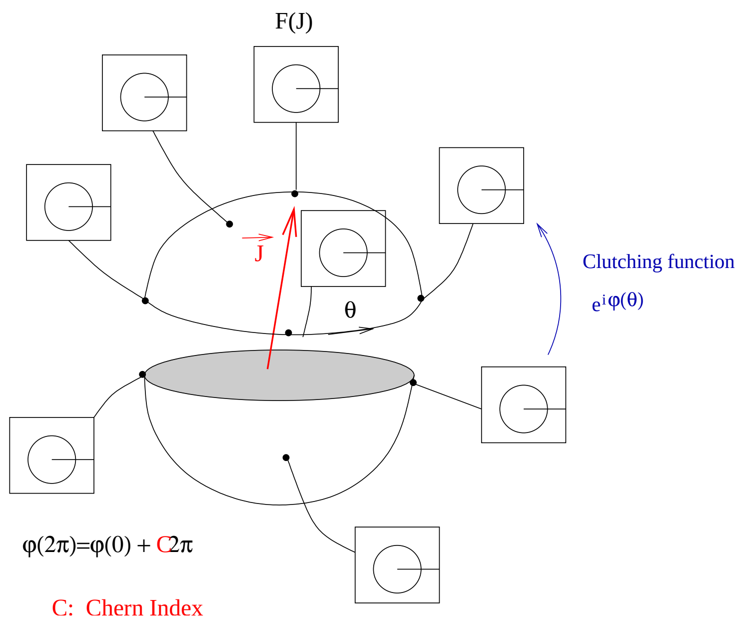


Figure 2.6: Complex line Bundle over S^2. The topology is characterized by the homotopy type of the clutching function, $C \in \mathbb{Z}$.

Property:

$$Chern(TS^2) = +2$$

(See other examples below.)

proof: see figure.

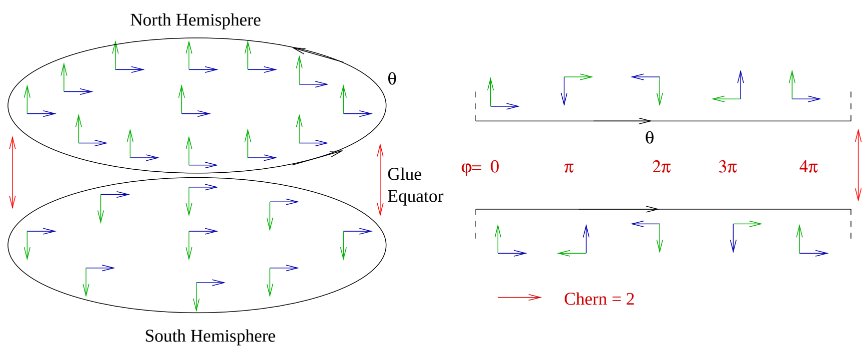


Figure 2.7: Topology of the tangent bundle TS^2

Remarks:

- The connection (curvature, holonomy,..) is a **geometric** structure on the fiber bundle (sensitive to continuous deformations of the metric).
- The Chern index $C \in \mathbb{Z}$ is **topological** property**,** robust (i.e. not sensitive) under continuous deformations.
- Geometrical structures can be used to compute topological properties. Example: Gauss-Bonnet curvature formula:

$$Chern\left(TS^2\right) = \frac{1}{2\pi}\int\int_{S^2} Curvature = \frac{4\pi}{2\pi} = 2$$

- The sign definition of the Chern index we use is from algebraic geometry conventions [7] and is opposite to algebraic topology conventions [8].

Topology from the zeros of a global section

A **Global section of the bundle** is a continuous choice of vectors in each fiber.

For a real vector bundle of rank 1 over S^1 (as the Moebius strip), the Stiefel-Whitney index SW is the parity of the number of zeros of a section ($0 =$ even number of zeros or $1 =$odd number zeros), see figure.

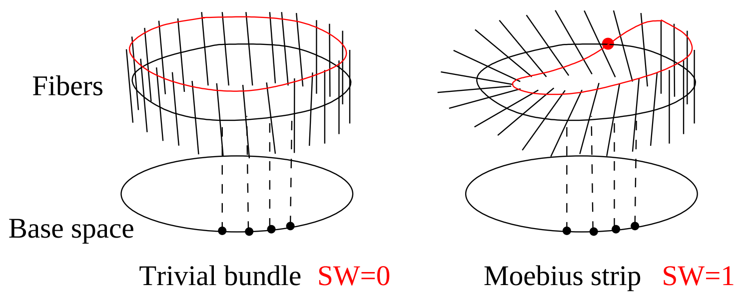


Figure 2.8: Moebius strip, Zero of sections.

For a complex vector bundle of rank 1 over S^2, the Chern index C is obtained by the opposite of the sum of the orientations (± 1) of isolated zeros of a generic section.

Remark: We saw two possibilities to compute the Chern index. This is very general. First from an **integral curvature**, which more generally use tools of **cohomology** (integrals). The second possibility is from zeros of global sections and use tools of **homology** (intersections) (historically the first definition of Chern classes). The two approaches are related by **Poincaré duality** [7].

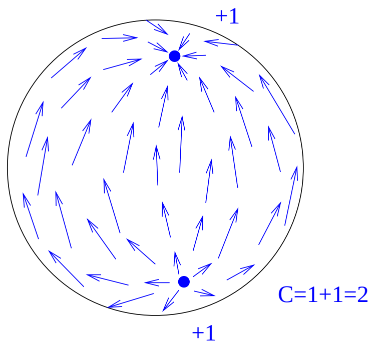


Figure 2.9: A section of TS^2 is a vector field on S^2. It gives the topology of the bundle TS^2.

2.3 The canonical quantum bundle over $\mathbb{P}$ (Hilbert space)

2.3.1 The projective space $\mathbb{P}(H)$

For a quantum system described by the state $|\psi(t)\rangle \in \mathcal{H}$ in Hilbert space $\mathcal{H}$, the Schrödinger equation is **linear**:

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

so if $|\varphi(0)\rangle = \lambda|\psi(0)\rangle$ then $|\varphi(t)\rangle = \lambda|\psi(t)\rangle$.

It is therefore natural to **identify vectors** $|\psi\rangle \sim \lambda|\psi\rangle$, for any $\lambda \in \mathbb{C}$. They are represented by an equivalence class $[\psi]$, which a dimensional one complex vector space in $\mathcal{H}$.

The set of equivalence class is the **projective space**:

$$\mathbb{P}(\mathcal{H}) = (\mathcal{H} \setminus \{0\}) / \sim$$

So $\mathcal{H} \to \mathbb{P}(\mathcal{H})$ is a complex fiber bundle of rank 1 over $\mathbb{P}(\mathcal{H})$.

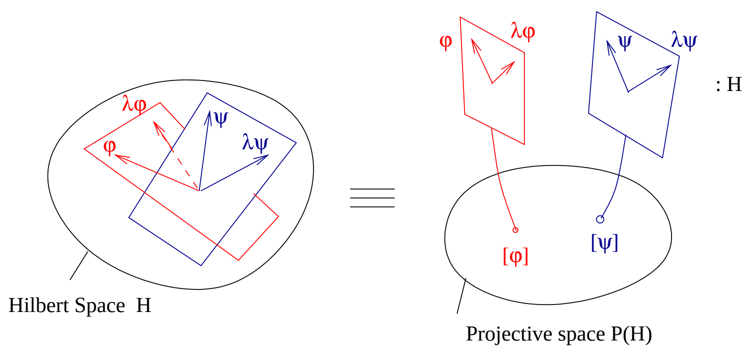


Figure 2.10: Projective Space $\mathbb{P}(\mathcal{H})$

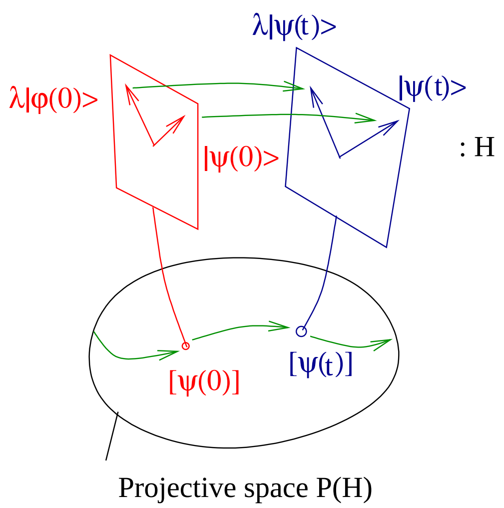


Figure 2.11: Quantum evolution in $\mathbb{P}(\mathcal{H})$

Because it is linear, the quantum dynamics in $\mathcal{H}$ projects onto $\mathbb{P}(\mathcal{H})$ (i.e. gives well defined trajectories on $\mathbb{P}(\mathcal{H})$).

Remark that if $dim_{\mathbb{C}}\mathcal{H} = n$ then $dim_{\mathbb{C}}\mathbb{P}(\mathcal{H}) = n - 1$.

Example of $\mathcal{H} = \mathbb{C}^2$

$\mathbb{P}(\mathbb{C}^2) = \mathbb{P}^1 \cong S^2$ is the **Riemann Sphere,** or **Bloch Sphere,** and $\mathcal{H} = \mathbb{C}^2$ is a complex fiber bundle over $\mathbb{P}(\mathbb{C}^2) \cong S^2$: (so called "**canonical bundle**") , with

$$Chern\left(\mathbb{C}^2 \to \mathbb{P}^1\right) = -1$$

Proof:

If $(|+\rangle, |-\rangle)$ is a orthonormal basis of $\mathbb{C}^2$,

$$\begin{aligned} |\psi\rangle = a|+\rangle + b|-\rangle \quad &= b\left(\tfrac{a}{b}|+\rangle + |-\rangle\right) \quad : \text{if } b \neq 0 \\ &\sim \quad z|+\rangle + |-\rangle = |\psi_z\rangle \quad : \ (z = a/b \in \mathbb{C}) \text{ unique representative in } P\left(\mathbb{C}^2\right) \end{aligned}$$

but if $b = 0$, i.e. $|z| \to \infty$,

$$|\psi_\infty\rangle \sim |+\rangle \quad : \text{unique point at infinity}$$

So we have shown that $\mathbb{P}\left(\mathbb{C}^2\right)$ is the complex plane $z \in \mathbb{C}$ with the infinity identified to a unique point. This is a sphere S^2.

The **stereographic** (or **inhomogeneous) coordinate** on $S^2 \cong \mathbb{P}\left(\mathbb{C}^2\right)$ are $z = cotg\,(\theta/2)\, e^{-i\varphi} \in \mathbb{C}$.

Consider now the orthogonal projection of $|-\rangle$ onto the fiber $Fiber_{[\psi]}$. This gives a global section of the bundle $|s_{[\psi]}\rangle = P_{[\psi]}|-\rangle = |\psi\rangle\langle\psi|-\rangle$ which is zero only if $[\psi] = [+]$. One can show that this zero has orientation -1.

Remark: the normalized states $\langle\psi|\psi\rangle = 1$, form the Hopf bundle $S^3 \to S^2$.

■

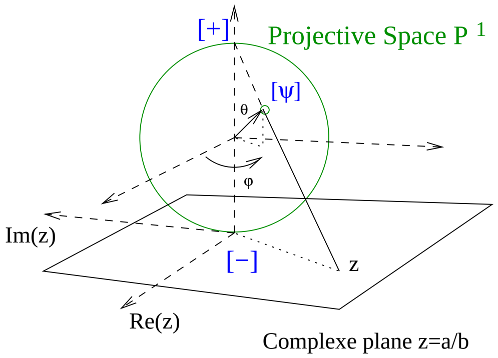


Figure 2.12: Stereographic coordinates on $\mathbb{P}\left(\mathbb{C}^2\right)$

Remarks

- If $|\psi\rangle = a|+\rangle + b|-\rangle$ is a spin 1/2 state, then $[\psi] \in \mathbb{P}\left(\mathbb{C}^2\right)$ is identical with the "mean spin direction" $\vec{s} = \langle\psi|\hat{\vec{S}}|\psi\rangle \in S^2$ in $\mathbb{R}^3$.

2.3.2 Berry's connection between the fibers of $\mathcal{H} \to \mathbb{P}(\mathcal{H})$

Similarly with the TS^2 case, the Scalar product in $\mathcal{H}$ defines a Levi-Civita connection on the bundle $\mathcal{H} \to \mathbb{P}(\mathcal{H})$.

A section $|\psi(X)\rangle$ is **parallel transported** over δX if

$$D|\psi\rangle = P\, d|\psi\rangle = 0$$

but $P = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$ so

$$D|\psi\rangle = \frac{|\psi\rangle\langle\psi|d\psi\rangle}{\langle\psi|\psi\rangle} = 0 \quad \Leftrightarrow \quad \langle\psi|d\psi\rangle = 0$$

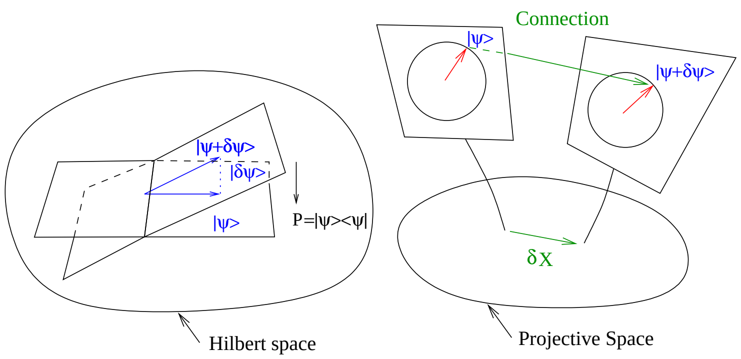


Figure 2.13: Connection on $\mathcal{H} \to P(\mathcal{H})$

If an other section has an additional phase $|\psi'(X)\rangle = e^{if(X)}|\psi(X)\rangle$ (and therefore is not parallel transported), then $|d\psi'\rangle = idf|\psi'\rangle + e^{if}|d\psi\rangle$,

$$\langle\psi'|d\psi'\rangle = i\,df\,\langle\psi'|\psi'\rangle$$

This connection is called the **Berry's connection** in physics (but is known since a long time in mathematics, see [7]).

Quantum evolution and the Berry's Connection

Consider any quantum dynamics defined by the Schrödinger equation (with possibly time dependent operator $\hat{H}(t)$)

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

This gives

$$\langle\psi|d\psi\rangle = -i\frac{\langle\psi|\hat{H}(t)|\psi\rangle}{\hbar}dt = i\,df\,\langle\psi|\psi\rangle$$

with

$$\frac{df}{dt} = -\frac{\langle\psi|\hat{H}(t)|\psi\rangle}{\hbar\langle\psi|\psi\rangle} = -\frac{E_{\psi(t)}}{\hbar}$$

so the quantum evolution follows the Berry's connection plus an additional **dynamical phase** (related to the mean energy $E_{\psi(t)}$).

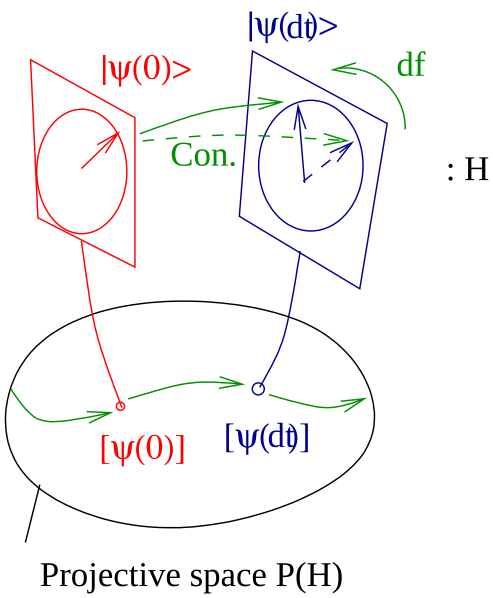


Figure 2.14: Quantum evolution in $\mathcal{H} \to \mathbb{P}(\mathcal{H})$ with the dynamical phase.

Suppose now that $[\psi(t)]$ is a closed trajectory in $\mathbb{P}(\mathcal{H})$. After a period T, the state comes back to the original fiber, so $|\psi(T)\rangle = e^{i\varphi}|\psi(0)\rangle$. The total phase is

$$\varphi = \varphi_{Berry} + \varphi_{Dyn} \tag{2.1}$$

$$\varphi_{Berry} = h(\gamma) \quad : \text{Holonomy or Berry's phase} \tag{2.2}$$

$$\varphi_{Dyn} = -\int_0^T \frac{E_{\psi(t)}}{\hbar} dt \qquad : \text{Dynamical phase} \tag{2.3}$$

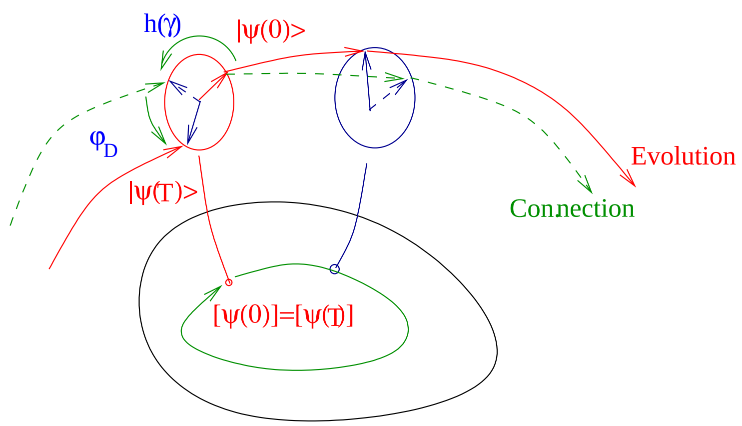


Figure 2.15: Berry's phase

As we have shown this Berry's phase is quite general in quantum mechanics and occurs in different contexts when there is a closed (or almost closed) trajectory $[\psi(t)]$ in $\mathbb{P}(\mathcal{H})$:

1. ***Adiabatic motion:*** a closed loop of in parameter space $X(t)$ gives (from quantum adiabatic theorem) an approximated closed loop of $[\psi(X(t))]$: this is the original adiabatic Berry's phase. See below.

2. ***Semi-classics:*** motion of a wave packet on a closed trajectory. See more details below. Then

$$\varphi_{Berry} = \frac{1}{\hbar}\oint p dq = \frac{Action}{\hbar},$$

   and gives quantization rules: $\varphi_{Berry} \equiv 0 \ [2\pi] \ \Leftrightarrow \ Action = n\, h, \quad n \in \mathbb{N}$.
   (This bundle description with wave packets is the basis of "geometrical quantization theory" with complex polarization, see [21][6]).

Proof: from $[\hat{q}, \hat{p}] = i\hbar$, and $\hat{T}_Q = e^{-iQ(\hat{p}-p)/\hbar}$, $\hat{T}_P = e^{iP(\hat{q}-q)/\hbar}$, one deduces $\hat{T}_P^{-1}\hat{T}_Q^{-1}\hat{T}_P\hat{T}_Q = e^{iAction/\hbar}$. On the other hand, as explained above, these unitary operators generate parallel tranport of wave packets at mean position (q, p). ■

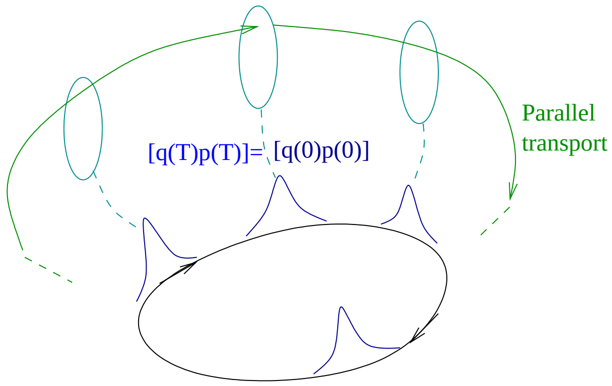


Figure 2.16: Quantization rule

Other properties (*) Natural metric (Fubiny-Study) on $\mathbb{P}(\mathcal{H})$, $ds^2 = d^2([\psi], [\psi + d\psi]) = 1 - |_n\langle\psi|\psi + d\psi\rangle_n|^2$

The velocity of $[\psi(t)]$ measured with this metric is $v = \frac{ds}{dt} = \frac{\Delta E}{\hbar}$, with $\Delta E^2 = \langle\psi|\hat{H}^2|\psi\rangle - \langle\psi|\hat{H}|\psi\rangle^2$ the **energy uncertainty.**

Reference: Anandan et al [1].

Chapter 3

The Semi-classical limit. Example of the Angular momentum dynamics

This chapter is an introduction to quantization of reduced phase space, coherent states, and some semi-classical limit concepts, in the simple example of angular momentum dynamics.

We will begin with the simple and concrete example of the free rigid body dynamics.

We explain at the end of the chapter, why and how ***the semi-classical limit is related to the adiabatic limit***.

3.1 The free rigid body motion

For a precise theory of the free rigid body motion, see Arnold [2], or Ratiu [9] for symplectic reduction theory.

Here, we only give a short description of some (known) results, inspired from [12].

See also [10].

3.1.1 In classical mechanics

Consider a free rigid body, that is a rigid body with no external forces (for example a falling rigid object).

Consider a fixed inertial frame $\mathcal{R}_e$ with origin at the body's center of mass, and a frame $\mathcal{R}_b$ fixed with respect to the body.

A configuration of the rigid is specified by its orientation with respect to an inertial frame, that is by the rotation matrix $\mathbf{R} \in SO(3)$ which relates frames $\mathcal{R}_e$ and $\mathcal{R}_b$. The **configuration space** is then the group SO(3) of rotation matrices which is 3 dimensional (2 angles for the direction of rotation, and one angle for the magnitude of rotation).

The **phase space** $P = T^*SO(3)$ includes the momenta denoted by $\vec{J}$ and is therefore 6 dimensional.

The reduced phase space: $S^2_{\vec{J}}$

Because of symmetry by rotation of the problem, the total angular momentum is conserved. This means that, with respect to the inertial frame $\mathcal{R}_e$, the total angular momentum $\vec{J}_e \in \mathbb{R}^3$ is a fixed vector.

Euler showed how to simplify the equations of motion by going to the frame $\mathcal{R}_b$ attached to the body. In this frame $\vec{J}(t)$ moves. But $\vec{J} = \mathbf{R}\vec{J}_e$ so $\left|\vec{J}\right| = \left|\vec{J}_e\right|$ is constant, so $\vec{J}(t)$ moves on the surface of a 2 dimensional sphere $S^2_{\vec{J}_e}$.

This sphere is called a **reduced phase space** of the problem (it is shown in [9] that $S^2_{\vec{J}_e}$ has indeed a canonical reduced symplectic two form).

The **kinetic energy** is

$$H\left(\vec{J}\right) = \frac{1}{2}\vec{J}\mathbf{I}^{-1}\vec{J} = \frac{1}{2}\left(\frac{J_x^2}{I_x} + \frac{J_y^2}{I_y} + \frac{J_z^2}{I_z}\right) \tag{3.1}$$

where $\mathbf{I}$ is the moment of inertia tensor, a symmetric positive definite matrix, we suppose diagonal in the frame $\mathcal{R}_b$, with eigenvalues (I_x, I_y, I_z).

The energy levels (which coincide with the trajectories) are depicted on figure 3.1. There are 6 fixed points, 2 minima of energy, 2 saddle points, and 2 maxima.

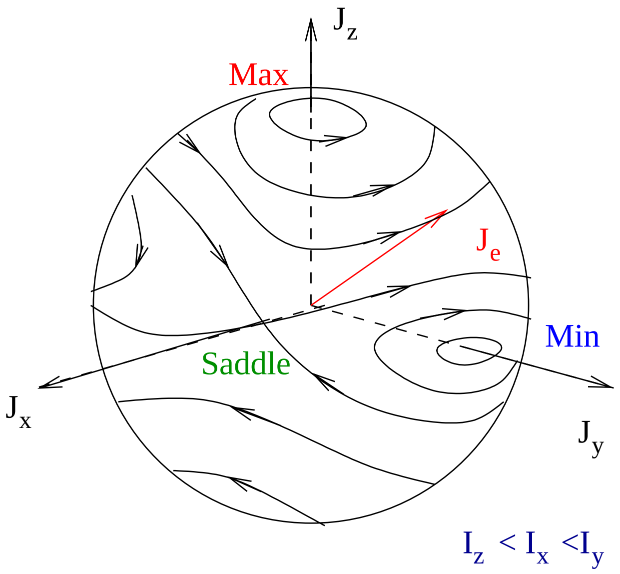


Figure 3.1: Rigid body trajectories on the reduced phase space $S^2_{\vec{J}_e}$.

The equation of motion of $\vec{J}$ can be written as:

$$\frac{d\vec{J}(t)}{dt} = \frac{\partial H(\vec{J})}{\partial \vec{J}} \wedge \vec{J}$$

Each fixed point on the sphere corresponds to special cases when $\vec{J}$ coincide with one of the principal axis of the body. The motion of the body in $\mathcal{R}_e$ is then a rotation around

$\vec{J}_e$. Try to launch a book, and observe these stationnary points, called relative equilibria (because the motion is still on a circle).

The fiber bundle over $S^2_{\vec{J}_e}$; *"A Berry's phase from the XVIII century"*

Let us denote by $M_{\vec{J}_e}$ the points of phase space P which corresponds to a given $\vec{J}_e$. Of course $M_{\vec{J}_e} \cong SO(3)$ is 3 dimensional. Because $\vec{J}_e$ is constant of motion, the dynamics stay inside $M_{\vec{J}_e}$.

We have seen that the reduced phase space $S^2_{\vec{J}_e}$ defined above, miss to describe the rotation of the body around the vector $\vec{J}_e$. This means that $S^2_{\vec{J}_e}$ is obtained from $M_{\vec{J}_e}$ by identification of points related by such a rotation:

$$S^2_{\vec{J}_e} = M_{\vec{J}_e} / \sim \equiv SO(3)/SO(2)$$

So $M_{\vec{J}_e}$ is actually seen as a fiber bundle over the sphere $S^2_{\vec{J}_e}$. The fibers are circles, and the dynamics of the body takes place in the fibers, whereas the reduced dynamics is on $S^2_{\vec{J}_e}$. See figure 3.2. With our conventions, the topology of this fiber bundle is $Chern = 2$, (because it is isomorphic to the unit subbundle of TS^2).

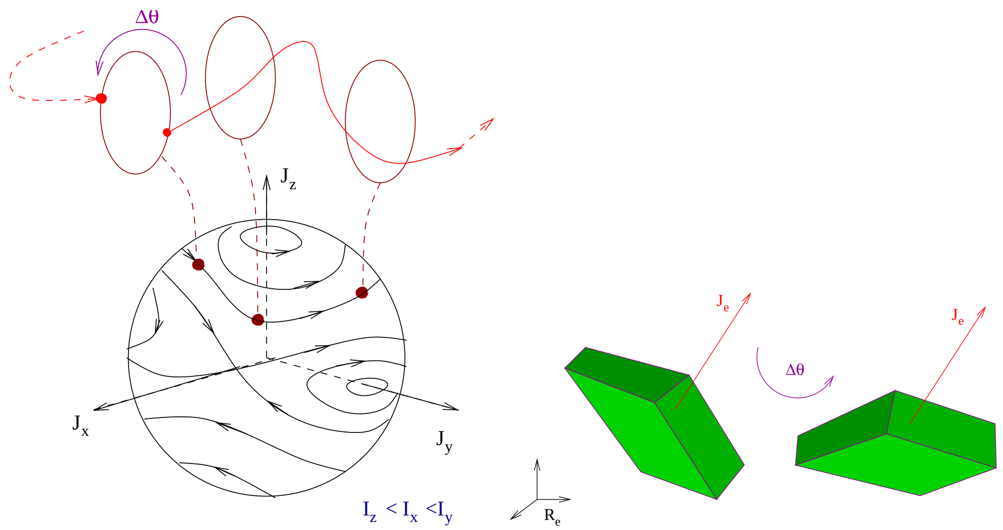


Figure 3.2: True trajectories: in a Circle bundle over the reduced phase space $S^2_{\vec{J}_e}$.

Consider now any closed reduced trajectory γ on the reduced phase space $S^2_{\vec{J}_e}$, with period T and energy E. The actual trajectory in $M_{\vec{J}_e}$ is not closed and after the period T, it comes back in the initial fiber, shifted by an angle $\Delta\theta$, measured in inertial frame $\mathcal{R}_e$. In [12], R.Montgomery showed that this angle can be express as:

$$\Delta\theta = \frac{2ET}{\left|\vec{J}\right|} - \Omega,$$

where Ω is the solid angle enclosed by the closed trajectory γ on the reduced phase space $S^2_{\vec{J}_e}$. The angle Ω is the holonomy of the path γ with respect to a natural connection in the fiber bundle $M_{\vec{J}_e}$. This connection is induced from the natural symplectic form in phase space $T^*SO(3)$.

The angle $2ET/J$ is a dynamical phase, and Ω is a geometrical phase, very similar with (2.1).

3.1.2 In quantum mechanics

The Hilbert space of the quantum free rigid body is

$$\mathcal{H} = L^2\left(SO(3)\right)$$

Angular momentum operators are acting in $\mathcal{H}$ with the usual commutation relations of the $so(3)$ Lie algebra:

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hat{J}_z, \quad \left[\hat{J}_y, \hat{J}_z\right] = i\hat{J}_x, \quad \left[\hat{J}_z, \hat{J}_x\right] = i\hat{J}_y.$$

Two rotations act in this problem. A first rotation which rotates together the rigid body and the vecteur $\vec{J}_e$, is a symmetry of the problem.

A second rotation which rotates the rigid body alone (or equivalently the vector $\vec{J}$ in the body frame), is not a symmetry of the problem.

With respect to these two rotations the Hilbert space decomposed as:

$$\mathcal{H} = L^2\left(SO(3)\right) = \bigoplus_{j\in\mathbb{N}} \mathcal{H}_j^{(1)} \otimes \mathcal{H}_j^{(2)}$$

where $\mathcal{H}_j$ is an irreducible representation space of the $so(3)$ algebra, with dimension $2j+1$.

In group theory, this decomposition is called the **Peter-Weyl formula**, see [17].

The quantum operator $\hat{H}$ obtained from (3.1) acts in $\mathcal{H}_j^{(2)}$ alone: this express the quantum reduced dynamics of the rigid body.

(Note that because $\hat{H}$ has no action in $\mathcal{H}_j^{(1)}$, every eigenvalue has multiplicity $(2j+1)$).

3.2 The Classical limit of the Angular momentum dynamics

In this section we recall some known results about the angular momentum coherent states, and their role to define the classical limit, see [14] and [20]. We would like to stress the correspondence between the quantum dynamics of an angular momentum with a fixed modulus j (integer or half integer: $2j \in \mathbb{N}$), and the classical dynamics of an angular momentum vector $\vec{J}$ **of length 1**. $\vec{J}$ belongs to a sphere noted S^2 with radius 1, which is the classical phase space of the angular momentum.

3.2.1 The $su(2)$ algebra and the coherent states

The quantum hermitian operators of the spin $\hat{J}_x, \hat{J}_y, \hat{J}_z$ form an irreducible representation of the $su(2)$ algebra, in a Hilbert space $\mathcal{H}_j$ with dimension $2j+1$:

$$\left[\hat{J}_x, \hat{J}_y\right] = i\hat{J}_z, \quad \left[\hat{J}_y, \hat{J}_z\right] = i\hat{J}_x, \quad \left[\hat{J}_z, \hat{J}_x\right] = i\hat{J}_y.$$

In order to have a nice correspondance with the classical limit, we now rescale these operators by:

$$\hat{\vec{J}}_{new} = \frac{1}{2j}\hat{\vec{J}}$$

We also write $\hat{\vec{J}}$ insteed of $\hat{\vec{J}}_{new}$, so:

$$\left[\hat{J}_x, \hat{J}_y\right] = i\frac{1}{2j}\hat{J}_z, \quad \left[\hat{J}_y, \hat{J}_z\right] = i\frac{1}{2j}\hat{J}_x, \quad \left[\hat{J}_z, \hat{J}_x\right] = i\frac{1}{2j}\hat{J}_y.$$

So define

$$\hbar_{eff} = \frac{1}{2j}$$

(remark that $\hbar_{eff} = \frac{1}{2j}$ plays the role of an effective Planck constant, $\hbar_{eff} \to 0$ is the classical limit).

A basis are the vectors $|m>$, $m = -j, -j+1, \ldots, +j$, eigen-vectors of the $\hat{J}_z$ operator: $\hat{J}_z|m> = \left(\frac{m}{j}\right)|m>$. An element of the group $g \in SU(2)$ is represented by the unitary operator

$$\hat{R}(\vec{\alpha}) = \exp\left(-i\alpha_3\hat{J}_z/\hbar_{eff}\right)\exp\left(-i\alpha_2(2j)\hat{J}_y/\hbar_{eff}\right)\exp\left(-i\alpha_1\hat{J}_z/\hbar_{eff}\right), \tag{3.2}$$

acting in $\mathcal{H}_j$, where $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ are the Euler angles.

The state $|m = -j>$ corresponds to the classical vector $\vec{J} = (0, 0, -1)$. In order to obtain a quantum state $|\vec{J}>$ associated to the classical vector $\vec{J}$ with any spherical coordinates (θ, φ) we only need to apply the rotation operator (3.2) on $|m = -j>$, with $\vec{\alpha} = (0, \theta - \pi, \varphi)$, see figure 3.3 (a). Such a state $|\vec{J}> = \hat{R}(\vec{\alpha})|-j>$ is called a **coherent state.** One can show that ([20]):

$$\left|<\vec{J}'|\vec{J}>\right|^2 = \cos^{4j}\left(\frac{\Theta}{2}\right) \simeq 1 - \frac{j\Theta^2}{2} + o(\Theta^2), \tag{3.3}$$

where Θ is the angle between $\vec{J}'$ and $\vec{J}$ on the sphere.

More generally, for every state $|\psi> \in \mathcal{H}_j$, one can define its **Husimi distribution** [20],[18, 19]:

$$Hus_\psi(\vec{J}) = \left|<\vec{J}|\psi>\right|^2,$$

which is a positive function on the sphere.

From (3.3), we see that in the **classical limit** $j \to \infty$, the Husimi distribution of a coherent state $|\vec{J}>$**becomes localized on the phase space**, at point $\vec{J}$ with a width $\simeq 1/\sqrt{j}$. Let us also remark that if $\vec{J}'$ and $\vec{J}$ are opposite, then the function $\left|<\vec{J}'|\vec{J}>\right|$ is zero with order $2j$.

As a second example, consider the state $|m>$. One obtains that $Hus_{|m>}(\vec{J}) = \left|<\vec{J}|m>\right|^2$ is maximum on the line $\left(\vec{J}\right)_z = m/j$ as expected, with a width of order $\simeq 1/\sqrt{j}$, and $\left|<\vec{J}|m>\right|$ has a zero of order $(j-m)$ at point $\vec{J} = (0,0,1)$, and a zero of order $(j+m)$ in $\vec{J} = (0,0,-1)$.

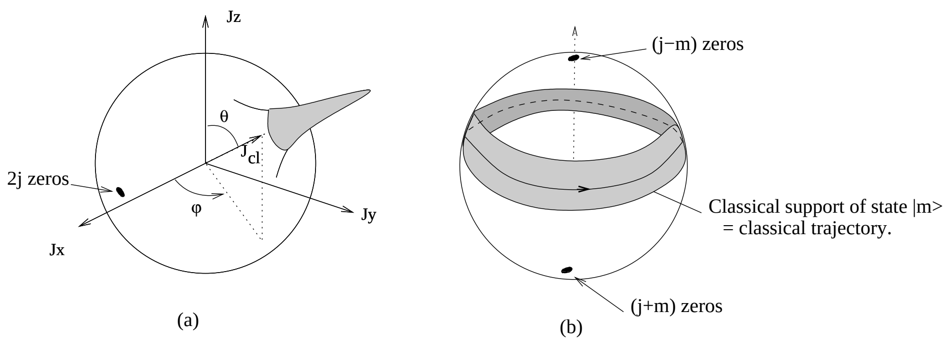


Figure 3.3: (a) Husimi distribution $Hus_{\vec{J}}(\vec{J}') = \left|<\vec{J}'|\vec{J}>\right|^2$ of a coherent state $|\vec{J}>$, with its zeros.
(b) Husimi distribution $Hus_{|m>}(\vec{J}') = \left|<\vec{J}'|m>\right|^2$ of the state $|m>$ with its zeros.

3.2.2 Expectation values of operators

One can compute [20]:

$$<\vec{J}|\hat{J}_z|\vec{J}>= J_z,$$
$$<\vec{J}|\hat{J}_x|\vec{J}>= J_x,$$
$$<\vec{J}|\hat{J}_z^2|\vec{J}>= (J_z)^2 + \hbar_{eff}\left(1 - J_z^2\right),$$

and more generally, the expectation value of an operator $\hat{O}$ over coherent states gives a function on the sphere, noted

$$O(\vec{J}) =<\vec{J}|\hat{O}|\vec{J}>$$

called the **Berezin symbol of the operator** (or Normal symbol). The operators constructed from the elementary operators $\hat{\vec{J}}$ as above, have a symbol which admits a formal series in power of $\hbar_{eff}$:

$$O(\vec{J}) = \underbrace{O_0(\vec{J})}_{\textbf{principal symbol}} + \hbar_{eff} O_1(\vec{J}) + \dots$$

The map $\hat{O} \to O$ is injective [4], so **the symbol characterizes the operator.** The first term $O_0(\vec{J})$ is the **principal symbol**, or **classical observable**. In the limit $\hbar_{eff} \to 0$ the symbols are dense in the space of C^∞ functions on the sphere. See [4][16] for the more general **"deformation quantization"** framework.

Thanks to the injectivity of the symbol, one can define the **star product** of two symbol $a * b$, to be the product of the two operators (see figure):

$$\widehat{a * b} = \hat{a}\,\hat{b}$$

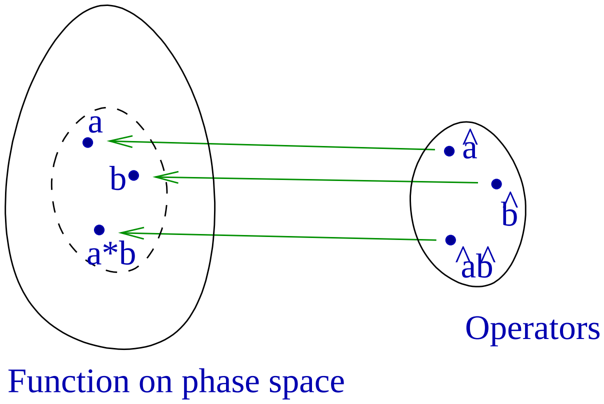


Figure 3.4: Symbols and star product.

Then one has the property (common to all star products, and choice of quantization):

$$a * b = ab + i\hbar_{eff}\,\{a, b\} + o\left(\hbar_{eff}\right)$$

where the second term involves the Poisson brackets of the symbols. The star product allows to work (as possible) with symbols on phase space insteed of operators.

3.2.3 Schrödinger equation and classical limit

The quantum dynamics is defined by **Hamiltonian** $\hat{H}$**,** a self-adjoint operator in $\mathcal{H}_j$. A quantum state $|\psi(t)\rangle$ evolves under the **Schrödinger equation**:

$$i\hbar_{eff}\frac{\partial|\psi(t)>}{\partial t} = \hat{H}|\psi(t)> \tag{3.4}$$

Remark: one put the factor $1/j$ in front of $\frac{\partial}{\partial t}$ in order to have a nice classical limit.

The symbol of $\hat{H}$ is written

$$H =< \vec{J}|\hat{H}|\vec{J} >= H_0 + \hbar_{eff}H_1 + \ldots$$

Consider a coherent state $|\psi(0) >= |\vec{J}(0) >$. One can show that this state is approximatively a coherent state for not too long time evolution:

$$\left\| |\psi(t) > -e^{i\alpha(t)}|\vec{J}(t) > \right\| = O(t)$$

where the dynamics of point $\vec{J}(t)$ on classical phase space S_j^2 is given by **classical Hamilton equations of motion:**

$$\frac{d\vec{J}(t)}{dt} = \frac{\partial H_0(\vec{J})}{\partial \vec{J}} \wedge \vec{J}$$

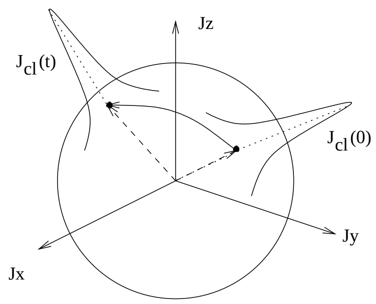


Figure 3.5: Evolution of Husimi distribution of a coherent state: it is approximativelly coherent, and its mean position $\vec{J}(t)$ evolves with the Classical Hamilton equations of motion.

Remarks:

- For example for $\hat{H} = \hat{J}_z$, the motion is a rotation around the z axis, with angular velocity $\omega = 1$.

- From a geometrical point of view, the symplectic two form on S^2 is (in spherical coordinates):

$$\Omega = \frac{1}{2} \sin\theta \, d\theta \wedge d\varphi$$

  and the equation of motion can be written as $dH(.) = \Omega(X_H, .)$, with $X_H = \dot{\theta}\frac{\partial}{\partial\theta} + \dot{\varphi}\frac{\partial}{\partial\varphi}$ the Hamiltonian vector field.

- **Important remark:** In order to have a well defined classical limit, we have put a factor $\hbar_{eff}$ in the Schrödinger equation (3.4). This is possible by a redefinition of time units.
  In the sequel, we will consider **Schrödinger equations without this** $1/j$ **factor**:

$$i\frac{\partial|\psi(\tilde{t})>}{\partial\tilde{t}} = \hat{H}|\psi(\tilde{t})>$$

  In other words we will use a time variable $\tilde{t} = t/\hbar_{eff}$. (Correspondingly, the two form is $\tilde{\Omega} = \Omega/\hbar_{eff}$).
  The main effect of this new definition, is that **in the classical limit, the classical motion viewed in time scale** $\tilde{t}$ **becomes slower and slower**, because typical velocities on the sphere are

$$\tilde{v}_\theta = \frac{d\theta}{d\tilde{t}} = \hbar_{eff}\frac{d\theta}{dt}$$

In this sense, **the classical limit $\hbar_{eff} \to 0$ will be equivalent to the adiabatic limit of slow motion**.

3.2.4 The quantizated line bundle over S^2

For each point $\vec{J} \in S^2$ we have defined a coherent state $|\vec{J}\rangle \in \mathcal{H}_j$. The choice of the phase in the definition of $|\vec{J}\rangle$ is quite arbitrary, so the correct geometrical object to consider is the one dimensional vector space of vectors proportionnal to $|\vec{J}\rangle$.

This defines a complex line bundle over S^2, whose topology is characterized by an integer Chern index.

The Chern index of this line bundle is

$$C = -(2j) \tag{3.5}$$

The easiest way is to see this is to construct a global section of the bundle and compute its zeros: Consider a reference coherent state $|\vec{J}_0\rangle$, its projection $|\vec{J}\rangle\langle\vec{J}|\vec{J}_0\rangle$ gives a global section. This section is zero if $\langle\vec{J}|\vec{J}_0\rangle = 0$. We said above that this happens for $\vec{J} = -\vec{J}_0$ with order $(2j)$. A correct inspection of the orientation gives $C = -(2j)$.

Remarks:

- In mathematical terms, the coherent states family defines a map $\vec{J} \in S^2 \to \left[|\vec{J}\rangle\right] \in \mathbb{P}(\mathcal{H}_j)$, and the line bundle in consideration is the pull back of the canonical bundle $\mathcal{H}_j \to \mathbb{P}(\mathcal{H}_j)$.)
- This line bundle, and its topology will be important for the application of the index formula below. (it plays also key role in geometric quantization, see [21, 16]).

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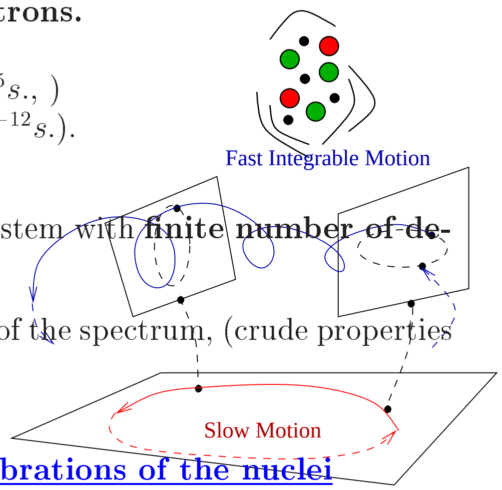
Chapter 4

Topological aspects in the Semi-quantum model of slow-fast coupled systems

4.1 Introduction

- A small molecule:

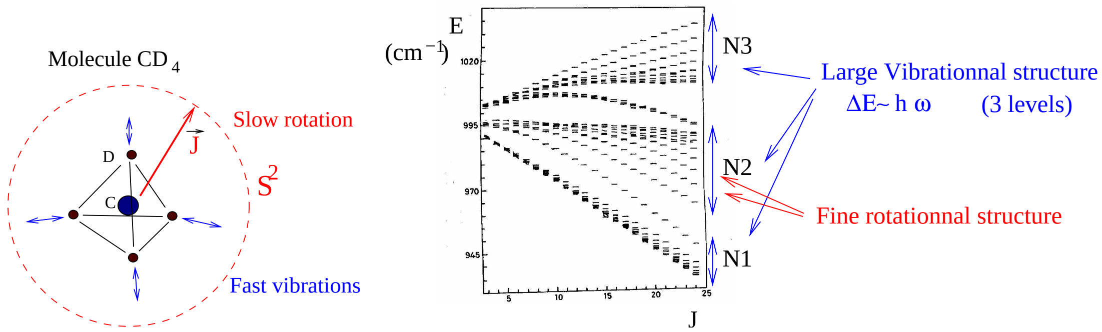
group of **interacting (quantum) nuclei and electrons.**
with **fast electrons** ($\tau_e \simeq 10^{-15} \to 10^{-16} s.$),
slower vibrations of the nuclei ($\tau_v \simeq 10^{-14} \to 10^{-15} s.,$)
slower rotation of the molecule ($\tau_{rot} \simeq 10^{-10} \to 10^{-12} s.$).



Characteristics:

- **Fast-Slow coupled, quantum, Hamiltonian** system with **finite number of degree of freedom.**
- We will be concerned with **Topological** properties of the spectrum, (crude properties but robust against perturbations).
  Works of D. Sadovskii, B. Zhilinskii, ...

First example: Slow rotation coupled with fast vibrations of the nuclei

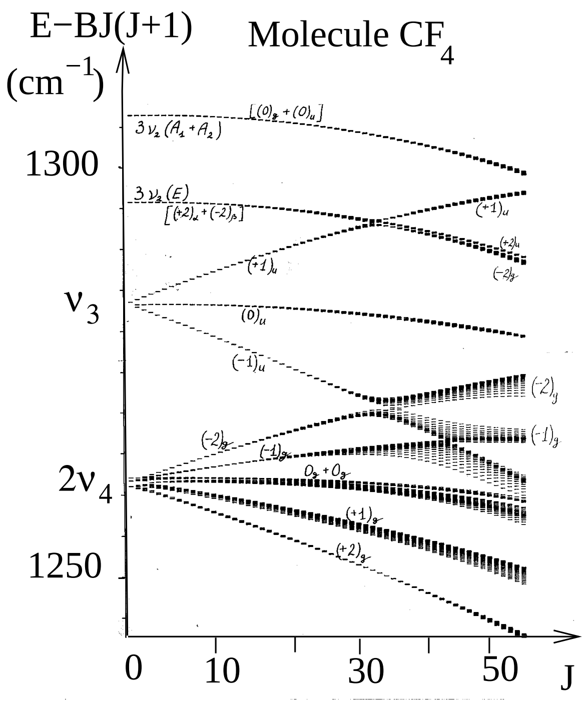


__Observations:__

- Group of rotational levels
- Restructuration of groups and exchange of levels with external parameter.

__Objectives:__ Understand these qualitative phenomena

These qualitative phenomena are very common in molecular spectra.



4.2 Model for coupling between: slow rotation and n quantum vibrational levels:

4.2.1 The semi-quantal model

Suppose $\hat{H}_{tot}$ acts in

$$\mathcal{H}_{tot} = \mathcal{H}_{slow} \otimes \mathcal{H}_{fast} = \mathcal{H}_j \otimes \mathbb{C}^n$$

Its **symbol** admits a formal power series in $\hbar_{eff} = 1/(2j)$:

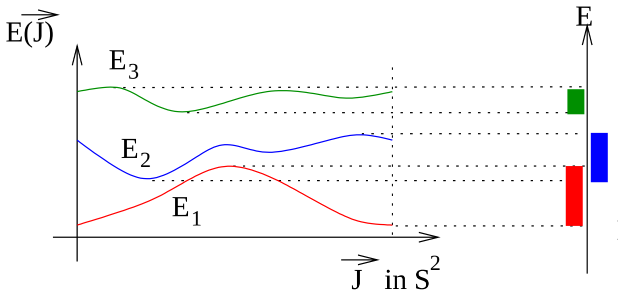
$$\hat{H}_{fast}(\vec{J}) = \langle \vec{J} | \hat{H}_{tot} | \vec{J} \rangle = \hat{H}_0(\vec{J}) + \hbar_{eff} \hat{H}_1(\vec{J}) + \dots.$$

- **This is a operator valued symbol** (the Born-Oppenheimer Approximation)**:**

$$\boxed{\left\{\begin{array}{ccc} \vec{J} & \rightarrow & \hat{H}_{fast}\left(\vec{J}\right) \\ S_J^2 & \rightarrow & \mathrm{Herm}\left(\mathcal{H}_{fast}=\mathbb{C}^n\right) \\ Slow & & Fast \end{array}\right.}$$

- **<u>Eigenvalues of</u>** $\hat{H}_0\left(\vec{J}\right)$ **<u>:</u>**

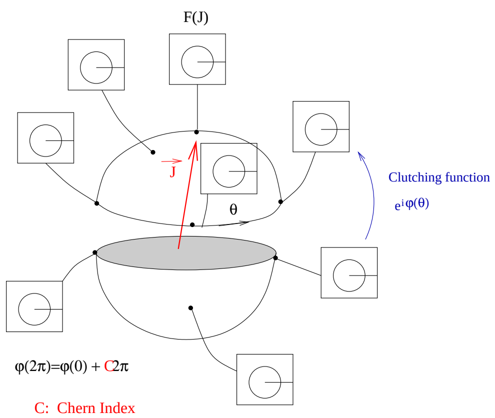
are $E_1\left(\vec{J}\right), E_2\left(\vec{J}\right), E_3\left(\vec{J}\right), \ldots,$ form n **bands**, ***provided there is no degeneracy.***



We discuss below the **important role of degeneracies**.

- **<u>The eigenspaces of</u>** $\hat{H}_0\left(\vec{J}\right)$**<u>:</u>**

$$\vec{J} \rightarrow F_i\left(\vec{J}\right) = \mathrm{Ker}\left(\hat{H}_0(\vec{J}) - E_i\left(\vec{J}\right)\, Id\right) \subset \mathbb{C}^n$$



define n **Complex Vector Bundle of rank 1**: F_1, F_2, F_3.

Their **topology** is characterized by **Chern indices:**

$$C_1, C_2, C_3, \ldots \in \mathbb{Z}$$

Additivity of the indices:
Because of the triviality of the total bundle $\mathcal{H}_{fast} \to P_{slow} = S_j^2$,

$$\sum_i C_i = \sum_i c_1(L_i) = c_1(\oplus_i L_i) = c_1(\mathcal{H}_{fast}) = 0.$$

4.2.2 Modifications of bands by an external parameter λ:

Property about degeneracies:
*If $\lambda \in \mathbb{R}^n \to \hat{H}(\lambda)$ is **generic** family of hermitian operators,then **degeneracies** between **two** eigenvalues occur with **codimension** 3. And more generally degeneracies with multiplicity $k = 2, 3, \ldots$ occur with codimension $k^2 - 1 = 3, 8, \ldots$*

Because the space of $k \times k$ Hermitian matrices is k^2 dimensional. Matrices with multiplicity k are: λId with $\lambda \in \mathbb{R}$.

Or because for a 2×2 matrix:

$$\hat{H}(\lambda) = \begin{pmatrix} \lambda_1 & \lambda_3 + i\lambda_4 \\ \lambda_3 - i\lambda_4 & \lambda_2 \end{pmatrix}, \qquad \Delta E = \sqrt{(\lambda_1 - \lambda_2)^2 + 4\lambda_3^2 + 4\lambda_4^2} : \text{ splitting}$$

Remarks:

- for the same reason, in the case of **real symmetric matrices**, the codimension for a multiplicity $k = 2, 3, \ldots$ event, is $\frac{1}{2}k(k+1) - 1 = 2, 5, \ldots$.
- In many physical problems, **constrains by particular symmetries**.

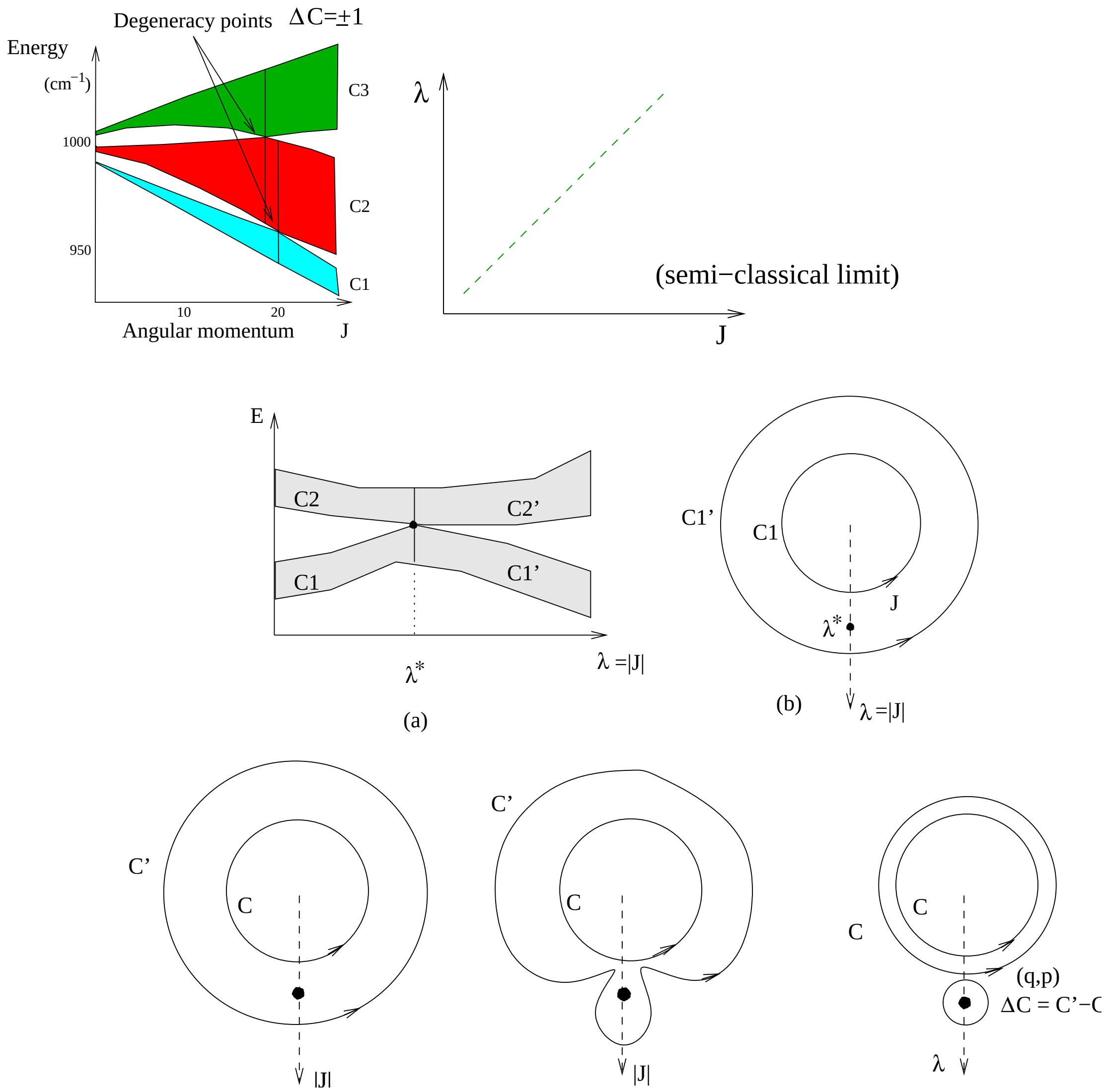
For model $\hat{H}_{fast}\left(\vec{J}\right)$,
the external parameters are:

$$\vec{J} = \left(\frac{\vec{J}}{\left|\vec{J}\right|}, \left|\vec{J}\right|\right) \in \left(S_J^2 \times \mathbb{R}^+\right) = \mathbb{R}^3$$

Modification of Chern index at a generic degeneracy:

$$\Delta C_2 = C_2' - C_2 = \pm 1$$

Proof: in $\vec{J} \in \mathbb{R}^3$ space,



Local model near an isolated degeneracy:

$$\hat{H}_\lambda(q,p) = \begin{pmatrix} \pm\lambda & q+ip \\ q-ip & \mp\lambda \end{pmatrix}, \quad \Delta E = 2\sqrt{\lambda^2+q^2+p^2}$$

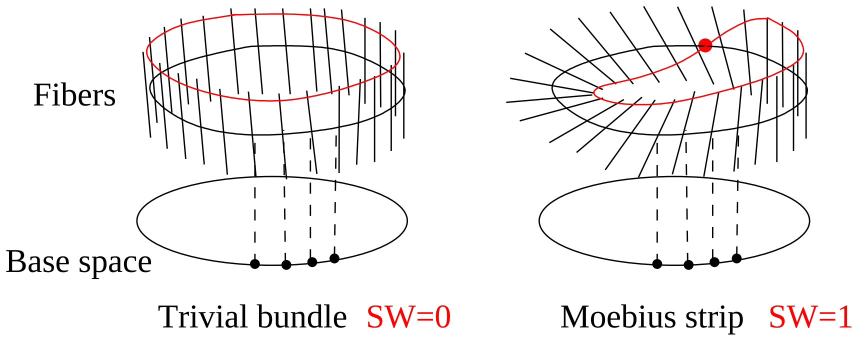
giving (Berry 84)

$$\boxed{\Delta C = \mp 1}$$

Because topology *can be computed from zeroes of a global section*:
Here

$$\hat{H}_\lambda \equiv \vec{B}.\hat{\vec{\sigma}}, \qquad \vec{B} = (\lambda, q, p)\,, \quad \hat{\vec{\sigma}} : \text{Pauli Matrices}$$

has eigenstates $|\psi_\pm\left(\vec{B}\right)\rangle$ define two complex vector bundles F_+, F_- of rank 1 over S^2.



A global section of the upper band is F_+ is obtained by projection of the fixed state $|+\rangle$ onto F_+:

$$|\psi_+\left(\vec{B}\right)\rangle\langle\psi_+\left(\vec{B}\right)|+\rangle \in F_+$$

and has one zero for $|\psi_+\left(\vec{B}\right)\rangle = |-\rangle$. Careful inspect of orientation gives $C_+ = -1$.

■

4.2.3 Quantum model: (rotation is quantized)

$$\text{Opérateur } \hat{H}_{tot} = \hat{H}_{fast}(\hat{\vec{J}}) \quad \text{sur } \mathcal{H}_j \otimes \mathbb{C}^n$$

Theorem :(C.Emmrich-A.Weinstein, CMP 176, p.701, 1998),

Construct ***projectors in*** *$\mathcal{H}_{tot}$, $\hat{P}_1, \hat{P}_2, \hat{P}_3, \ldots$ associated with bands, such that $\left[\hat{H}_{tot}, \hat{P}_i\right] = O(\hbar_{eff}^{\infty})$.*

($\hat{P}_i$ is given by its symbol $\hat{P}_{i,0}(\vec{J}) + \hbar_{eff}\hat{P}_{i,1}(\vec{J}) + \ldots$,
with $\hat{P}_{i,0}\left(\vec{J}\right)$: spectral projector of $\hat{H}_0\left(\vec{J}\right)$.)

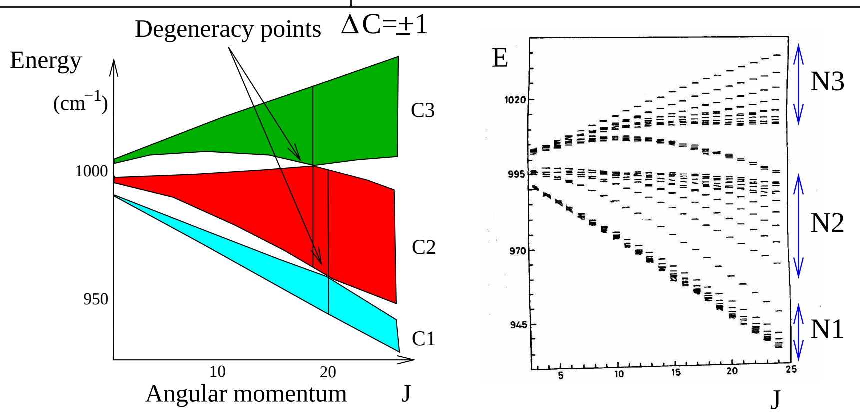
So define: $\mathcal{N}_i = Rank\left(\hat{P}_i\right)$: number of levels in band i

Remarks:

•This result is no so obvious **if bands overlap** in energy; (figure above).
•Corrections are due to possible **tunnelling effect** between bands.
•General theorem and Proof below.

Summary:

$1/2$ Quantum (B.O.)	Quantum
$\vec{J} \rightarrow H_{fast}\left(\vec{J}\right)$ $S_j^2 \rightarrow Herm\left(\mathbb{C}^n\right)$	Operator $\hat{H} = H_{fast}(\hat{\vec{J}})$ sur $\mathcal{H}_j \otimes \mathbb{C}^n$
Chern indices C_i for bands	Number of levels in bands: $\mathcal{N}_i$



Question: relation between band topology C_i and $\mathcal{N}_i$?

Property: (F.Faure, B.Zhilinskii, Phys.Rev.Lett. **85,** p.960, 2000)

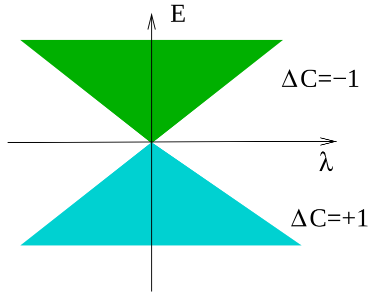
$$\mathcal{N}_i = (2j+1) - C_i$$
$$\textbf{i}.e. \quad \Delta\mathcal{N}_i = -\Delta C_i$$

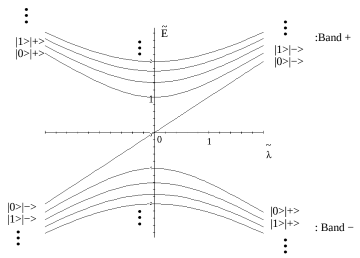
Proof (simple):
For a generic contact, the local model gives $\Delta C = \mp 1$,
Its quantization:

$$\hat{H}_\lambda = \begin{pmatrix} \pm\lambda & \hat{q} + i\hat{p} \\ \hat{q} - i\hat{p} & \mp\lambda \end{pmatrix}, \qquad \text{gives } \Delta\mathcal{N} = \pm 1$$

So $\Delta\mathcal{N}_i = -\Delta C_i$.
Consider a **generic deformation** of the given symbol $\hat{H}\left(\vec{J}\right)$ to the trivial (uncoupled) situation $\hat{H}_0 = \hat{S}_z$, where $\mathcal{N}_i = (2j+1)$, $C_i = 0$.
$\blacksquare$.

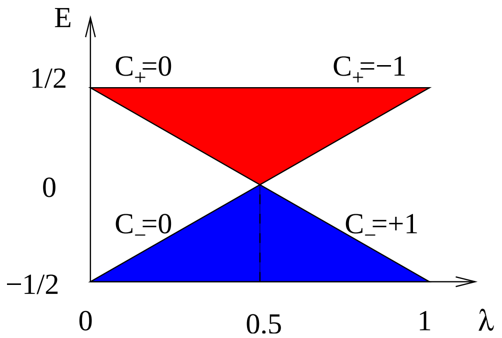
Simple example: Spin-orbit coupling
A two state (fast) spin $\vec{S}$ $(s = 1/2)$,
coupled with a (slow) angular momentum $\vec{J}$ with $2j+1$ states, with $j \gg 1$:

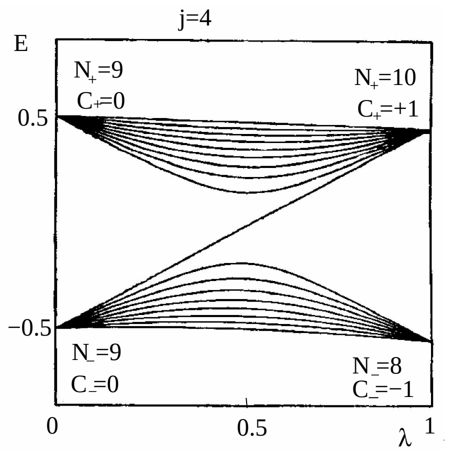




$$H\left(\vec{J}_{slow}, \vec{S}_{fast}\right) = (1-\lambda)\ S_z + \lambda\ \vec{J}.\vec{S}, \qquad \lambda \in [0,1] : \text{parameter}$$

- For $\lambda = 0$, $H = S_z$: Two trivial bands, $C_\pm = 0$; with $\mathcal{N}_\pm = (2j+1)$ levels.
- For $\lambda = 1$, $H = \vec{J}.\vec{S}$: Two non trivial bands, $C_\pm = \mp 1$, with $\mathcal{N}_\pm = (2j+1) \pm 1$ levels.
- At $\lambda = 1/2$, $\vec{J} = (0,0,-1)$, gives $H = 0$; an isolated degeneracy between the two bands.





What is particular here:

•Dim(*phase space* S^2)=2 $<$ Codim(*degeneracies*)=3.
So Vector bundles have **rank 1.**

With external parameter $\lambda \in \mathbb{R}$, isolated degeneracies; local model.

•Rank 1 vector bundles over S^2 are characterized by

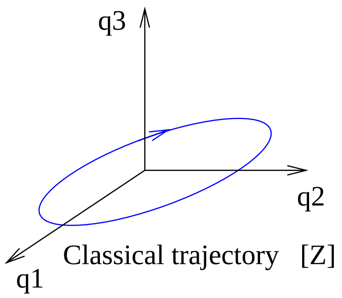
$$\text{Chern Index :}\quad C \in H^2\left(S^2, \mathbb{Z}\right) \equiv \mathbb{Z}$$

Question: what happends with **4-dimensional** compact slow phase space?

4.3 Model with more interesting topological phenomena: Slow motion on $\mathbb{C}P^2$, dimension 4.

4.3.1 Classical mechanics:

Three vibrations in 1:1:1 resonance on $T^*\mathbb{R}^3 = \mathbb{R}^6$:



$$H_{vib} = \sum_{i=1}^{3} \frac{1}{2}\left(p_i^2 + q_i^2\right) = \sum_{i=1}^{3} |Z_i|^2 = \langle Z|Z\rangle,$$

$$\text{with } Z_i = \frac{1}{\sqrt{2}}(q_i + ip_i) \in \mathbb{C}, \quad Z = (Z_1, Z_2, Z_3) \in \mathbb{C}^3$$

so $Z(t) = Z(0)e^{-it}$.

For a fixed energy $E = \langle Z|Z\rangle$, a trajectory is associated to a point $[Z]$ in **reduced phase space (dim 4)**

$$\mathbb{C}P^2 = \left(\mathbb{C}^3 \setminus \{0\}\right) / \sim, \qquad with\; Z \sim \lambda Z, \quad \lambda \in \mathbb{C}$$

4.3.2 Quantum mechanics:

on $L^2(\mathbb{R}^3)$,

operators $\hat{q}_i : \psi(\vec{q}) \to q_i\psi(\vec{q}) \qquad \hat{p}_i : \psi(\vec{q}) \to -i\frac{\partial\psi(\vec{q})}{\partial q_i}$,

$$\hat{H} = \sum_{i=1}^{3} \frac{1}{2}\left(\hat{p}_i^2 + \hat{q}_i^2\right),$$

- **Spectrum:**

$$E = \sum_{i=1}^{3}\left(n_i + \frac{1}{2}\right) = n_1 + n_2 + n_3 + \frac{3}{2} = N + \frac{3}{2}$$

$$\text{multiplicity}: \frac{1}{2}(N+2)(N+1)$$

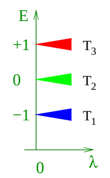
$$\text{Phase space } \mathbb{C}P^2 \Leftrightarrow \text{Hilbert space } \mathcal{H}_{Polyad\,N}$$

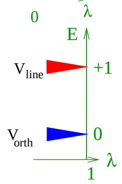
- **Semi-classical limit:** $N \to \infty$

4.3.3 Slow Vibrations coupled with 3 electronic states:

Matrix symbol: with parameter $\underline{\lambda \in [0,1]}$ *":magnetic field",*

$$\left\{ \begin{array}{lll} [Z] & \rightarrow & \hat{H}_{fast,\lambda}(Z) = (1-\lambda)\,\hat{H}_{fast,0} + \lambda\,\hat{H}_{fast,1}(Z) \\ \mathbb{C}P^2 & \rightarrow & Herm\left(\mathbb{C}^3_{fast}\right) \\ \text{Slow} & & \text{Fast} \end{array} \right.$$





•For $\lambda = 0$,

No dependence on $[Z] \in \mathbb{C}P^2$: $\hat{H}_{fast,0} = \begin{pmatrix} -1 & & \\ & 0 & \\ & & 1 \end{pmatrix}$, giving

three trivial fibers bundles, rank 1, on $\mathbb{C}P^2$: T_1, T_2, T_3.

•For $\lambda = 1$,

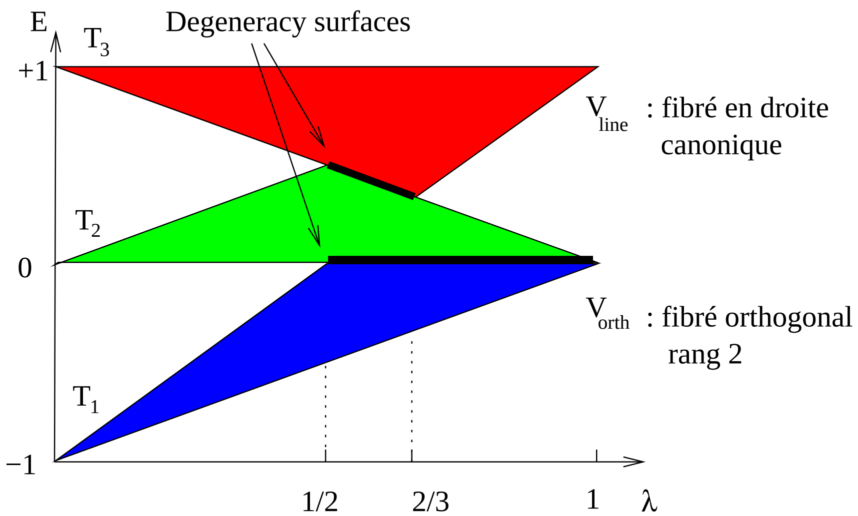
$\hat{H}_{fast,1}(Z) \equiv |Z\,\rangle\langle\,Z| = \frac{1}{<Z|Z>}\left(\overline{Z_i}Z_j\right)_{i,j}$: Projector onto line $[Z] \subset \mathbb{C}^3_{fast}$

Eigenvalue $(E_3 = 1)$: **rank 1 fiber bundle** V_{line} **:"the canonical bundle"**

Eigenvalue $(E_1 = 0,\ E_2 = 0)$: **rank 2 fiber bundle** V_{orth}.

4.3.4 Band spectrum in B.O approximation:

One compute $E_1(\lambda,[Z]) \le E_2(\lambda,[Z]) \le E_3(\lambda,[Z])$, $\lambda \in \mathbb{R}, [Z] \in \mathbb{C}P^2$.



represents the decomposition of the trivial bundle $\mathbb{C}P^2 \times \mathbb{C}^3$:

$$\begin{array}{ccc} T_1 \oplus T_2 \oplus T_3 & = \mathbb{C}^3 = & V_{line} \oplus V_{orth} \\ Rank\,1,\ trivial & Rank\,3,\ trivial & Rank\,1 \oplus Rank\,2 \end{array}$$

4.3.5 Topology of a vector fiber bundle F over $\mathbb{C}P^2$:

Characterized by its **Chern Class** $C(F) \in H^*(\mathbb{C}P^2, \mathbb{Z})$

$$C(F) = 1 + Ax + Bx^2, \qquad A, B \in \mathbb{Z}$$

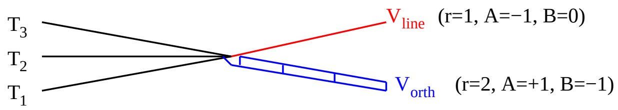
and its **rank**: $r \in \mathbb{N}^*$, $\quad (B = 0 \text{ if } r = 1)$.
(x is symplectic two form on $\mathbb{C}P^2$).

- **Composition property**:

$$C(F \oplus F') = C(F) \wedge C(F') = 1 + (A + A')\, x + (AA' + B + B')\, x^2$$

- **In the model,**

$$1 = C(\mathbb{C}^3) = C(V_{Line}) \wedge C(V_{Orth})$$



$$C(V_{Line}) = 1 + x, \qquad C(V_{Orth}) = 1 - x + x^2$$

but

$$C(V_{Orth}) \neq (1 + A\,x) \wedge (1 + A'\,x) = 1 + (A + A')\,x + (AA')\,x^2$$

no solution with integers A, A'.
So V_{Orth} is a **rank 2 undecomposable bundle.**

Physical interpretation:

A **spectral gap can not appear** inside the band V_{orth}, **under any perturbation**.

- **Remark:** *One needs at least **three bands** because:*

$$(1 + A\,x) \wedge (1 + A'\,x) = 1 + (A + A')\,x + (AA')\,x^2 = 1$$
$$\Rightarrow\ A = A' = 0 : \quad 2 \text{ trivial bands}$$

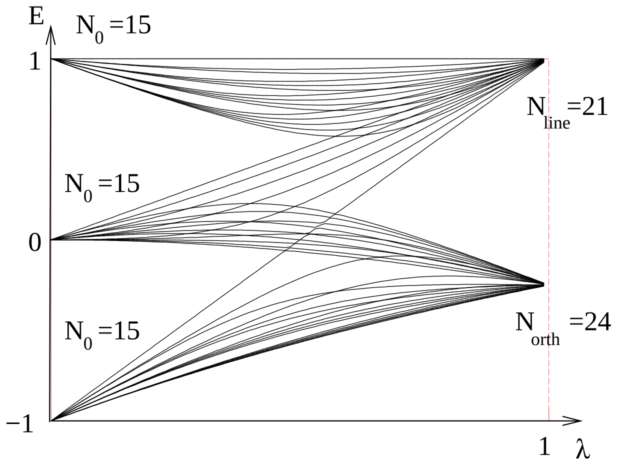
4.3.6 Quantization of vibrations:

$\mathbb{C}P^2 \rightarrow$ Hilbert space $\mathcal{H}_{Polyad\,N}$, $\quad Z = \frac{1}{\sqrt{2}}(q + ip) \rightarrow \hat{Z} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})$,
$\hat{H}_{fast}(Z) \rightarrow \hat{H}_{total}$

Total Hilbert space:

$$\mathcal{H}_{tot} = \mathcal{H}_{Polyad\,N} \otimes \mathbb{C}^3_{Electronics}$$

Numerical results for $N = 4$:



One observs the exchange of **"elementary group"** of $\Delta N = N + 2 = (N + 1) + 1 = 6$ levels.

Question: relation between $\mathcal{N}$ and band topology (r, A, B)?

Atiyah-Singer Index formula (1965), Fedosov (1990)
(A twist version of the *Hirzebruch-Riemann-Roch Formula*)
relating Analysis (number of levels) and topology of bundles:

$$\boxed{\mathcal{N}(F) = \left[Ch(F^*) \wedge Ch(Polyad_N) \wedge Todd(T\mathbb{C}P^2)\right]_{/\text{coef de } x^2}}$$

with

$$\begin{aligned} Ch(F^*) &= r - Ax + \frac{1}{2}\left(A^2 + 2B\right)x^2 && : \text{Band topology of the dual bundle} \\ Ch(Polyad_N) &= \exp(Nx) && : \text{geometric quantization of } \mathbb{C}P^2 \\ Todd(T\mathbb{C}P^2) &= 1 + \frac{3}{2}x + x^2 && : \text{Base space} \end{aligned}$$

In the above model:

$$\mathcal{N}(V_{Line}) = \left[\left(1+x+\frac{x^2}{2}\right)\wedge\left(1+Nx+\frac{(Nx)^2}{2}\right)\wedge\left(1+\frac{3}{2}x+x^2\right)\right]_{/x^2} = \frac{1}{2}(N+3)(N+2)$$

$$\mathcal{N}(V_{Orth}) = \left[\left(2-x-\frac{x^2}{2}\right)\wedge\left(1+Nx+\frac{(Nx)^2}{2}\right)\wedge\left(1+\frac{3}{2}x+x^2\right)\right]_{/x^2} = N(N+2)$$

4.3.7 Summary:

•**Semi-classical correspondence** between the ***Topological aspects of Semi Quantum*** and the ***Qualitative aspects of the Quantum*** problem :

The semi-quantum **Born-Oppenheimer** approximation for ***rotation-vibration-electronic*** coupling in molecules, shows **bands with non trivial topology** (vector bundles of any ranks)**.**

This topology is related to the **number of energy levels** in each group of the quantum problem.

•**Bifurcations : A change of band topology** gives **an exchange of levels** between groups of levels.

•**in Q.C.D., Instantons** are solitons of the gluon field, with a non trivial topology. The index formula gives them an axial charge. The consequences is a breaking of the chiral symmetry and **explains the important mass of the mesons** η, η'**.**

The index theorem is "one of the deepest and hardest results of mathematics" which "is probably enmeshed more widely with topology and analysis than any other single result" (Hirzebruch-Zagier 1974).

4.3.8 Remark on Index formula for the sphere (angular momentum phase space)

Chern Class of a line bundle is $C(F^*) = 1 - Cx \in H^*(S^2, \mathbb{Z})$, with $C \in \mathbb{Z}$.

$$\mathcal{N}(F) = \left[Ch(F^*)\wedge Ch(Quant_j)\wedge Todd(TS^2)\right]_{/\text{coef de } x^2}$$

with

$$\begin{aligned} Ch(F^*) &= 1 - Cx && : \text{band} \\ Ch(Quant_j) &= \exp((2j)x) && : \text{geometric quantization of } S^2 \\ Todd(TS^2) &= 1 + (1-g)x && : \text{Base space, genre } g = 0 \end{aligned}$$

gives

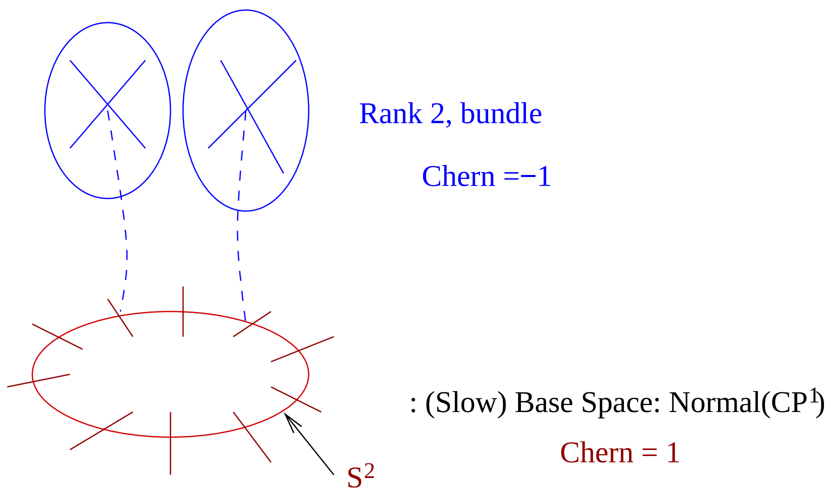
$$\begin{aligned}\mathcal{N}(F) = [(1 - Cx) \wedge (1 + (2j)x) \wedge (1 + (1 - g)x)]_{/x} &= (2j) + (1 - g) - C \\ &= (2j + 1) - C\end{aligned}$$

4.3.9 Remark on the surface of degeneracy $\mathcal{S}$ in the model between bands 2-3

In Parameter space $(\lambda, [Z]) \in \mathbb{R} \times \mathbb{C}P^2$,

This surface $\mathcal{S} \subset \mathbb{R} \times \mathbb{C}P^2$ is homotopic to $\mathbb{C}P^1 \subset \mathbb{C}P^2$ (Sphere: $Z_1 = 0$)

Locally, one has a rank 2 bundle over Normal($\mathbb{C}P^1$):



This gives transfert of states:

$$\Delta\mathcal{N} = (N + 1) + 1$$

4.3.10 Remark on Semi-classical expansion for $\hbar \to 0$; Weyl formula with correction

For a line bundle over a Riemann surface,

$h_{eff} = 1/(2j)$, Vol(S^2)=1.

$$\mathcal{N}(F) = \frac{Vol}{h_{eff}} + (1 - g) - C$$

The first term is Usual Weyl **"number of quanta"** in total phase space
(Below, this will give **the local density of states**.)

For a line $(r=1)$ bundle $\mathcal{F}$ over $\mathbb{C}P^2$,

number of levels $\mathcal{N}(F)$ is a polynomial in N:

$$\begin{aligned}\mathcal{N}(F) = &\left[\left(1 - Ax + \frac{1}{2}A^2x^2\right) \wedge \left(1 + Nx + \frac{(Nx)^2}{2}\right) \wedge \left(1 + \frac{3}{2}x + x^2\right)\right]_{/x^2} \\ &= \frac{1}{2}N^2 + N\left(-A + \frac{3}{2}\right) + \left(\frac{1}{2}A^2 - \frac{3}{2}A + 1\right)\end{aligned}$$

Interpretation: $h_{eff} = 1/N$, $\mathrm{Vol}(\mathbb{C}P^2) = 1/2$.
So

$$\mathcal{N}(F) = \frac{Vol}{h_{eff}^2} + \frac{1}{h_{eff}}\left(\frac{3}{2} - A\right) + \ldots$$

4.3.11 Remark on "Naturality" of index formula

The Chern Class is a map:

$$C: \; F \in Vect(M) \to C(F) \in H^*(M, \mathbb{Z})$$

The main interest of Chern class $C(F)$ is that coefficients are *integers*.
But $C(F \oplus F') = C(F) \wedge C(F')$.
•For two bundles over (dim $2n$) phases spaces,

$$F_1 \to M_1, \qquad F_2 \to M_2$$

one expects:

$$\mathcal{N}((F_1 \otimes F_2) \to (M_1 \times M_2)) = \mathcal{N}(F_1 \to M_1)\mathcal{N}(F_2 \to M_2) \quad \text{: product of Hilbert spaces}$$
$$\mathcal{N}((F_1 \oplus F_2) \to M) = \mathcal{N}(F_1 \to M) + \mathcal{N}(F_2 \to M) \quad \text{: Sum of bands}$$

This comes from

$$\begin{aligned} Ch(F_1 \otimes F_2) &= Ch(F_1) \wedge Ch(F_2) \\ Ch(F_1 \oplus F_2) &= Ch(F_1) + Ch(F_2) \\ Todd\left(T\left(M_1 \times M_2\right)\right) &= Todd\left(TM_1\right) \wedge Todd\left(TM_2\right) \end{aligned}$$

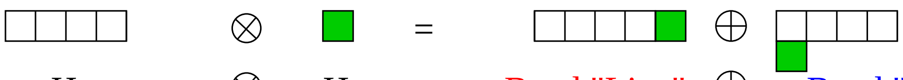
So the index formula is an expected formula:

$$\mathcal{N}(F_i) = \left[Ch(F_i \otimes Line_N) \wedge Todd(TM_i)\right]_{/\text{coef de } x^n}$$

But $Ch, Todd \in H^*(M, \mathbb{Q})$ (not integer classes).

4.3.12 Index theorem and group theory:

In the model, for $\lambda = 1$, $\hat{H}_1$ is constructed from **equivariance by SU(3)** :

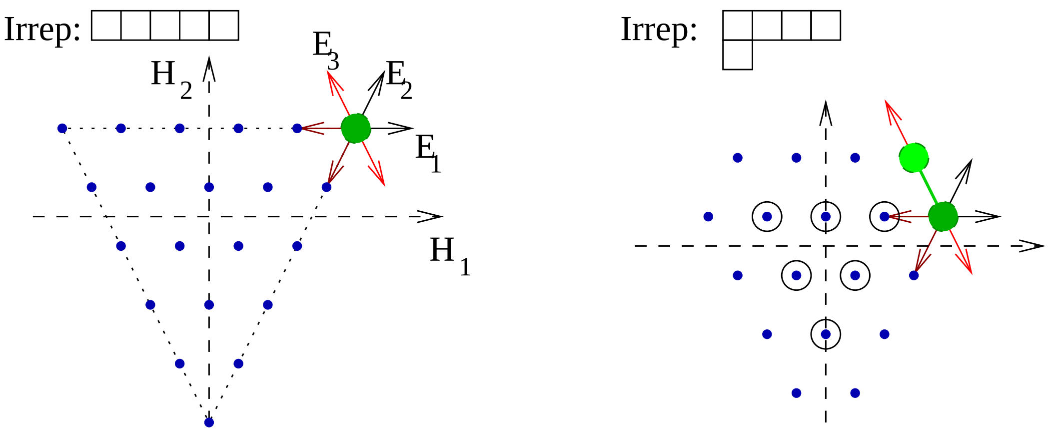


H_{tot} = H_{polyad} $\otimes$ H_{elec} = Band "Line" $\oplus$ Band "Orth"

15 * 3 = 21 + 24

Weyl formula of group theory gives correct dimensions $\mathcal{N}_{Line}, \mathcal{N}_{orth}$.

Remark on relations with vector coherent states, and weight diagramm, induced representations, equivariant vector bundles:



Orbit of :

Line bundle over: SU(3)/U(2)=CP 2

(Perelomov coherent states)

Orbit of :

Line bundle over: SU(3)/U(1)*U(1)

Orbit of :

Rank 2 bundle over SU(3)/U(2)=CP 2

4.4 Main "Born-Oppenheimer" theorem of adiabaticity

(C.Emmrich-A.Weinstein, CMP 176, p.701, 1998)

Consider:

- *a **Phase space** P_{slow} (a symplectic manifold for slow motion),*
- *an **Hilbert space** $\mathcal{H}_{fast}$ (for fast motion)*

- *a* ***Matrix symbol*** $p \in P_{slow} \to \hat{H}(p) \in Herm(\mathcal{H}_{fast})$ *which can be written*

$$\hat{H}(p) = \hat{H}_0(p) + \hbar \hat{H}_1(p) + \hbar^2 \hat{H}_2(p) \ldots,$$

- ***Hypothesis:*** $\forall p \in P_{slow}$, *eigenvalues* $(\lambda_i)_{i=1,\ldots m}$ *of* $\hat{H}_0(p)$ *are separated from the other part of the spectrum* $(\mu_j)_{j=\ldots}$*:*

$$\forall i, j, p \ \lambda_i(p) - \mu_j(p) \neq 0$$

- *So eigenvalues* $(\lambda_i(p))_{i=1,\ldots m}$ *define a subspace* $E(p) \subset \mathcal{H}_{fast}$*, with orthogonal projector* $\hat{\pi}_0\,(p)$*.*
- $E \to P_{slow}$ *is a rank* m ***complex vector bundle*** *over* P_{slow}*.*
- *Then for any* $k \in \mathbb{N}$*, there is a* ***unique*** *matrix valued symbol:*

$$\hat{\pi}(p) = \hat{\pi}_0(p) + \hbar \hat{\pi}_1(p) + \ldots \hbar^k \hat{\pi}_k(p)$$

which defines a self-adjoint operator $\hat{\pi}_{tot}$ *in* $\mathcal{H}_{tot}$*, such that:*

$$\begin{aligned} \hat{\pi}_{tot}^2 = \hat{\pi}_{tot} + \mathcal{O}(\hbar^{k+1}) \quad &: \ quasi - projector, \\ \left[\hat{H}_{tot}, \hat{\pi}_{tot}\right] = \mathcal{O}(\hbar^{k+1}) \quad &: \textit{almost commute.} \end{aligned}$$

Remarks

- One can thus modify $\hat{\pi}_{tot}$ (move slightly the eigenvalues towards 1 or 0, without moving the eigen-spaces) to obtain a true projector $\hat{\pi}'_{tot}$ (i.e. $\hat{\pi}'^2_{tot} = \hat{\pi}'_{tot}$). Let:

$$\mathcal{N} = Rank(\hat{\pi}'_{tot})$$

$\mathcal{N}$ is the number of eigenvalues close to 1 of the principal symbol $\hat{\pi}_0(\vec{J})$.

- The **index formula** above gives $\mathcal{N} = Rank(\hat{\pi}'_{tot})$ in terms of topology of the bundle E.
- **Generic case:** each eigenvalue E_i and eigenvector $|\phi_i>$ of $\hat{H}_{tot}, \quad i \in [1, \ldots \dim \mathcal{H}_{tot}]$, can be associated with the vector bundle E or its complement $E^\perp$; i.e. $|\phi_i\rangle \in Im(\hat{\pi}(p))$ *or* $\hat{\mathrm{K}}\mathrm{er}\,(\hat{\pi}(p))$.
- **Consequence:** a quantum state which initially belongs to the space $Im(\hat{\pi}(p))$, will stay in this space forever during its evolution, with a good approximation (if k high).
- **Non generic case:** by resonances between two eigenvalues the associated states can be equidistributed on$Im(\hat{\pi}(p))$ and $\hat{\mathrm{K}}\mathrm{er}\,(\hat{\pi}(p))$., as it occurs usually in the **tunneling effect**.

Indications for the proof :

By induction on $k \in \mathbb{N}$. One works only with symbols.

Hypothesis for a given k:

$$\begin{aligned} \pi * \pi - \pi &= \hbar^{k+1} A + O\left(\hbar^{k+2}\right) \\ [\pi, H]_* &= \hbar^{k+1} F + O\left(\hbar^{k+2}\right) \end{aligned}$$

Check that the hypothesis is true for $k = 0$.

Because $[\pi_0, H_0] = 0$, one can find a basis (for a given $p \in P$) such that:

$$\pi_0 = \left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right), \quad H_0 = \left(\begin{array}{cc} (\lambda_i)_i & 0 \\ 0 & (\mu_j)_j \end{array}\right) \equiv \left(\begin{array}{cc} H_{00} & 0 \\ 0 & H_{11} \end{array}\right),$$

and write in this basis:

$$A = \left(\begin{array}{cc} A_{00} & A_{01} \\ A_{10} & A_{11} \end{array}\right), \quad idem\ for\ F.$$

Lemme 1: $[A, \pi_0] = 0$, so $A = \left(\begin{array}{cc} A_{00} & 0 \\ 0 & A_{11} \end{array}\right)$.

Lemme 2: $F_{00} = [A_{00}, H_{00}]\,, F_{11} = [A_{11}, H_{11}]$.

Write:

$$\tilde{\pi} = \pi + \hbar^{k+1} K$$

with unknown $K = \left(\begin{array}{cc} K_{00} & K_{01} \\ K_{10} & K_{11} \end{array}\right)$ such that:

$$\begin{aligned} \tilde{\pi} * \tilde{\pi} - \tilde{\pi} &= O\left(\hbar^{k+2}\right) \\ [\tilde{\pi}, H]_* &= O\left(\hbar^{k+2}\right) \end{aligned}$$

Lemme 3: $K_{00} = -A_{00}$, $K_{11} = A_{11}$.

Lemme 4: $H_{00}K_{01} - K_{01}H_{11} = F_{01}$ and $H_{11}K_{10} - K_{10}H_{00} = F_{10}$, i.e.:

$$(K_{01})_{ij} = (\lambda_i - \mu_j)^{-1} (F_{01})_{ij}\,, \quad idem\ for\ K_{10}.$$

So Matrix $K(p)$ is determined, giving $\tilde{\pi}$.

Lemma 1,2,3,4 are not difficult to prove.

■

4.5 Berry's connection, Chern Class and Characteristic Classes

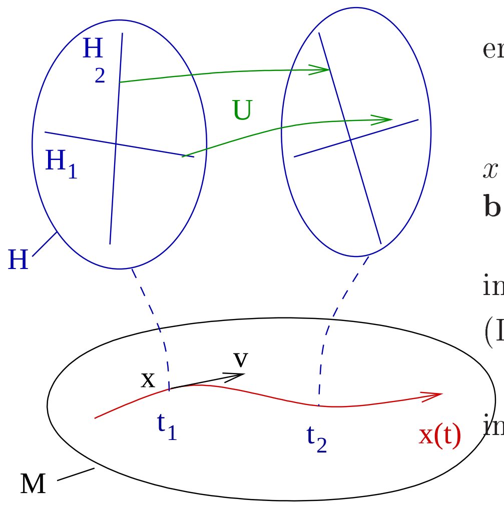
We gives here the definitions of the Characteristic classes used in Index formula above.

Consider

$$\mathcal{H}: \quad \text{fixed Hilbert space}$$
$$x \in M: \quad \text{Parameter space } (Phase\ space\ Manifold)$$

A x-dependent decomposition of $\mathcal{H}$:

$$\mathcal{H} = \bigoplus_i \mathcal{H}_{i,x}, \quad \mathcal{H}_{i,x} = Im\left(\hat{P}_{x,i}\right), \qquad \hat{P}_{x,i} : projector$$



•Think that $\hat{H}_x$ is a x-dependent Hermitian operator, with eigen-spaces $\mathcal{H}_{i,x}$.

•If $\hat{P}_{x,i}$ has a smooth dependence with respect to $x \in M$, then $F_i : \mathcal{H}_{i,x} \to M$ is a well defined **vector bundle** over M of rank $m_i = dim_{\mathbb{C}}(\mathcal{H}_{i,x})$.

•Consider a parametrized path $x(t) \subset M$. Lift x in $\mathcal{H} \times M$ with respect to the **parallel transport** (Levi-Civita) in each subspace $Im\left(\hat{P}_i\right)$.

This defines a *unitary* family of operators $\hat{U}(t_1, t_2)$ in $\mathcal{H}$, with *Hermitian* generator $\hat{K}^{Berry}(t_2)$:

$$i\hbar \frac{d}{dt} \hat{U}(t_1, t_2) = \hat{K}^{Berry}(t_2)\, \hat{U}(t_1, t_2)$$

Remark:
•Operator $\hat{K}^{Berry}$ express the **Berry's connection**.

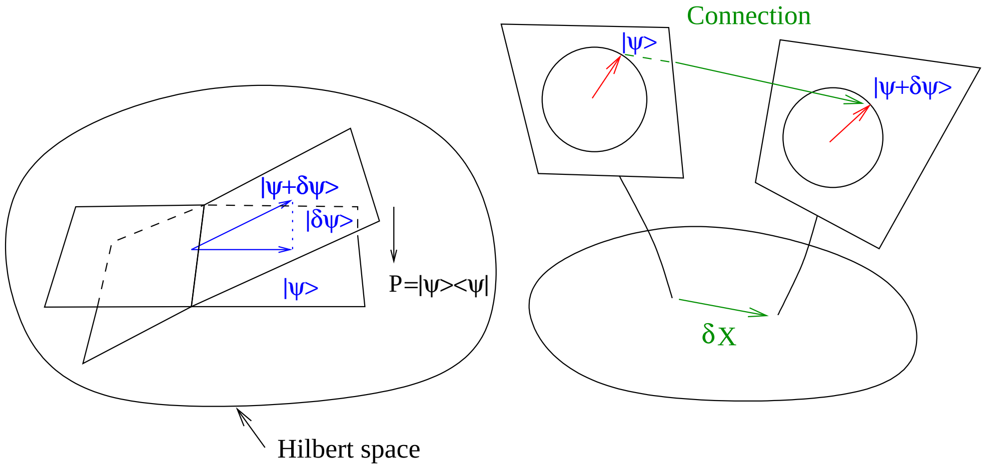
•$\hat{K}^{Berry}$ depends only on the tangent vector $v = \frac{dx}{dt} \in T_x M$ so $\hat{K}^{Berry}$ **is a 1-form on** M **with values in** $Herm(\mathcal{H})$.

Property:

$$\boxed{\hat{K}^{Berry}_{x,v} = i\hbar \sum_i \frac{d\hat{P}_{x,i}}{dt} \hat{P}_{x,i}}$$

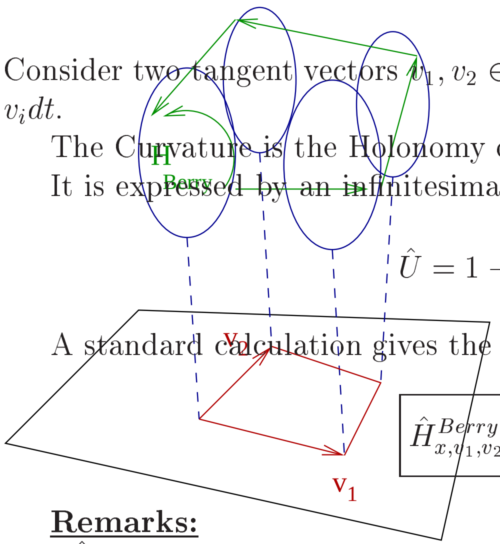
proof:
We saw that the Levi-Civita connection on space $\mathcal{H}_{i,x}$ can be expressed by:

$$|\psi + d\psi\rangle_i = P_i(x + dx)\, |\psi\rangle_i, \quad where\ |\psi_i\rangle \in \mathcal{H}_{i,x}$$



so $|\psi + d\psi\rangle = \sum_i |\psi + d\psi\rangle_i = \sum_i (P_i + dP_i)\,|\psi\rangle_i = |\psi\rangle + \sum_i dP_i P_i|\psi\rangle$. Identify with $i\hbar\frac{|d\psi\rangle}{dt} = \hat{K}^{Berry}|\psi\rangle$.■.

4.5.1 Berry's Curvature



Consider two tangent vectors $v_1, v_2 \in T_xM$, defining an infinitesimal loop in M, with sides $v_i dt$.

The Curvature is the Holonomy on this loop.

It is expressed by an infinitesimal unitary operator

$$\hat{U} = 1 - \frac{i}{\hbar}\hat{H}^{Berry}_{v_1,v_2} dt_1 dt_2 + o(dt^2)$$

A standard calculation gives the ***Hermitian generator*** of this **Berry's curvature**:

$$\boxed{\hat{H}^{Berry}_{x,v_1,v_2} = \frac{-i}{\hbar}\left[\hat{K}^{Berry}_{x,v_1}, \hat{K}^{Berry}_{x,v_2}\right]}$$

<u>**Remarks:**</u>

•$\hat{H}^{Berry}$ **is a 2-form on** M **with values in** $Herm\,(\mathcal{H})$.

•By construction $\hat{H}^{Berry}_{x,v_1,v_2}$ leaves $\mathcal{H}_{i,x}$ invariant, $\forall i$. The restriction is:

$$\hat{\Omega}^{Berry}_{i,v_1,v_2} = \hat{P}_i\left(\hat{H}^{Berry}_{x,v_1,v_2}\right)\hat{P}_i \ \in \ Herm\,(\mathcal{H}_{i,x})$$

•If $dim\mathcal{H}_{i,x} = 1$, then $\Omega^{Berry}_{i,v_1,v_2} \in \mathbb{R}$ is called the **(Scalar) Berry's curvature** for level i.

•One can check the formula:

$$\hat{H}^{Berry}_{x,v_1,v_2} = \sum_i P_i\left[d_{v_1}P_i, d_{v_2}P_i\right]P_i$$

•We will see below that in the semi-classical limit, if the **dynamics is integrable**, then $\hat{H}^{Berry}$ is the **quantization of a classical Hamiltonian** H^{Hannay} corresponding to the **Hannay connection** between Tori.

4.5.2 Characteristic Class

Consider a complex vector bundle $F : \mathcal{H}_x \to M$, over compact manifold M.

Define

$$\boxed{C(F) = det\left(1 + \frac{1}{2\pi i}\hat{\Omega}^{Berry}\right); \quad \textbf{Total Chern Class}}$$

<u>**Remarks and Properties:**</u>

- $\hat{\Omega}^{Berry}$ is a 2-form on M so $C(F)$ is a *differential form with even degree* only.
  One writes also: $C(F_i) = 1 + C_1 + C_2 + \ldots$,
  with $C_k \in H^{2k}(M, \mathbb{R})$: **k**st **Chern Class**.
- If $Rank_{\mathbb{C}}(F) = r$, then $C_k = 0$ for $k > r$.
  If $n = dim_{\mathbb{R}} M$, then $C_k = 0$ for $2k > n$.
- $C(F)$ is an **integral class** $C(F) \in H^{even}(M, \mathbb{Z})$; which means that C_k gives integers after integration over any closed submanifold S $\in H_{2k}(M, \mathbb{Z})$.
  (One check this in the Universal Classifying Grassmanian bundle $\mathbb{C}^{m+n} \to G_m(M)$, and use invariance of differential forms by pull-back; see Hatcher's Book, or Eguchi).
- if $r = Rank_{\mathbb{C}}(F) = 1$, then

  $$C_1 = \frac{1}{2\pi i}\hat{\Omega}^{Berry} \in H^2(M, \mathbb{Z})$$

  characterizes the topology of the bundle F**.** (See Well's book).
  This is not true in general for higher ranks.
- On $\mathbb{C}P^2$, we used the fact that

  $$H^*\left(\mathbb{C}P^2\right) = \mathbb{Z} + \mathbb{Z}x + \mathbb{Z}x^2$$

  where x is the (normalized) symplectic 2-form.
- More generally, for **any polynomial** P (or formal serie) on $\mathbb{R}$, then

  $$\mathrm{Tr}\left(P\left(\frac{1}{2\pi i}\hat{\Omega}^{Berry}\right)\right) \in H^{even}(M, \mathbb{R})$$

  is a topological invariant (does not depend on the connection).
  To have nice relations with $\oplus, \otimes$, (important for the index formula) define:

  $$Ch(F) = \mathrm{Tr}\left(e^{\frac{1}{2\pi i}\hat{\Omega}^{Berry}}\right); \quad \textbf{Chern Character}$$

$$Todd(F) = det\left(\frac{\frac{1}{2\pi i}\hat{\Omega}^{Berry}}{e^{\frac{1}{2\pi i}\hat{\Omega}^{Berry}} - 1}\right); \quad \textbf{Todd Class}$$

Then:

$$\begin{aligned} Ch(F_1 \otimes F_2) &= Ch(F_1) \wedge Ch(F_2) \\ Ch(F_1 \oplus F_2) &= Ch(F_1) + Ch(F_2) \\ Todd\,(F_1 \oplus F_2) &= Todd\,(F_1) \wedge Todd\,(F_2) \end{aligned}$$

4.5.3 Important physical remarks:

We show here that the Index formula is more precise than just giving the total number of states.

- The Index formula can be written:

$$\mathcal{N}\,(F) = \int_M \mu$$

$$\mu = \left[Ch(F^*) \wedge Ch(Polyad_N) \wedge Todd(T\mathbb{C}P^2)\right]_{/\mathrm{Vol}}$$

The Volume form μ is interpreted as **the local density of states in phase space M.**

- μ is still well defined if M *is not compact*.
- By the Semi-classical Symbol of the Hamiltonian $p \in M \to H(p) \in \mathbb{R}$, one obtains then the **Energy density of states**.
- For $h_{eff} = 1/N \to 0$, the expansion of μ is the **Weyl formula**. ("Averaged part" of the Gutwiller Trace-Formula), and involves no dynamics.

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Chapter 5

Topological aspects in the Classical model of slow-fast coupled systems

5.1 A simple class of models. Topology of the tori bundle.

•**Model:** A slow angular momentum $\vec{J}(t)$ coupled with fast Angular momentum $\vec{S}(t)$.

•Total *classical phase space*:

$$P_{tot} = P_{slow} \times P_{fast} = S_j^2 \times S_s^2$$

•Total *quantum Hilbert space*:

$$\mathcal{H}_{tot} = \mathcal{H}_{slow} \otimes \mathcal{H}_{fast} = \mathcal{H}_j \otimes \mathcal{H}_s, \quad dim = (2j+1)(2s+1)$$

•with the **adiabatic assumption**:

$$j \gg s$$

and the *(optional)* **semi-classical limit for fast variable**:

$$s \gg 1$$

•The **classical model** is specified by a **total symbol**:

$$H\left(\vec{J}, \vec{S}\right)$$

•Total Dynamics is **nearly integrable** (well identified tori: $S_{fast}^1 \times S_{slow}^1$).

•Simple example **"Spin-orbit coupling"**:

$$H\left(\vec{J},\vec{S}\right) = (1-\lambda)S_z + \lambda\vec{J}\vec{S}, \qquad \lambda \in [0,1]$$

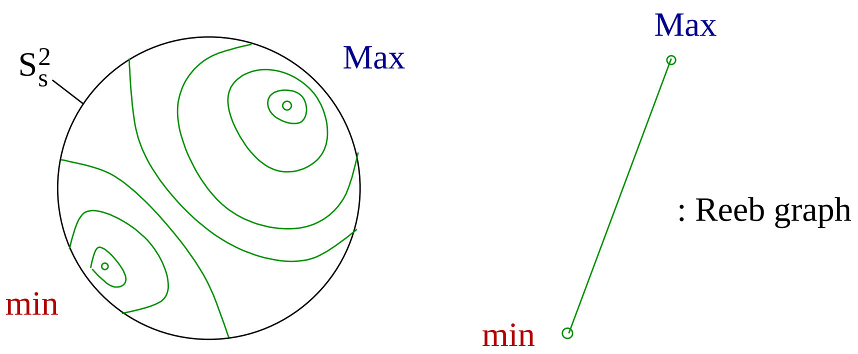
•Summary:

Slow $\vec{J}$ \ Fast $\vec{S}$	Classical in $P_{Fast} = S_s^2$	Quantum in $\mathcal{H}_{Fast} = \mathcal{H}_s$
Classical in $P_{Slow} = S_j^2$	Function $H_{tot}(\vec{J},\vec{S})$ (***Classical***, phase space $S_j^2 \times S_s^2$)	Operator Symbol $\vec{J} \to \hat{H}_{fast}(\vec{J})$ (***Semi-Quantum***)
Quantum in $\mathcal{H}_{Slow} = \mathcal{H}_j$	No meaning	$\hat{H}_{tot}$ (***Quantum*** in $\mathcal{H}_{tot} = \mathcal{H}_{slow} \otimes \mathcal{H}_{fast}$)

Restricted Hypothesis:

•For every $\vec{J}$ fixed, $H_{\vec{J}}\left(\vec{S}\right)$ is a function on S_s^2, with only a minimum min and a Maximum Max.

$\mathcal{C}$: this class of models.

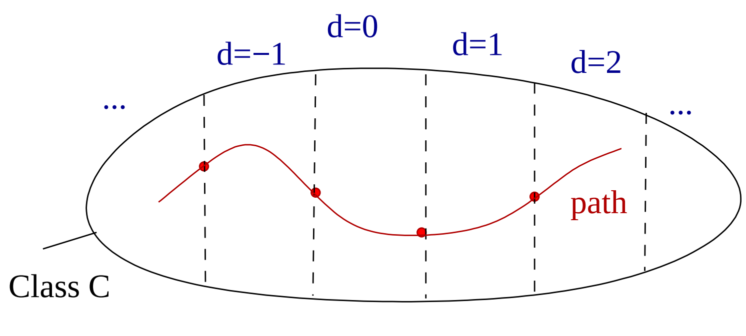


•If $Max > min$, Topology of the fast trajectories, characterized by **degree** $d \in \mathbb{Z}$ of:

$$degree\ of: \quad \vec{J} \in S_j^2 \to \text{Max} \in S_s^2$$

So Topological subclass of models

$$\mathcal{C} = (\cup_d \mathcal{C}_d) \cup Singulars$$



Topology of tori bundle ($T^1 \to S^2_{slow}$):

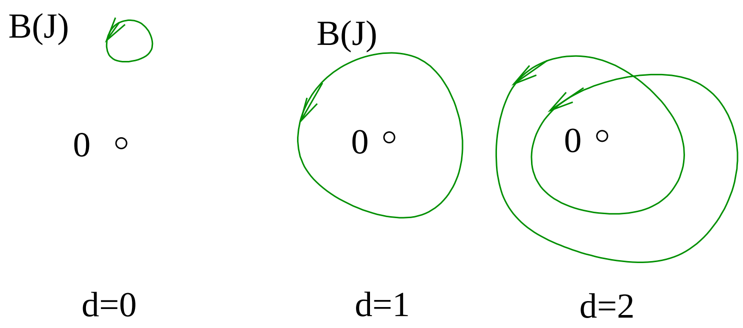
$$Chern_{Hannay} = 2\,d$$

Examples:

$$H = \vec{B}(\vec{J}).\vec{S} \in \mathcal{C}_d$$

with $\vec{J}\,(\theta,\varphi) \to \vec{B}\,(\theta',\varphi')$ of degree d:

$$\begin{array}{llll}
\bullet d = 1, & \vec{B} = \vec{J}, & H = \vec{J}.\vec{S} & C_{Hannay} = 2 \\
\bullet d = 0, & \vec{B} = (0,0,1) & H = S_z, & C_{Hannay} = 0 \\
\bullet d \neq 0, & \vec{B}(\theta' = \theta, \varphi' = d\varphi) & H = \vec{B}(\vec{J})\vec{S}, & C_{Hannay} = 2d
\end{array}$$



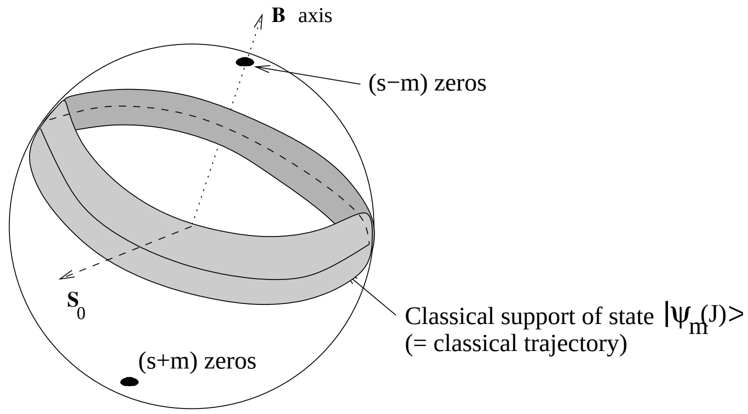
5.2 Semi-quantum model; Energy Bands and their topology by semi-classical calculation

For $\mathcal{H} \in \mathcal{C}_d$, there are $dim\mathcal{H}_{fast} = 2s+1$ isolated bands,
with Chern index $C_{Berry,m}$, $m = -s \to +s$.
Property:

$$C_{Berry,m} = -\,(2m)\,d,$$
$$C_{Hannay} = -\frac{\partial C_{Berry,m}}{\partial m} = 2d$$

Proof: Count the zeros of a global section
of band F_m: $\vec{J} \to \hat{H}_{\vec{J}}|\psi_{\vec{J},m}\rangle = E_{\vec{J},m}|\psi_{\vec{J},m}\rangle$.
Consider a **fixed coherent state** $|\vec{S}_0\rangle$. A **global section** is $|\psi_{\vec{J},m}\rangle\langle\psi_{\vec{J},m}|\vec{S}_0\rangle$.
Same zeroes as the Husimi distribution at point $\vec{S}_0$:

$$Hus_{\Psi}\left(\vec{S}\right) = \left|\langle\vec{S}_0|\psi_{\vec{J},m}\rangle\right|^2$$



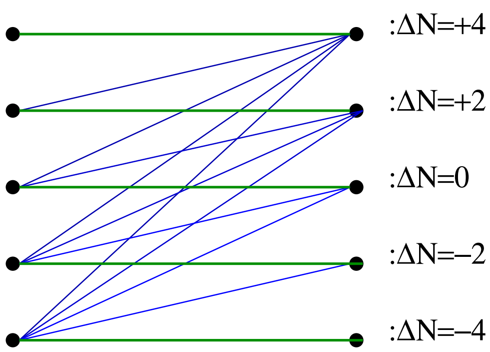
$$C_{Berry,m} = ((s-m) - (s+m))\, d = -\,(2m)\, d$$

Example: $s = 2$, $m = -2 \to +2$ so 5 bands,

$$\begin{array}{ll} d = 1, & C_{-2} = +4,\ \ C_{-1} = +2,\ \ C_0 = 0,\ \ C_1 = -2,\ \ C_2 = -4, \\ d = 2, & C_{-2} = +8,\ \ C_{-1} = +4,\ \ C_0 = 0,\ \ C_1 = -4,\ \ C_2 = -8, \end{array}$$

Remember in the *Quantum model* : $\mathcal{N}_m = (2j+1) - C_{Berry,m}$
So transition $d \to d+1$ gives a **redistribution of levels** $\Delta\mathcal{N}_m = 2m$**.**

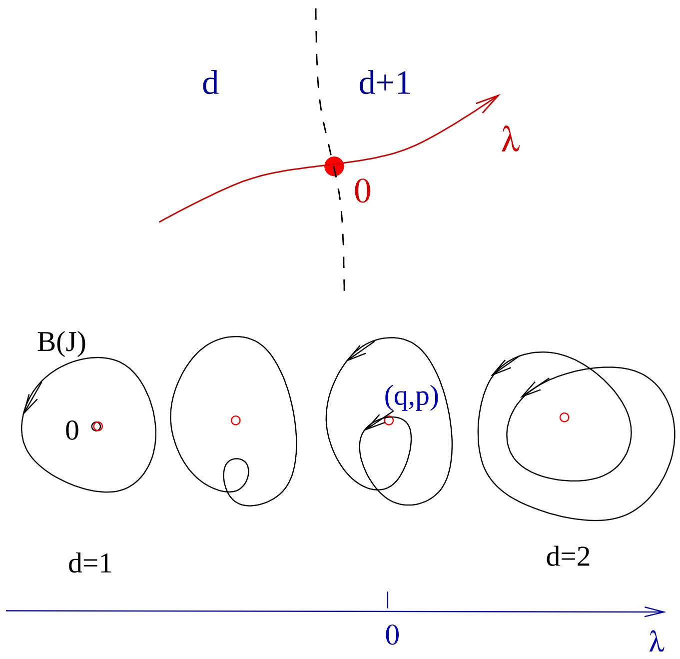
$$\Delta\mathcal{N}_{-2} = -4,\ \ \Delta\mathcal{N}_{-1} = -2,\ \ \Delta\mathcal{N}_0 = 0,\ \ \Delta\mathcal{N}_1 = +2,\ \ \Delta\mathcal{N}_2 = +4,$$



5.3 Relation with classical and quantum monodromy:

Local model at a transition between $\mathcal{C}_d$ and $\mathcal{C}_{d+1}$ Transition occurs if $\vec{B}\left(\vec{J}\right) \sim 0$, for $\vec{J} \simeq \vec{J}^*$.

(q,p) : local coordinates for $\vec{J} \in S_j^2$.



Generic local model in $\left(q, p, \vec{S}\right) \in \mathbb{R}^2 \times S_s^2$:

$$H_{loc}\left(q, p, \vec{S}\right) = qS_y + pS_x - \lambda S_z$$

Parameter space $(q, p, \lambda) \in \mathbb{R}^3$.
Singularity at $(0, 0, 0)$ gives:

$$\Delta C_{Hannay} = 2, \qquad \Delta C_{Berry,m} = -2m, \qquad \Delta \mathcal{N}_m = 2m$$

•For $s = 1/2$, already considered:

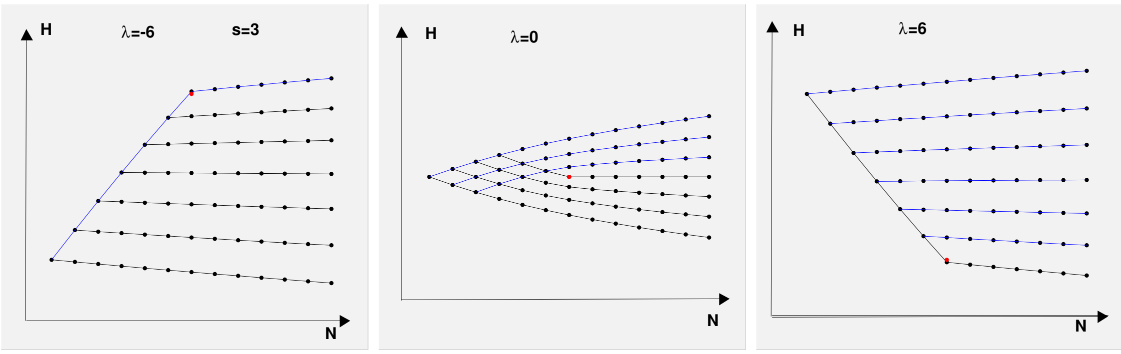
$$\hat{H}_{loc} = \begin{pmatrix} -\lambda & p + iq \\ p - iq & \lambda \end{pmatrix}$$

•This local model is **integrable**:

$$N = S_z + \frac{1}{2}\left(p^2 + q^2\right), \quad \{H_{loc}, N\} = 0$$

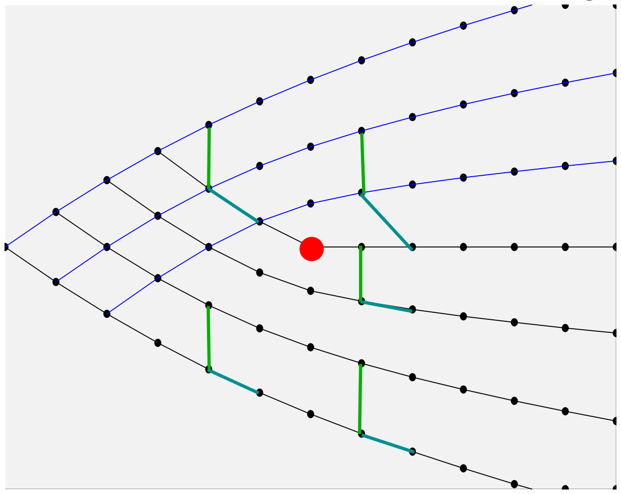
<u>This local integrable model has a generic (classical and quantum) monodromy defect</u>

Observed by D.A. Sadovskii,B.I. Zhilinskii, *"Monodromy, diabolic points, and angular momentum coupling"* Physics Letter A, **256**, p235 (1999).



See **Movie on web-page.**

Remark: generic only with the special assumption on Reeb graphs.



Monodromy matrix:

$$M = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \in SL(2, \mathbb{Z})$$

Remark: Monodromy is a generic event in integrable systems.

5.4 Classical Hannay connection; Semi-classical correspondence with Berry's connection

5.4.1 Classical Hannay connection

<u>**General SetUp:**</u>

- A ***fixed*** **Phase space** $p \in P_{fast}$.
- A **Parameter space** $x \in M$
- A **familly of Hamiltonian** H_x on P_{fast}, **Integrable** for any $x \in M$.
  We write (I_x, θ_x) local (x-dependent) **action-angle coordinates** on P_{fast}.

- **Adiabatic limit:** $x(\varepsilon t) \in M$ varies slowly, $\varepsilon \ll 1$.
  The **Classical Adiabatic theorem:** the trajectories follows tori with (approximatively) **constant action**.

Objective: explain the precise motion in the tori, in terms of a geometric Hannay connection.

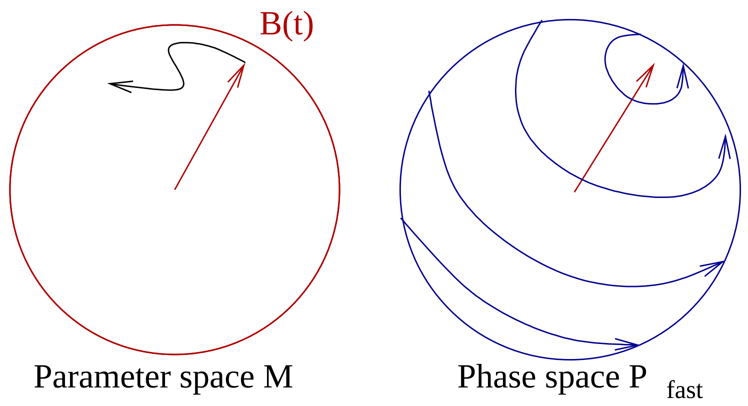
"Spin precession" example:
Hamiltonian on $P_{fast} = S_s^2$:

$$H_x\left(\vec{S}\right) = \vec{B}.\vec{S}$$

with **imposed Slow varying** "Parameter":

$$x(\varepsilon t) = \vec{B}(\varepsilon t) \in M = S^2, \quad \text{with } \varepsilon \ll 1$$

Tori trajectories are Circles around $\vec{B}$ on S_s^2.



Adiabatic Averaging method:
The evolution vector field on $M \times S_s^2$

$$V = (V_x, V_S) = \left(\frac{dx}{dt}, \frac{\partial H_x(\vec{S})}{\partial \vec{S}} \wedge \vec{S}\right) \in T\left(M \times S_s^2\right)$$

is **approximated by its averaged** over the motion of $\vec{S}$:

$$\begin{array}{rlll} \langle V \rangle_{fast} = \langle (V_x, V_S) \rangle_{fast} & = \langle (0, V_S) \rangle_{fast} & + \langle (V_x, 0) \rangle_{fast} \\ & = (0, V_S) & +V^{Hannay} \\ & \quad Dynamical & \quad Geometric \end{array}$$

decomposed

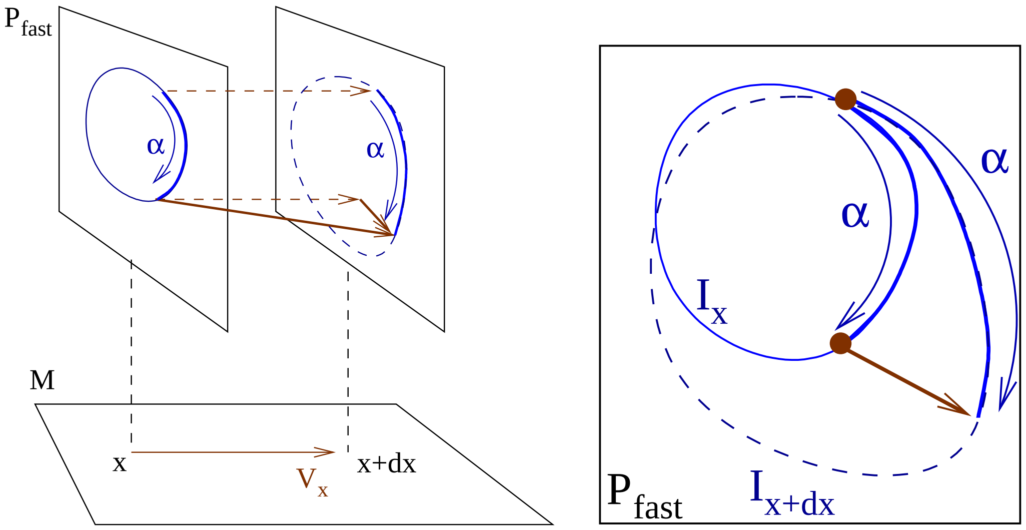
- in the **"trivial" "Dynamical"** fast motion (In Action-Angle coordinates, V_S : $\frac{dI}{dt} = 0$, $\frac{d\theta}{dt} = \omega(I) = \frac{\partial H}{\partial I}$).

- and the **Hannay Hamiltonian Vector field** V^{Hannay}**.**

More explicitly:

On S^2_s, define $R_{x,\alpha} : (I_x, \theta_x) \to (I_x, \theta_x + \alpha)$ the rotation by the same angle α on each Tori.

$$V^{Hannay} = \int_0^{2\pi} \left(\frac{d\alpha}{2\pi}\right) \frac{dR_{x,\alpha}}{dx} R^{-1}_{x,\alpha} V_x$$



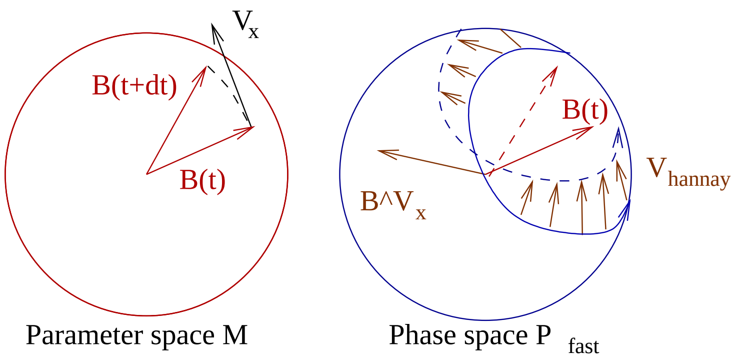
- $V^{Hannay} = \langle (V_x, 0) \rangle_{fast} = \left(\frac{dx}{dt}, V_S^{Hannay}\right)$ has component in $P_{fast} = S^2_s$

- Vector field V_S^{Hannay} is generated by a Hamiltonian K^{Hannay}_{x,V_x}.
  Hannay Hamiltonian function K^{Hannay} is a **one-form on** M **valued in Hamiltonian function** in P_{fast}.

It defines the **Hannay Connection** between tori, which connects tori with same actions "$I = \int pdq$".

Example of spin precession:

$$K^{Hannay}_{V_x} = \left(\vec{B} \wedge \vec{V_x}\right).\vec{S},$$



Hannay's curvature:
is the Hamiltonian vector field (valued two- form):

$$\Omega_{v_1,v_2}^{Hannay} = \left[V_{v_1}^{Hannay}, V_{v_2}^{Hannay}\right]$$

or Hamiltonian function (valued two- form):

$$H_{v_1,v_2}^{Hannay} = \left\{K_{v_1}^{Hannay}, K_{v_2}^{Hannay}\right\}$$

By construction, they preserve the Tori. The Hannay curvature is then just a shift angle Ω_θ^{Hannay} in each Tori:

$$\Omega_\theta^{Hannay} = \frac{\partial H^{Hannay}}{\partial I}$$

Example of spin precession:

$$H_{v_1,v_2}^{Hannay} = \left((\vec{v}_1 \wedge \vec{v}_2)\,.\vec{B}\right)\vec{B}.\vec{S} = \left((\vec{v}_1 \wedge \vec{v}_2)\,.\vec{B}\right)\, H_x\left(\vec{S}\right)$$

Remark: the Tori bundle has global topology: $C^{Hannay} = \int \Omega_\theta^{Hannay} = 2$

5.4.2 Semi-classical correspondence between Hannay and Berry's connection.

•Now $\hat{H}_x$ is the quantization of H_x, on fixed Hilbert space $\mathcal{H}$.
•The eigenspaces of $\hat{H}_x$ define a x-dependent decomposition of $\mathcal{H}$:

$$\mathcal{H} = \bigoplus_m \mathcal{H}_{m,x}, \quad \mathcal{H}_{m,x} = Im\left(\hat{P}_{x,m}\right), \qquad \hat{P}_{x,m} : projector$$

Where m is the quantum number of quantized Tori, with Action: $I_m = m\,h$.
•The quantization of $R_{x,\alpha}$ is the unitary operator:

$$\hat{R}_{x,\alpha} = \sum_m e^{-i\frac{I_m(\alpha/2\pi)}{\hbar}}\hat{P}_m = \sum_m e^{-im\alpha}\hat{P}_m$$

•The quantization of $K_{x,v}^{Hannay}$ is then

$$\hat{K}_{x,v}^{Hannay} = i\hbar\int \frac{d\alpha}{2\pi}\frac{d\hat{R}_{x,\alpha}}{dx}\hat{R}_{x,\alpha}^{-1}v$$

Property:

$$\boxed{\begin{array}{c}\hat{K}^{Hannay}_{x,v} = \hat{K}^{Berry}_{x,v} : \text{Hamiltonian connection} \\ \\ \hat{H}^{Hannay}_{x,v} = \hat{H}^{Berry}_{x,v} : \text{Hamiltonian curvature}\end{array}}$$

proof:

$$\begin{aligned}\frac{1}{i\hbar}\hat{K}^{Hannay}_{x,v} = \int \frac{d\alpha}{2\pi}\frac{d\hat{R}_{x,\alpha}}{dx}\hat{R}^{-1}_{x,\alpha}v &= \sum_{m,m'}\int \frac{d\alpha}{2\pi}e^{i(m-m')\alpha}\frac{d\hat{P}_{m'}}{dx}\hat{P}_m \\ &= \sum_m \frac{d\hat{P}_m}{dx}\hat{P}_m = \frac{1}{i\hbar}\hat{K}^{Berry}_{x,v}\end{aligned}$$

■

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Chapter 6

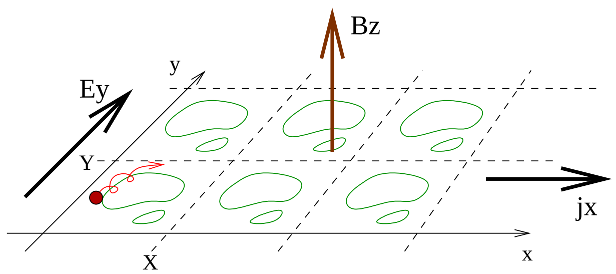
Topological Chern indices and the Integer Quantum Hall effect

6.1 Introduction

Non interacting bi-dimensional electrons in a ***Magnetic field*** B, in a periodic ***potential*** V,

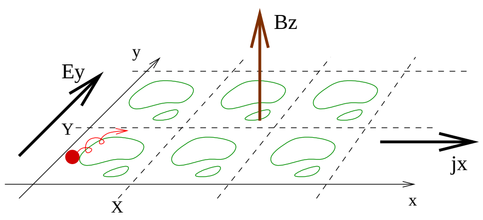
$$H(x, p_x, y, p_y) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + V(x, y), \qquad \vec{A} = \left(-\frac{1}{2}B\, y, \frac{1}{2}B\, x\right)$$

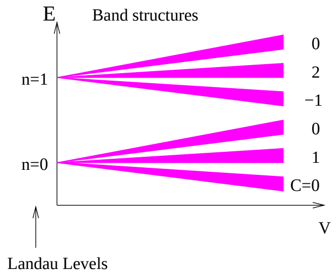
with a ***weak external electric field*** E.

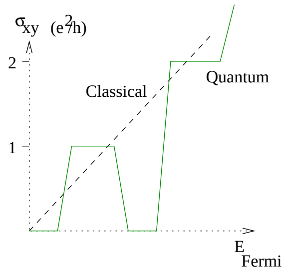


•**Motion of electrons;**
Slower motion of quasi-momentum over the Brillouin zone.

•**If** B **is strong** (not assumed for now)**: Fast Cyclotron motion** on circles; **Slower precession** of the circles;







Prop: (Thouless et al. 82)

$$\sigma_{xy} = \frac{j_x}{E_y} = \frac{e^2}{h} \sum_{\text{filled bands}} C_n, \qquad C_n \in \mathbb{Z}$$
$$h/e^2 = 25812.807\,\Omega$$

Observed by V.Klitzing et al. (1980).
Remarks:

- Recent experiments of Albrecht et al. (PRL **86**,147 2001) to observe Hofstader Spectrum.
- **Plateaux** are explains by intermediates localized states, due to **disorder**.
- **Strong** B is important: gives Landau gaps and plateaux.
- The **Fractionnal Quantum Hall** effect is related to **interactions** between electrons.

6.2 Band Spectrum and topology for the Quantum Hamiltonian

6.2.1 A dimensionless model

- We consider **non-interacting** electrons.
- Electron of mass m in plane (x, y) subject to a **bi-periodic potentiel** $V(x, y)$ (period X)
- a transverse **constant magnetic field** $\vec{B} = B\,\vec{e}_z$.
- The **classical phase space** is $T^*\mathbb{R}^2 \equiv \mathbb{R}^4$, with coordinates (x, p_x, y, p_y).

- The **Hamiltonian function** is:

$$H(x,p_x,y,p_y) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + V(x,y)$$

  with $\vec{B} = rot\left(\vec{A}\right) = (\partial_x A_y - \partial_y A_x)\,\vec{e}_z$.

- The **symetric Gauge** is the choice: $\vec{A} = \left(-\frac{1}{2}B\,y, \frac{1}{2}B\,x\right) = -\frac{1}{2}\vec{r}\wedge\vec{B}$, and gives:

$$H = \frac{1}{2m}\left(\left(p_x + \frac{eB}{2c}y\right)^2 + \left(p_y - \frac{eB}{2c}x\right)^2\right) + V(x,y)$$

- For the **quantum dynamics**, $\hat{x}, \hat{p}_x, \hat{y}, \hat{p}_y$ are operators ($[\hat{x}, \hat{p}_x] = i\hbar, \ldots$),

- The **Hilbert space** is

$$\mathcal{H}_{tot} = L^2\left(\mathbb{R}^2\right) = \mathcal{H}_x \otimes \mathcal{H}_y$$

  and the **Schrodinger equation** reads:

$$i\hbar\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

  with Hamiltonian operator $\hat{H}$ obtained by quantization of H.

- Consider canonical linear transformation, with new **dimensionless "fast and slow" variables** (and idem for quantum operators):

$$X_{fast} = \begin{cases} x_f = \frac{\sqrt{S}}{\hbar}p_x + \frac{1}{2\sqrt{S}}y \\ p_f = \frac{\sqrt{S}}{\hbar}p_y - \frac{1}{2\sqrt{S}}x \end{cases}$$

$$X_{slow} = \begin{cases} x_s = \frac{S}{\hbar X}p_x - \frac{1}{2Y}y \\ p_s = -\frac{S}{\hbar X}p_y - \frac{1}{2X}x \end{cases}$$

with the **quanta of surface**:

$$S = \frac{hc}{eB}$$

One can check that indeed:

$$[\hat{x}_f, \hat{p}_f] = i, \qquad [\hat{x}_s, \hat{p}_s] = i\,h_{eff}$$

(and other commutators are zero).
with the dimensionless parameter **"effective Planck constant"**:

$$h_{eff} = \frac{S}{X^2} \text{ : inverse of number of quanta flux per cell}$$

$$h_{eff} \to 0 \quad \text{is the adiabatic limit } (not\, assumed\, yet)$$

Define the **dimensionless time**

$$\tilde{t} = \omega t$$

with the **cyclotron frequency**

$$\omega = \frac{eB}{mc}.$$

and the **dimensionless Hamiltonian and potential**

$$\tilde{H} = \frac{1}{\hbar\omega} H, \quad \tilde{V}(a,b) = \frac{1}{\hbar\omega} V(-Xa, -Xb)$$

Then the **Schrödinger equation** reads:

$$i\frac{d|\psi\rangle}{d\tilde{t}} = \hat{\tilde{H}}|\psi\rangle, \qquad \text{in } \mathcal{H}_{tot} = L^2(\mathbb{R}_{slow}) \otimes L^2(\mathbb{R}_{fast}) = \mathcal{H}_{slow} \otimes \mathcal{H}_{fast}$$

and

$$\boxed{\tilde{H}(X_s, X_f) = \frac{1}{2}\left(p_f^2 + x_f^2\right) + \tilde{V}\left(p_s + \sqrt{h_{eff}} p_f\,,\, x_s + \sqrt{h_{eff}} x_f\right)}$$

Remark that $\tilde{H}(X_s, X_f)$ is **bi-periodic** w.r.t. $X_s = (x_s, p_s)$.
We write now:

$$h = h_{eff}$$

6.2.2 Band Spectrum and topological Chern indices

Translation operators in $L^2(\mathbb{R}_{slow})$

$$\begin{aligned}(\hat{T}_x\psi)(x_s) &= \psi(x_s - 1)\\ (\hat{T}_p\tilde{\psi})(p_s) &= \tilde{\psi}(p_s - 1): \quad \text{(Fourier)}\end{aligned}$$

$$\hat{T}_x = \exp(-i\hat{p}_s/\hbar), \quad \hat{T}_p = \exp(i\hat{x}_s/\hbar).$$

From **periodicity** of $\hat{H}$:

$$[\hat{H}, \hat{T}_x] = [\hat{H}, \hat{T}_p] = 0.$$

but:

$$\hat{T}_x\hat{T}_p = e^{-i/\hbar}\hat{T}_p\hat{T}_x,$$

So if

$$N = \frac{1}{2\pi\hbar} \in \mathbb{N}^*.$$

then

$$[\hat{T}_x, \hat{T}_p] = 0 : \qquad \textbf{Hypothesis}$$

Remark:

$$N = \frac{1}{2\pi\hbar} \to \infty \quad : \quad \text{Semi} - \text{classical limit (and adiabatic limit)}$$

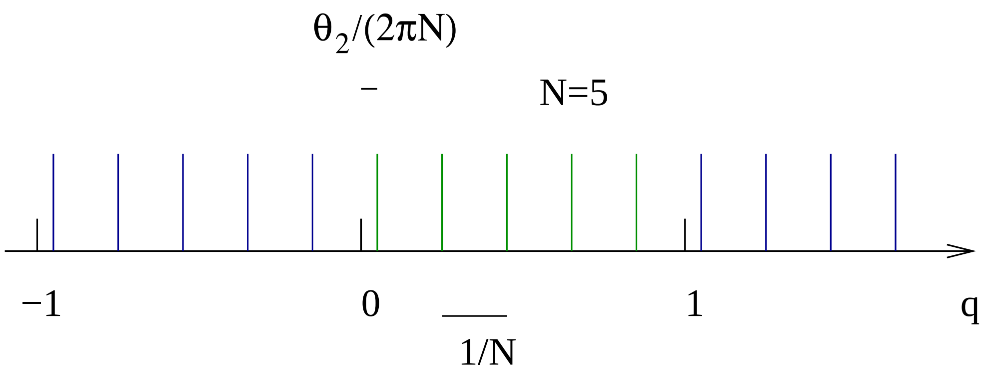
(if $\frac{1}{2\pi\hbar} = \frac{A}{B} \in \mathbb{Q}$, consider $\hat{T}_x = \exp(-iB\hat{p}_s/\hbar_{eff})$, then $[\hat{T}_x, \hat{T}_p] = 0$).

6.2.3 Decomposition of $L^2(\mathbb{R}_{slow})$ in eigenspaces of $\hat{T}_x$ and $\hat{T}_p$:

$\mathcal{H}_{Tore}(\theta_1, \theta_2) = \left\{ |\psi> \text{ such that } \begin{cases} \hat{T}_x|\psi >= \exp(i\theta_1)|\psi > \\ \hat{T}_p|\psi >= \exp(i\theta_2)|\psi > \end{cases} \right\}$, $L^2(\mathbb{R}_{slow}) = \int\int \mathcal{H}_{Tore}(\theta_1, \theta_2) \, \frac{d\theta_1 d\theta_2}{(2\pi)^2}$

$\vec{\theta} = (\theta_1, \theta_2) \in \mathcal{T}_\theta$ are Bloch Parameters

$\tilde{\psi}(p_s)$ is 1-périodique so $\psi(x_s)$ is $(h = 1/N)$-discrete, and also 1-periodic.



A basis of $\mathcal{H}_{Tore}(\theta_1, \theta_2)$ is then:

$$|j, \vec{\theta} >\equiv \psi_{j,\vec{\theta}}(x) = \frac{1}{\sqrt{N}} \sum_{n_1 \in \mathbb{Z}} \exp(-in_1\theta_1)\, \delta(x - q_j - n_1), \quad j = 1, \dots, N$$

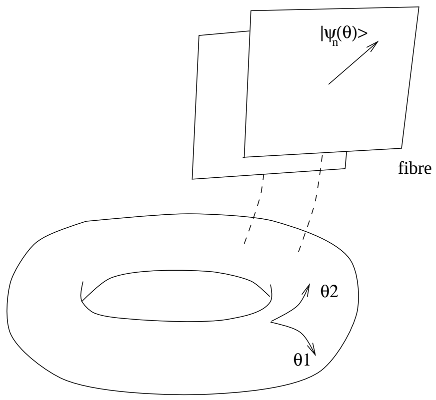
$$\text{with } q_j = \frac{1}{N}\left(j + \frac{\theta_2}{2\pi}\right).$$

So

$$\dim_{\mathbb{C}} \ \mathcal{H}_{Tore}(\theta_1, \theta_2) = N.$$

Band spectrum of $\hat{H}$ in $\mathcal{H}_{Tore}(\theta_1, \theta_2) \otimes L^2(\mathbb{R}_{fast})$:

$$\hat{H}|\varphi_n(\theta_1, \theta_2) >= E_n(\theta_1, \theta_2)|\varphi_n(\theta_1, \theta_2) >, \quad n \in \mathbb{N}.$$



6.2.4 Topological indices of the bands

Suppose that $E_n(\theta_1, \theta_2)$ is **isolated eigenvalue** $\forall\theta$. (true for generic $\hat{H}$).

The eigenspaces define **Complex line bundle**s:

$$F_n \to \mathcal{T}_\theta$$

With topology characterized by **Chern index**:

$$C_n \in \mathbb{Z} \quad : \text{ Chern index of band } n$$

(Formula to compute C_n below).

6.3 Interpretation of the Topological Chern indices: the Quantized Hall conductivity

The usual proof of

$$\sigma_{xy} = \frac{j_x}{E_y} = \frac{e^2}{h} \sum_{\text{filled bands}} C_n$$

uses Kubo formula.

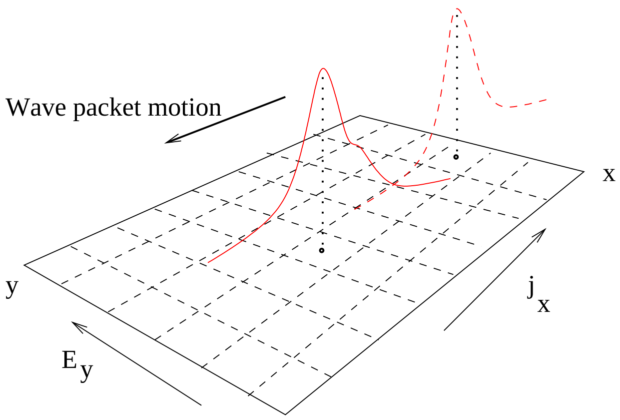
We present an equivalent but more **"dynamical"** proof, which relates C_n with the **adiabatic transport of a wave packet**.

6.3.1 Delocalized Bloch waves and Localized Wannier waves

In a fixed band n, consider a C^∞ section $|\psi\rangle$ of the vector bundle $F_n \to \mathcal{T}_\theta$:

$$|\psi>= \int\int d\theta_1 d\theta_2 |\psi(\theta_1, \theta_2)>, \qquad |\psi(\theta_1, \theta_2)>\in \mathcal{H}_{tore}\,(\theta)$$

Each state $|\psi\,(\theta)\rangle \in \mathcal{H}_{tore}\,(\theta)$ is a **delocalized Bloch wave**,
but $|\psi>\in L^2\,(\mathbb{R}^2)$ is a **localized Wannier wave**.



Consider the **translated localized Wannier state**

$$|\psi_{n_1,n_2}>= T_x^{n_1} T_p^{n_2} |\psi>= \int\int d\theta_1 d\theta_2 e^{in_1\theta_1+in_2\theta_2} |\psi(\theta_1,\theta_2)> .$$

Conversely:

$$|\psi(\theta_1,\theta_2)>= \sum_{n_1,n_2\in\mathbb{Z}^2} e^{-in_1\theta_1-in_2\theta_2} |\psi_{n_1,n_2}> .$$

Generalization: if

$$|\phi>= \int\int d\theta_1 d\theta_2 e^{if(\theta_1,\theta_2)} |\psi(\theta_1,\theta_2)>,$$

with any function f such that:

$$f(\theta_1+2\pi,\theta_2) = f(\theta_1,\theta_2) + N_1 2\pi$$
$$f(\theta_1,\theta_2+2\pi) = f(\theta_1,\theta_2) + N_2 2\pi,$$

(Integers $N_1, N_2 \in \mathbb{Z}$ characterize the homotopy type of f)

Define the **mean position** of $|\phi\rangle$ on the plane by:

$$< n_1 >= \sum_{n_1,n_2} n_1 . \left|< \psi_{n_1,n_2}|\phi >\right|^2$$
$$< n_2 >= \sum_{n_1,n_2} n_2 . \left|< \psi_{n_1,n_2}|\phi >\right|^2 ,$$

Then:

$$< n_1 >= N_1, \qquad < n_2 >= N_2,$$

So the **mean position of $|\phi>$ is "quantized".**

(This is a simple property of Fourier Series: if $g(\theta) = \sum_n c_n e^{in\theta} = e^{if(\theta)}$ with $f(2\pi) = f(0) + N2\pi$ then $\sum_n n|c_n|^2 =< g|\hat{p}_\theta|g >= \frac{1}{2\pi}\int_0^{2\pi} f' d\theta = N$, with courant operator $\hat{p}_\theta = \frac{1}{i} d/d\theta$.).

6.3.2 Physical consequence on temporal evolution

$$|\psi(t)>= e^{-i\hat{H}t/\hbar}|\psi_{0,0}>= \int\int d\theta_1 d\theta_2 e^{-iE(\theta_1,\theta_2)t/\hbar}|\psi(\theta_1,\theta_2)> .$$

has a "dynamical" phase $f(\theta_1,\theta_2) = -E(\theta_1,\theta_2)t/\hbar$ with homotopy type $N_1 = N_2 = 0$.

So $|\psi(t)>$ spreads on the plane, but its mean position $< n_1 >,< n_2 >$ is zero.

6.3.3 Addition of a weak external electric field $\vec{E} = \frac{\partial U}{\partial \vec{r}} = E_y \vec{u}_y$

Potential energy $\mathcal{E} = -eU(\vec{r})$, gives **a slow motion of the quasi-impulsion** $\vec{k}(t) = \hbar\vec{\theta}(t)/X$:

$$\frac{d\vec{k}}{dt} = -\frac{\partial \mathcal{E}}{\partial \vec{r}} = e\vec{E} = eE_y \vec{u}_y$$

gives

$$\theta_1(t) = \theta_1(0)$$
$$\theta_2(t) = -\omega t \qquad \text{with } \omega = eE_y X/\hbar$$

Then each Bloch state $|\psi(\vec{\theta}(t))\rangle$ **follows Berry's connection** plus **Dynamical phase** in the fibers.

After one period $T = 2\pi/\omega$,

$$e^{-i\hat{H}T/\hbar}|\psi(\theta_1,\theta_2)>= \exp\left(i\phi_D(\theta_1,\theta_2) + i\phi_B(\theta_2)\right)|\psi(\theta_1,\theta_2)>,$$

with **dynamical phase** $\phi_D(\theta_1,\theta_2)$ with homotopy $N_1 = N_2 = 0$

and **Berry's phase** $\phi_B(\theta_1,\theta_2)$ of the path $\theta_2(t)$, which is homotopic to $\phi_B(\theta_1) \equiv 2\pi C\theta_1$, so $N_1 = C$, $N_2 = 0$.

(Exponentially small "Landau-Zener" corrections).

Consequence:

after one period T, **the mean position has shifted** by **integer** number of cells

$$\delta < n_1 >= C, \qquad \delta < n_2 >= 0$$

The mean velocity of the electron is then:

$$V_x = \frac{\delta < n_1 > X}{T} = \frac{CX}{T}$$

If the band is filled by electrons, the density is one electron per cell: $\rho = 1/X^2$.

The current density is then

$$j_x = \rho e V_x = \frac{e^2}{h} C\, E_y$$

So

$$\sigma_{xy} = \frac{j_x}{E_y} = \frac{e^2}{h} C$$

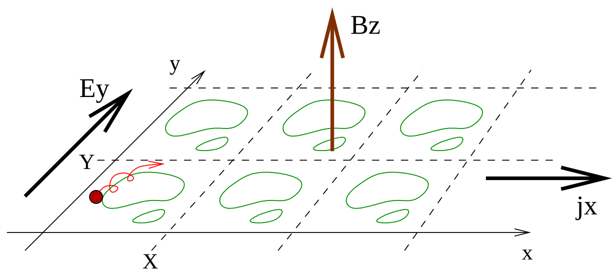
■

6.4 Born-Oppenheimer Approximation with Strong Magnetic field; Effective dynamics in a Landau Level

- With no hypothesis on B, the dynamics of electrons **has two degrees of freedom:** not integrable.
- Suppose now the **adiabatic limit:**

$$h_{eff} = \frac{hc}{eBX^2} \ll 1$$

Then the classical electron has a **fast cyclotron rotation**, and a **slower precession** of these circles.



Born-Oppenheimer description:
We treat $X_{slow} = (x_s, p_s)$ as **fixed classical parameters**,
$\hat{X}_{fast} = (\hat{x}_f, \hat{p}_f)$ as **quantum operators**, and consider the spectrum of:

$$X_s \to \hat{H}_{X_s} = \tilde{H}\left(X_s, \hat{X}_f\right)$$

it gives a **discrete spectrum** (fast motion):

$$E_1(X_s), \ldots, E_m(X_s), \ldots : \quad \text{Landau Levels}$$

The slow dynamics (precession of circles) **in Landau Level** m is described by the **effective bi-periodic Hamiltonian**:

$$H_{m,eff}(x_s, p_s) = E_m(x_s, p_s), \qquad X_{slow} = (x_s, p_s) \in T^2_{slow}$$

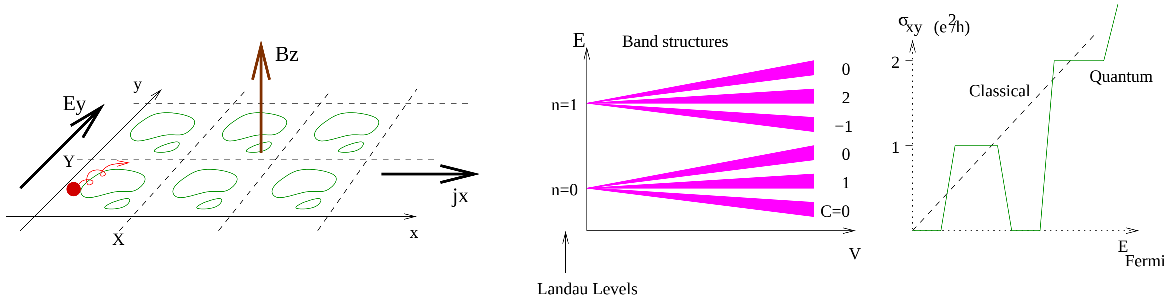
Below, we consider a **fixed Landau Level**, and write:

$$\boxed{H(q,p) = H_{m,eff}(q,p), \qquad m\,\text{fixed}}$$

which is an effective **Bi-periodic** Hamiltonian on $\mathbb{R}^2$:

$$H(q,p) = H(q+1,p) = H(q,p+1) \simeq V(q,p)$$

Remark: no degeneracies between lnadau Bands: $E_m(X_s) < E_{m+1}(X_s)$.
So the quantized operator$\hat{H} = H(\hat{q},\hat{p})$ acts in a space $\mathcal{H}_N(\theta)$ with **dimension** N**.**
The Landau Level m **has** N **subbands,** $n = 1 \rightarrow N$, which Chern indices C_n.



6.4.1 Formula for Chern indices C_n:

1) Integral curvature:

$$C_n = \frac{i}{2\pi}\int_{T_\theta} \mathrm{Tr}\left(P_n\left[\frac{\partial P_n}{\partial\theta_1},\frac{\partial P_n}{\partial\theta_2}\right]P_n\right)d\theta_2 d\theta_2 \qquad , \quad P_n = |\varphi_n(\theta)\rangle\langle\varphi_n(\theta)|$$

$$= \frac{i}{2\pi}\int_{T_\theta}\left(<\partial_{\theta_1}\varphi_n|\partial_{\theta_2}\varphi_n> - <\partial_{\theta_2}\varphi_n|\partial_{\theta_1}\varphi_n>\right)d\theta_2 d\theta_2$$

2) From the zeros of a global section $P_n|z_0\rangle = |\varphi_n(\theta)\rangle\langle\varphi_n(\theta)|z_0\rangle$, with a fixed coherent state $|z_0\rangle$, $z_0 \in T_{qp}$.
So from the zeros of Bargmann or Husimi functions $b_{\varphi(\theta)}(z_0) = \langle z_0|\varphi_n(\theta)\rangle$:

$$C_n = \sum_{\theta \text{ tq } b_{\varphi(\theta)}(z_0)=0} (\pm 1),$$

with sign ± 1 depending on orientation of the zero.

6.4.2 Sum of Chern indices in a Landau Level

$$\boxed{\sum_{n=1}^{N} C_n = c_1(F_1 \oplus \ldots \oplus F_N) = c_1(\mathcal{H}_{tore}) = +1}$$

Which means that the rank N **vector bundle** $\mathcal{H}_{tore} \rightarrow \mathcal{T}_\theta$ **is non trivial**.

This formula gives the Classical Hall conductivity in the semi-classical limit.

Five Different Proofs:

Proof 1: We saw a basis of $\mathcal{H}_{tore}(\theta)$, with states $|j,\theta\rangle$, $j = 1 \rightarrow N$.

This gives a trivialization of the bundle $\mathcal{H}_{tore} \rightarrow \mathcal{T}_\theta$ over $\theta_1 \in [0, 2\pi[$, $\theta_2 \in]0, 2\pi[$, with transition function at $\theta_2 \equiv 0$:

$$T(\theta_1) = \begin{pmatrix} 0 & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ e^{i\theta_1} & & & 0 \end{pmatrix}$$

Remark that $c_1(\mathcal{H}_{tore}) = c_1(det(\mathcal{H}_{tore}))$ (from $c_1(L_1 \otimes \ldots \otimes L_N) = c_1(L_1 \oplus \ldots \oplus L_N)$), and the line bundle $det(\mathcal{H}_{tore})$ has transition function $det(T(\theta_1)) = e^{i\theta_1}$.

We deduce that $c_1(\mathcal{H}_{tore}) = c_1(det(\mathcal{H}_{tore})) = +1$. ■

Proof 2: Consider $E = Vect(|0>, \ldots, |N>) \subset \mathcal{H}_{plan}$ a fixed space of dimension $N+1$, spanned by $N+1$ first states of Harmonic oscillator. Consider the orthogonal projection: $P_\theta : \ \mathcal{H}_{tore}(\theta) \rightarrow E$.

One shows that P_θ is into, so the rank N vector bundle $\mathcal{H}_{tore}(\theta) \rightarrow \mathcal{T}_\theta$ is realized as a subbundle of the rank $N+1$ trivial bundle: $E \rightarrow \mathcal{T}_\theta$.

Its orthogonal is a rank 1 bundle $L \rightarrow \mathcal{T}_\theta$ (i.e. $L_\theta \oplus \mathcal{H}_{tore}(\theta) = E$), and we calculate its Chern index with the zeros of a global section. One find $c_1(L) = -1$. So $c_1(\mathcal{H}_{tore}) = c_1(E) - c_1(L) = 0 + 1 = +1$.

Proof 3: There is a more standard presentation of $\mathcal{H}_{tore}(\theta)$ as the space of Holomorphic sections of a line bundle over $\mathcal{T}_{qp}$. The space $\mathcal{T}_\theta$ is the Jacobi variety and $\sum_n C_n = 1$ results from the Abel inversion theorem.

Proof 4: By computation, from integral curvature formula.

Proof 5: By semi-classical analysis, from the topology of the classical Reeb Graph. see below.

6.5 Semi-classical calculation of Chern indices in a Landau Level

(Generalization of the T.K.N.N. calculation)

$H(q,p)$ is bi-periodic on $(q,p) \in \mathbb{R}^2$:

$$H(q,p) = \sum_{n_1, n_2 \in \mathbb{Z}^2} c_{n_1,n_2} \exp(i2\pi n_1 q) \exp(i2\pi n_2 p).$$

$$c_{n_1,n_2} = \bar{c}_{-n_1,-n_2} \in \mathbb{C}, \quad (n_1, n_2) \in \mathbb{Z} : \text{ Fourier coeficients}$$

Hilbert space of the plane:

$$\mathcal{H}_{Plan} = L^2(\mathbb{R}_{slow}),$$

Quantization of $H(q,p)$:

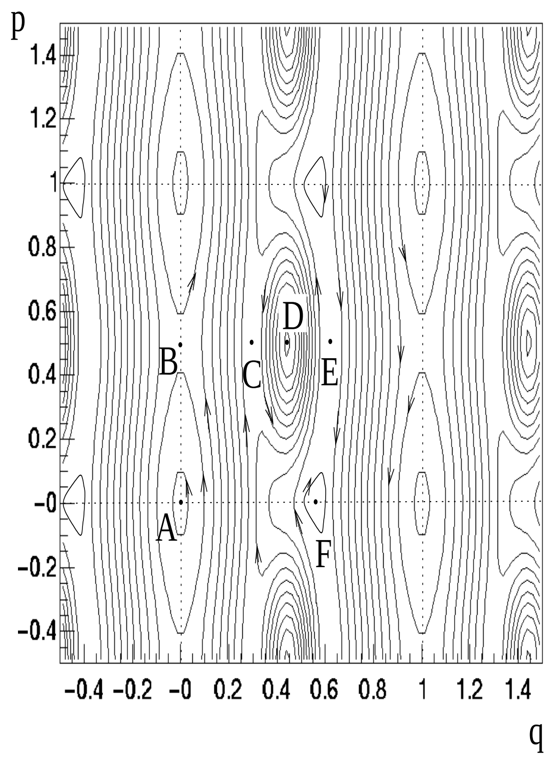
$$\hat{H} = \sum_{n_1,n_2 \in Z^2} \frac{1}{2} c_{n_1,n_2} \exp\left(i2\pi n_1 \hat{q}\right) \exp\left(i2\pi n_2 \hat{p}\right) + \text{hermitian conjugate.}$$

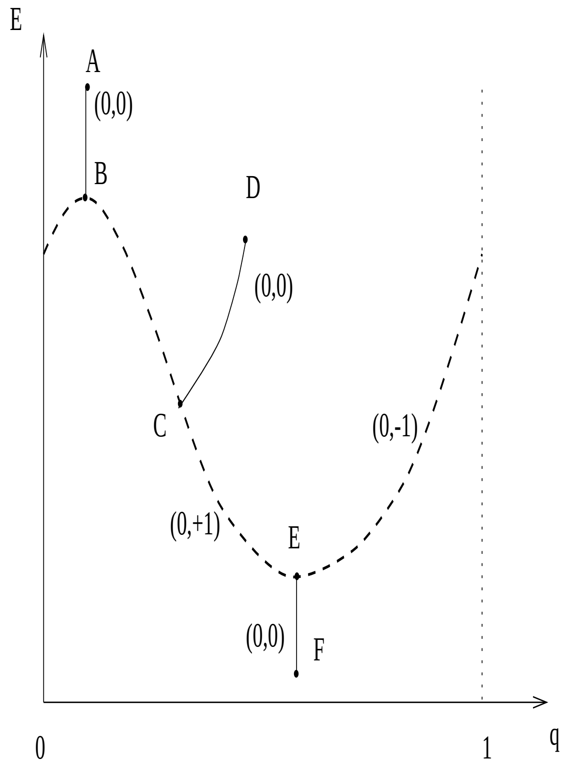
6.5.1 Classical Hamiltonian and trajectories of $H(q,p)$

Example :

$$H(q,p) = H_0(q,p) + H_1(q,p),$$
$$H_0(q,p) = \cos(2\pi q) + 0.1\cos(2\pi p),$$
$$H_1(q,p) = P\left[\exp\left(-100(q-q_0)^2 - 10(p-p_0)^2\right)\right], \quad q_0 = 0.45 \quad p_0 = 0.5$$

(operator P makes periodic on the plane).





Question : Understand the values of Chern indices C_n from the classical trajectories, or Reeb Graph ?

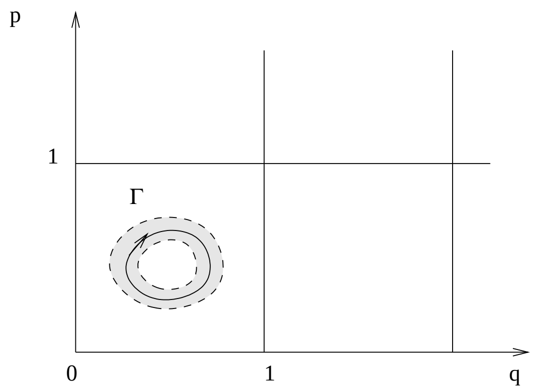
Solution :

the classical dynamics is integrable, so **stationnary states are approximated by quasi-modes** (WKB approach) :

$$|\tilde{\psi}_n(\theta_1, \theta_2) > \simeq |\varphi_n(\theta_1, \theta_2) >$$

We just have to study the dependence of the quasi-modes with (θ_1, θ_2).

6.5.2 Quasi-modes : Quasi-mode on a contractible trajectory of type $(0, 0)$:

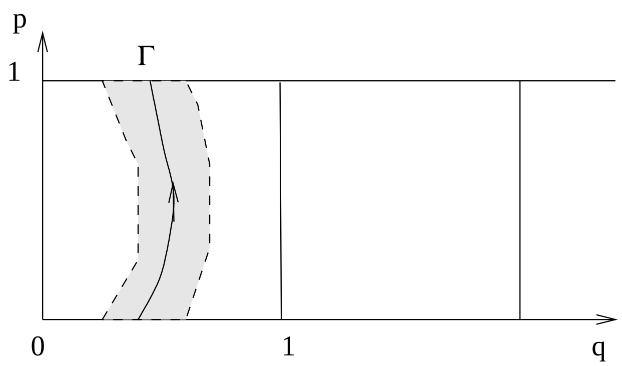


Energy $\tilde{E}$ **:**

$$S(\tilde{E}) = (k + 1/2)h + o(h), \quad k \in \mathbb{Z}$$

$$with\ S(\tilde{E})\ :\ \text{enclosed surface}$$

Remark : $\tilde{E}$ does not depend on (θ_1, θ_2).
Quasi-mode on a non-contractible trajectory of type $(0, \pm 1)$:



Energy $\tilde{E}(\theta_2)$ **:**

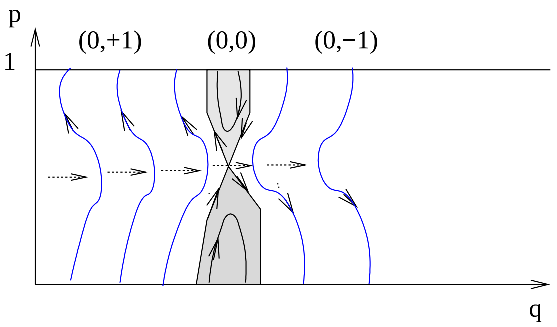
$$S(\tilde{E}) = (k - \theta_2/2\pi)h + o(h), \quad k \in \mathbb{Z}, \quad \text{with } S(\tilde{E}) \quad : \text{right side surface}$$

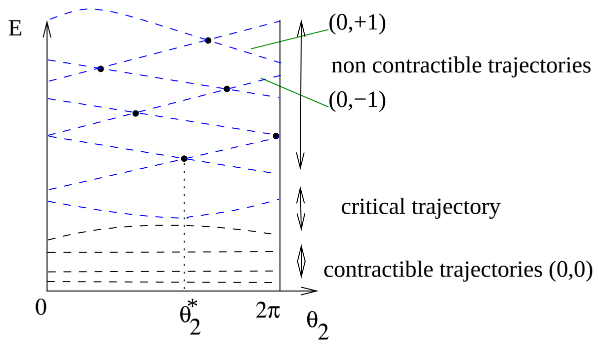
proof :

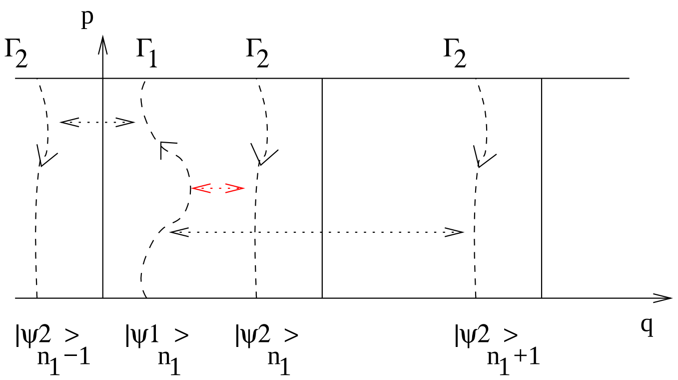
after one period on trajectory $q(t), p(t)$ the phase is $\varphi = -\int_\Gamma q dp/\hbar = S/\hbar$, and periodicity condition is $\varphi = \theta_2 \quad [2\pi]$.■.

Remark : $\tilde{E}(\theta_2)$ and the support $\Gamma(\theta_2)$ depend on θ_2.

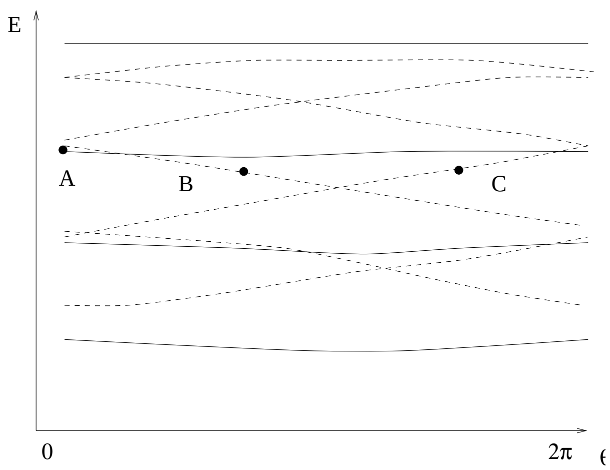
6.5.3 Semi-classical spectrum and tunnelling effect :





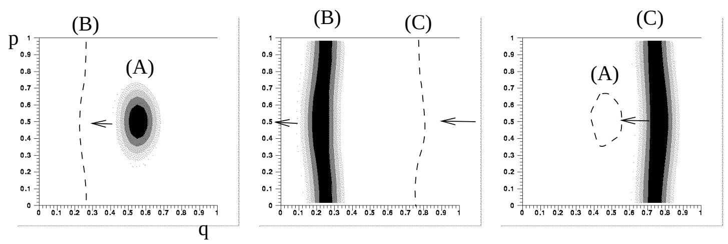


Numerical spectrum :



Above example, with $N = 11$, band $n = 6$:

$C_{1\to4}$	C_5	C_6	C_7	$C_{8\to11}$
0	$+1$	-1	$+1$	0



6.5.4 General result :

Consider the support of the quasi-mode of band n :

$$S_n : \quad \theta_2 \in \mathbb{R} \to \mathrm{Supp}\,(|\psi_n(\theta_2)>)\,.$$

With homotopy $I_n = I(S_n) \in \mathbb{Z}$:

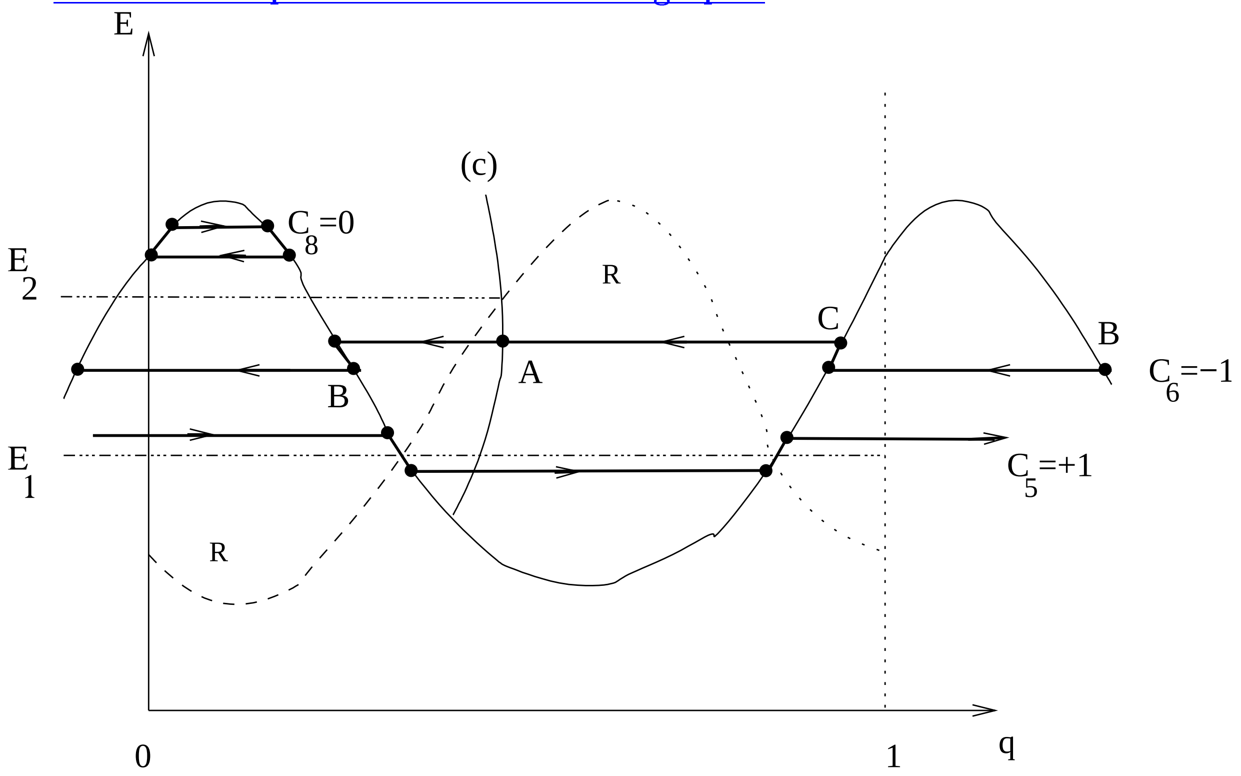
$$T_Q^{I_n}\,[\mathrm{Supp}\,(|\psi_n(0)>)] = [\mathrm{Supp}\,(|\psi_n(2\pi)>)]\,.$$

Theorem :

$$\boxed{C_n = I(S_n)}$$

proof : uses zeros of Husimi function.

Practical computation from the Reeb graph :

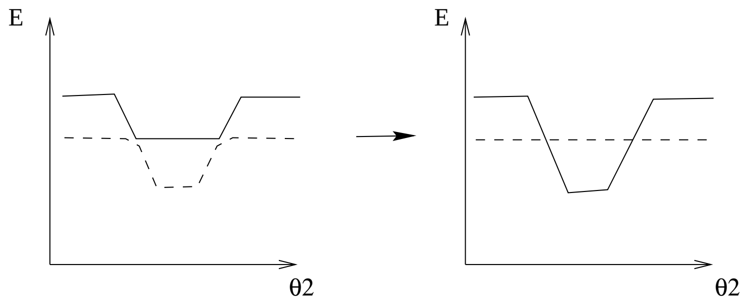


6.5.5 Total Chern index :

In order to recover :

$$\sum_{n=1}^{N} C_n = +1$$

First define $(S_n + S_{n+1})$ by removing the jumps (does not change the homotopy) :

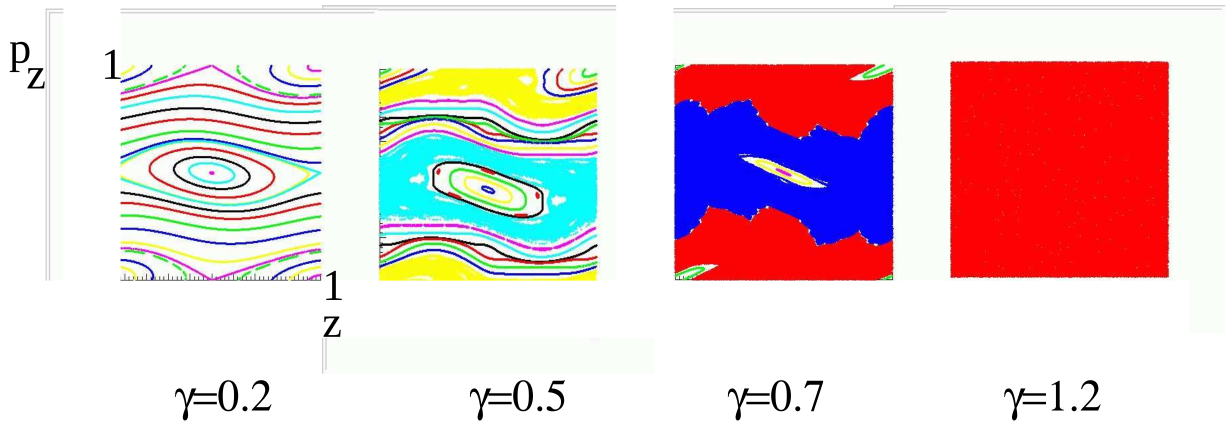


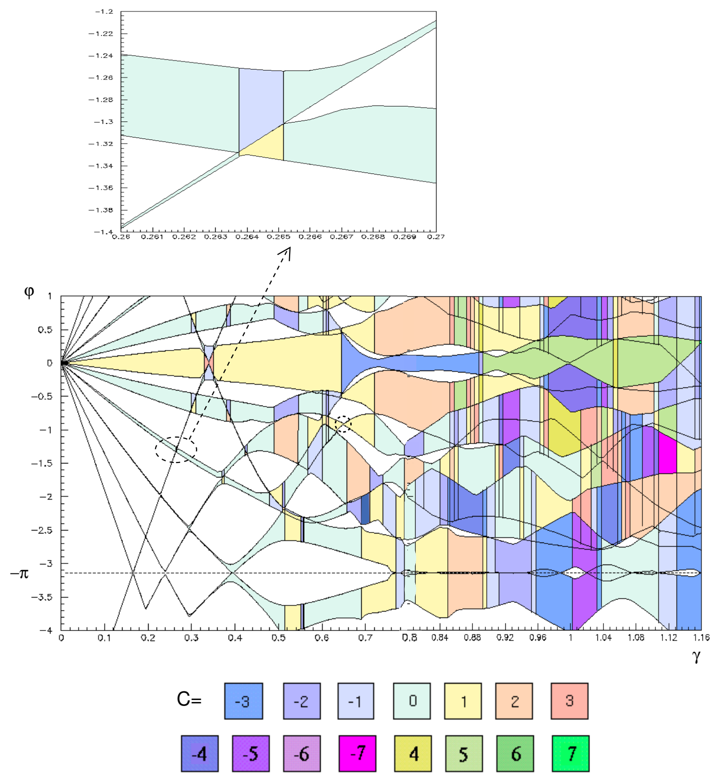
Then

$$\sum_{n=1}^{N} C_n = \sum_{n=1}^{N} I(S_n) = I\left(\sum_{n=1}^{N} S_n\right) = +1.$$

6.5.6 The Chern indices for a chaotic dynamics :

There are no more nice WKB quasi-modes.
Numerical results, in the Kicked Harper model : (time-dependent model, parameter γ)
Poincaré sections :





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