Some Geometrical / topological aspects of **slow / fast coupled** dynamical systems in **quantum / classical** dynamics.

1) Introduction

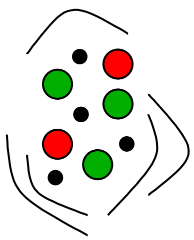
A small molecule:

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 ($\tau_{rot} \simeq 10^{-10} \to 10^{-12} s.$).

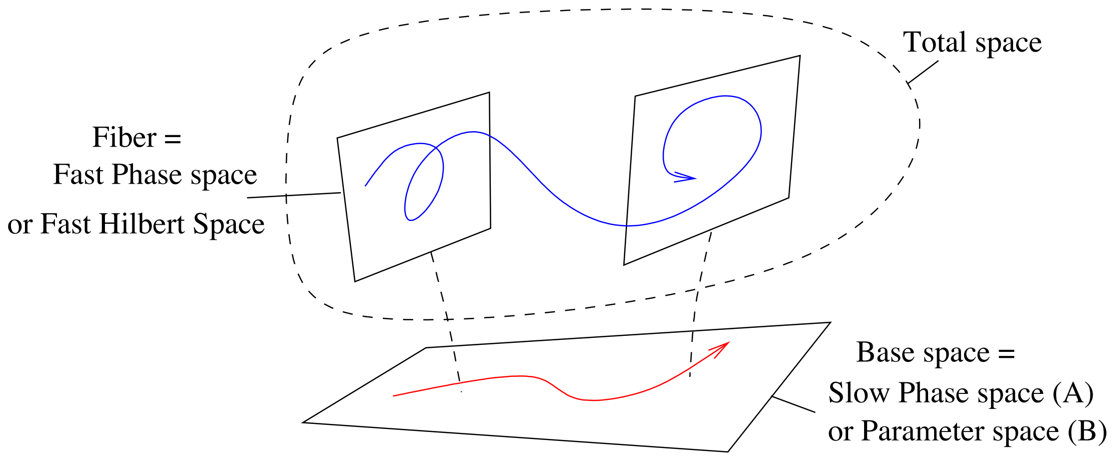


Characteristics:

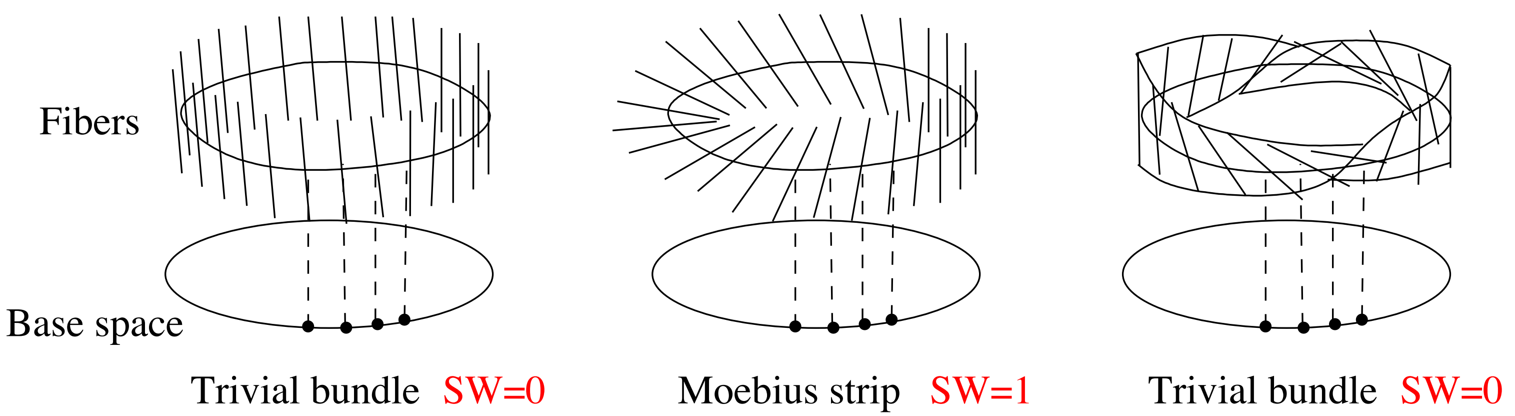
- **Fast-Slow coupled, quantum, Hamiltonian** system with **finite number of degree of freedom.**
- We will be concerned with **Topological** properties of the spectrum, (crude properties but robust against perturbations).
  Collaboration with Boris Zhilinskii (Dunkerque).

Geometrical and topological aspects:

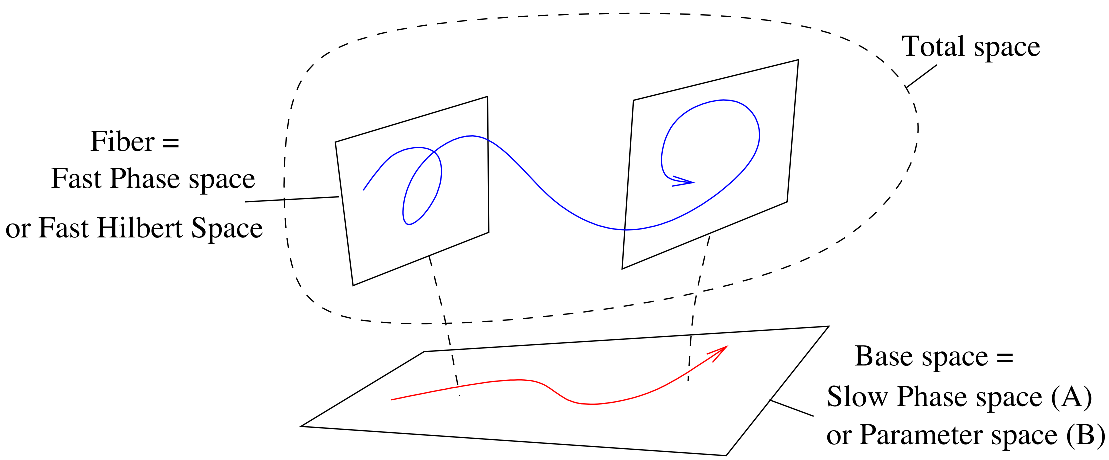
They concern **fiber bundles** with **connections** which naturally occur in the previous situations.

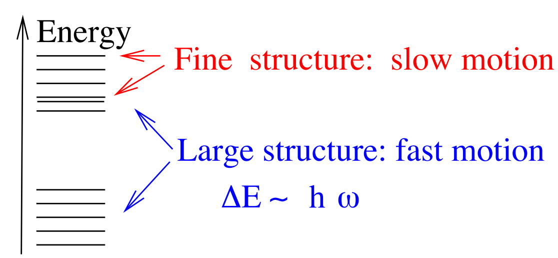


Topology of the bundle due to possible twists:



Slow \ Fast	Classical, Integrable in P_{Fast}	Quantum in $\mathcal{H}_{Fast}$
Classical in P_{Slow}	(***Classical***) Function $H_{tot}(X_{slow}, X_{fast})$ *Topology of tori bundle* Hannay's connection	(***Semi-Quantum***) Matrix Symbol $X_{slow} \to \hat{H}_{fast}(X_{slow})$ *Topology of eigenstates bundle* Berry's connection
Quantum in $\mathcal{H}_{Slow}$	No meaning (?)	(***Quantum***) $\hat{H}_{tot}$ in $\mathcal{H}_{slow} \otimes \mathcal{H}_{fast}$ *Number of states in group of levels* Density of states





Contents

- Correspondances between the semi-quantum and quantum description:
  - Slow motion on S^2: rotation coupled with fast fibrations.
    Line bundles with C_1 Chern index.
  - Slow motion on $\mathbb{CP}^2$: degenerate vibrations coupled with fast electronic motion.
    Vector bundles with C_1, C_2 Chern indices.
    Non-decomposable vector bundles. The index formula.
- Correspondances between the classical and semi-quantum description:
  Monodromy and bifurcation of eigenstate bundles.

References

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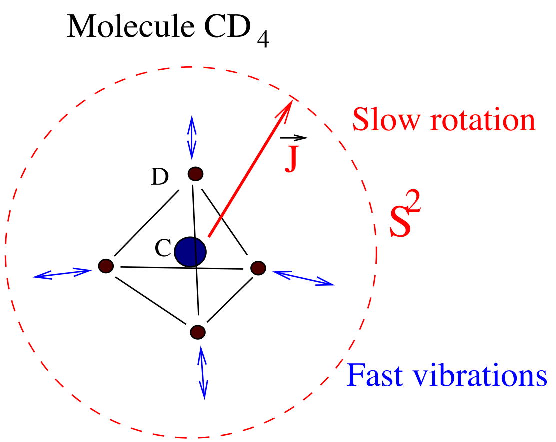
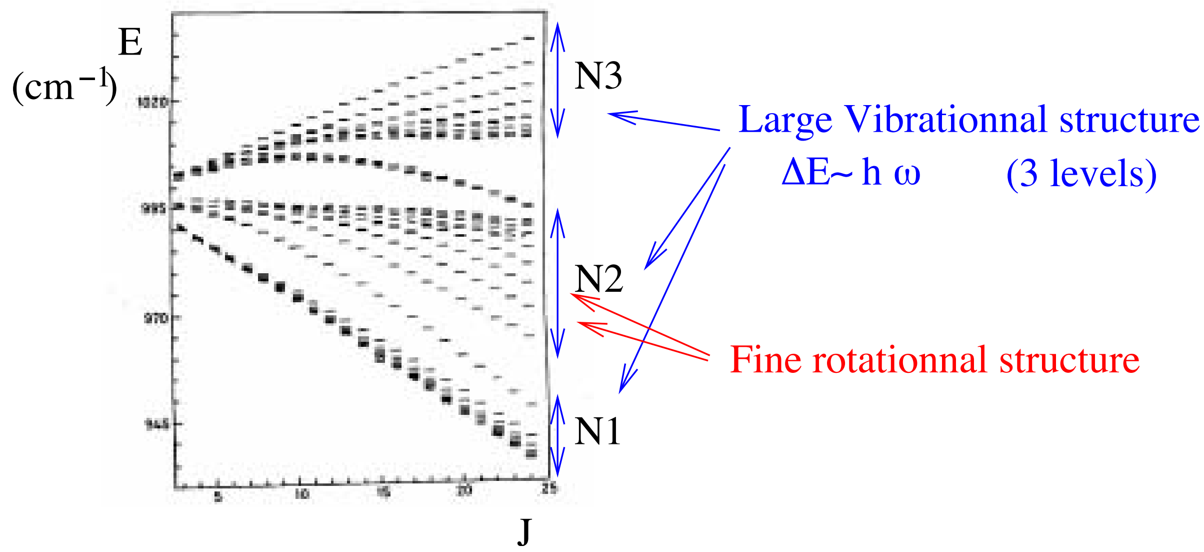
2) Slow rotation coupled with fast vibrations of the nuclei

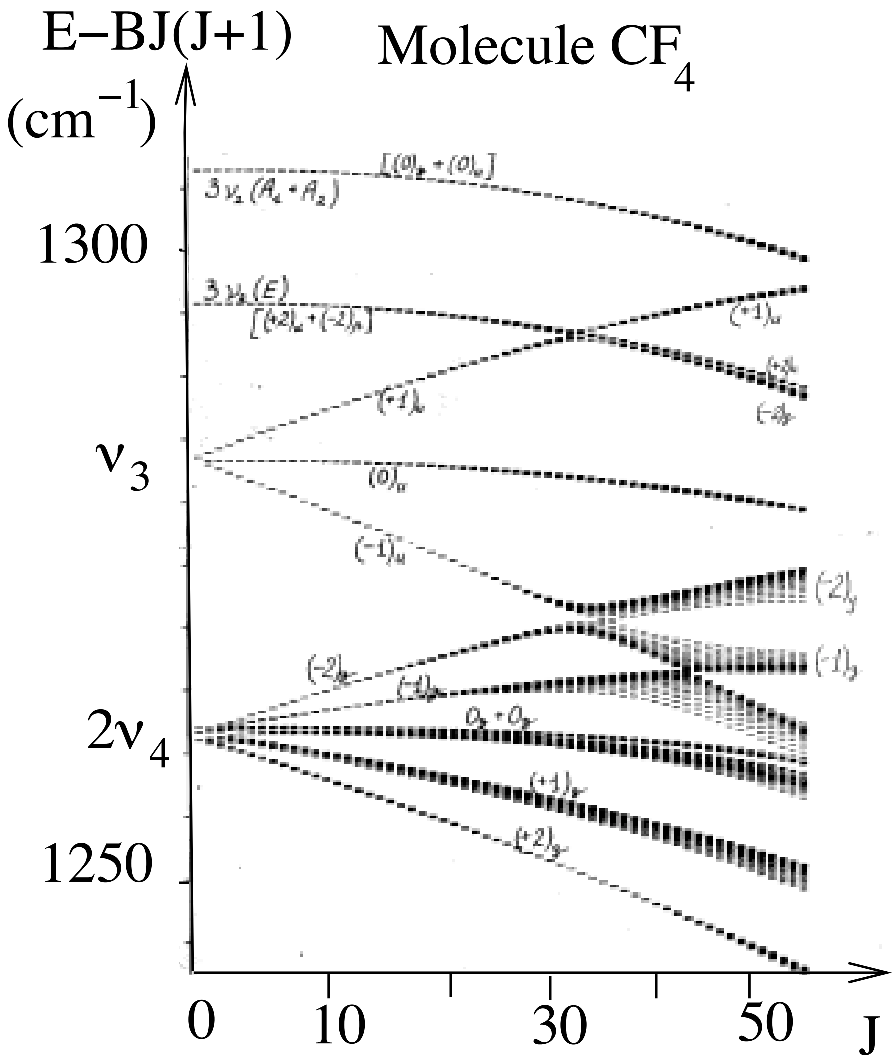




Observations:

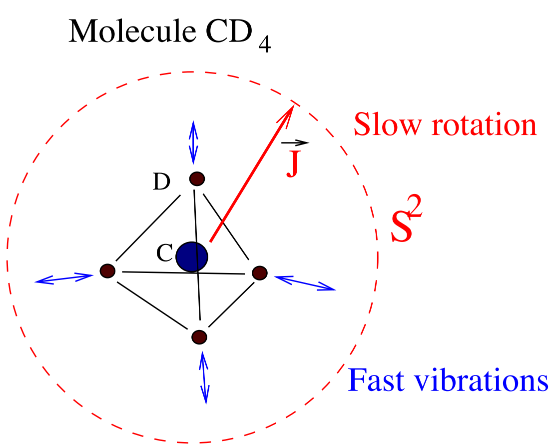
- Group of rotational levels
- Restructuration of groups and exchange of levels with external parameter.

These qualitative phenomena are very common in molecular spectra.



Objectives: Understand these qualitative phenomena

2.1) Angular momentum of a molecule



Isolated molecule

$\rightarrow$ the total angular momentum $\vec{J} = \sum_i \vec{x}_i \wedge \vec{p}_i$

is conserved in any inertial frame.

Rotational motion of a *rigid* molecule:

- **In classical dynamics, In the body frame** $\vec{J}(t)$ moves on the sphere **phase space** S_J^2, with energy: $H(\vec{J}) = \frac{J_x^2}{I_x} + \frac{J_y^2}{I_y} + \frac{J_z^2}{I_z}$.

- **In quantum dynamics**
  $j = \left|\vec{J}\right| \in \mathbb{N}$ **fixed**, and angular momentum operators $\left[\hat{J}_x, \hat{J}_y\right] = i\hat{J}_z$ of $so(3)$ acting in **Hilbert space** $\mathcal{H}_j$ with dimension $(2j+1)$.

- **Semi-classical limit** is

$$\hbar_{eff} = 1/(2j) \to 0$$

- We will use:

$$\hat{\vec{J}}_{new} = \frac{1}{j}\hat{\vec{J}}, \qquad \text{and write } \hat{\vec{J}} \text{ instead of } \hat{\vec{J}}_{new}$$

- **Berezin symbol of the operator** of $\hat{O}$ (or Normal symbol):

$$\hat{O} \in L(\mathcal{H}_j) \ \to \ O(\vec{J}) = < \vec{J}|\hat{O}|\vec{J} > \in C^\infty$$

Operator Symbol

with

$$|\vec{J} >= \hat{R}(\vec{\alpha})|m = -j >, : \text{coherent state}, \quad \vec{\alpha} = (0, \theta - \pi, \varphi)\text{:Euler angles}$$

$$\hat{R}(\vec{\alpha}) = \exp\left(-i\alpha_3 j\hat{J}_z\right)\exp\left(-i\alpha_2 j\hat{J}_y\right)\exp\left(-i\alpha_1 j\hat{J}_z\right) : \text{ Rotation operator} \tag{1}$$

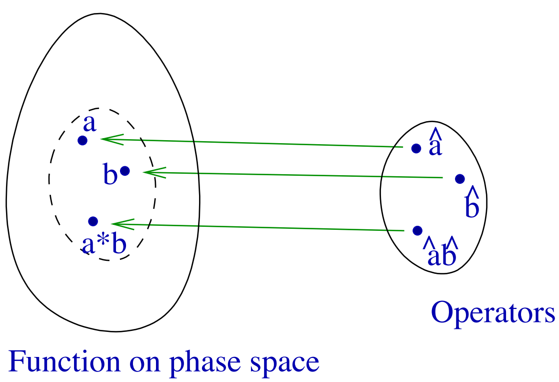
<u>Example:</u>

$$< \vec{J}|\hat{J}_z|\vec{J} >= J_z = \cos\theta, \qquad < \vec{J}|\hat{J}_x|\vec{J} >= J_x, \qquad < \vec{J}|\hat{J}_z^2|\vec{J} >= (J_z)^2 + \frac{1}{2j}\left(1 - J_z^2\right),$$

One consider operators with symbols such that:

$$O(\vec{J}) = \qquad O_0(\vec{J}) \qquad + \hbar_{eff}\, O_1(\vec{J}) + \dots$$

principal symbol



The map $\hat{O} \to O$ is injective.$\Rightarrow$ allows to work (as possible) with symbols on phase space instead of operators.

•Define the **star product** of two symbols:

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

<u>Property:</u>

$$a * b = ab + \frac{i}{2}\hbar_{eff}\,\{a, b\} + o\left(\hbar_{eff}\right)$$

2.2) Model for coupling between:

slow rotation and n quantum vibrational levels:

•In the quantum description: Suppose

$$\hat{H}_{tot} \text{ acts in } \quad \mathcal{H}_{tot} = \mathcal{H}_{slow} \otimes \mathcal{H}_{fast} = \mathcal{H}_j \otimes \mathbb{C}^n$$

Schrödinger equation is:

$$\begin{aligned} i\frac{d|\psi\rangle}{dt} &= \hat{H}_{tot}|\psi\rangle \\ \Leftrightarrow \quad i\hbar_{eff}\frac{d|\psi\rangle}{d\tilde{t}} &= \hat{H}_{tot}|\psi\rangle, \quad \text{with } \tilde{t} = \hbar_{eff}\, t \to 0 \end{aligned}$$

So **semi-classical limit** $\hbar_{eff} \to 0$ gives **slow (adiabatic) motion** for $\vec{J}\,(\tilde{t})$.

•In the semi-quantum description, its **symbol** is:

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

Symbol $\hat{H}_{fast}(\vec{J})$ is a operator valued symbol:

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

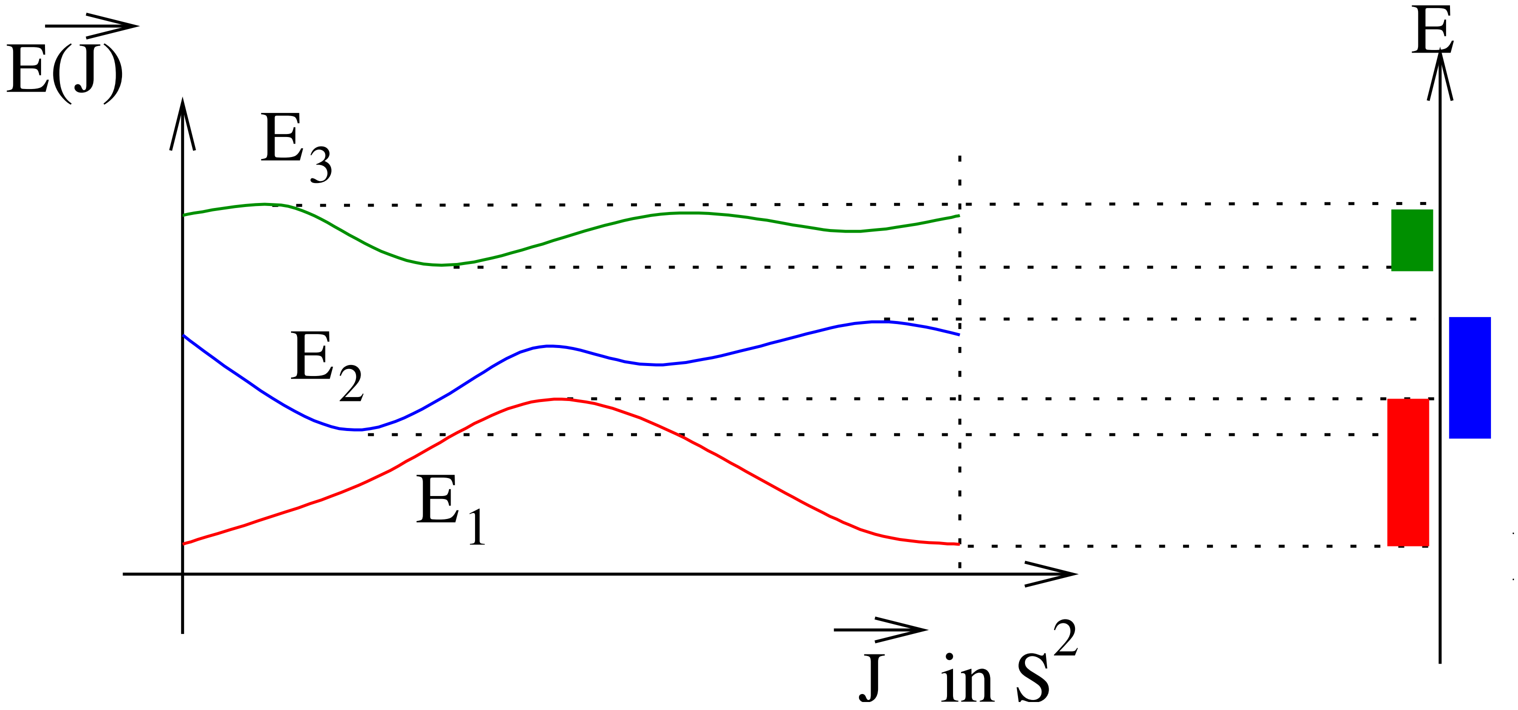
(This is the Born-Oppenheimer Approximation)

•Simple example: $(n = 2)$ the **Spin-Orbit** coupling $(\lambda \in [0, 1])$:

$$\hat{H}_{fast}\left(\vec{J}\right) = (1 - \lambda) \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + (\lambda) \frac{1}{2} \begin{pmatrix} J_z & J_x + iJ_y \\ J_x - iJ_y & -J_z \end{pmatrix}$$
$$= (1 - \lambda) \hat{S}_z + \lambda \vec{J}.\hat{\vec{S}}.$$

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

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



Property about degeneracies:

If $\lambda \in \mathbb{R}^n \to \hat{H}(\lambda)$ is ***generic*** *family of hermitian operators,*

then

degeneracies *between* ***2*** *eigenvalues occur with* ***codimension*** *3.*

More generally degeneracies with multiplicity $k = 2, 3, \ldots$

occur with codimension $k^2 - 1 = 3, 8, \ldots$

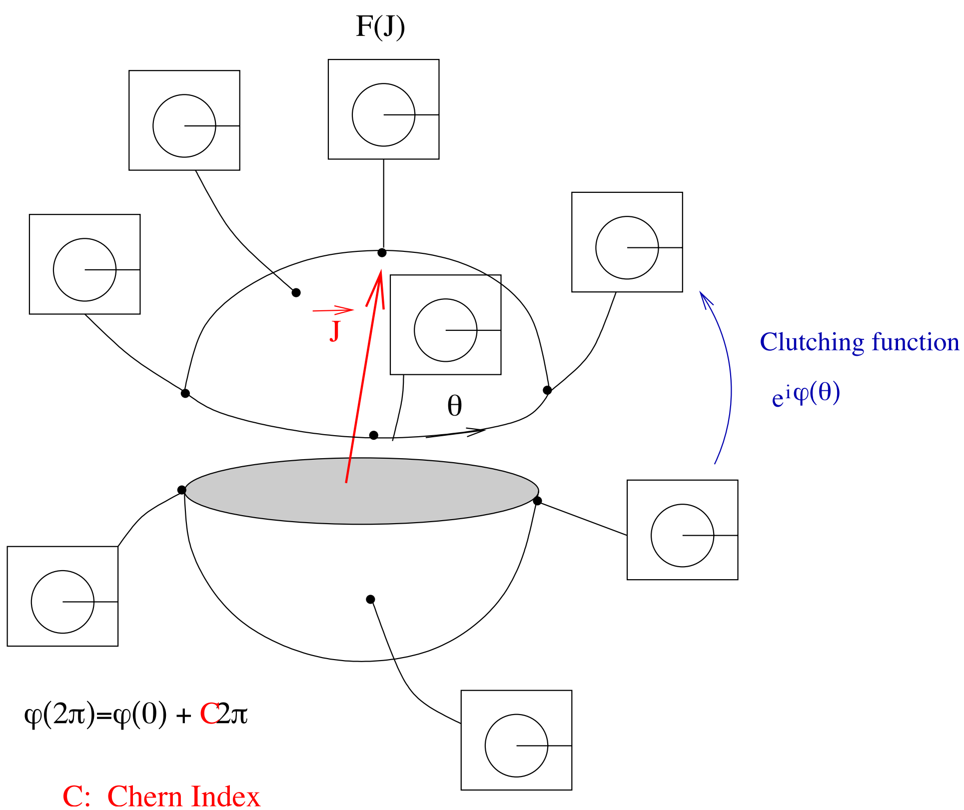
Proof:

Because the space of $k \times k$ Hermitian matrices is k^2 dimensional.

Matrices with multiplicity k are: $\lambda \hat{I}$ with $\lambda \in \mathbb{R}$.

The eigenspaces of $\hat{H}_0\left(\vec{J}\right)$:

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



define n **Complex Vector Bundle of rank 1**: $F_1, F_2, \ldots F_n$.

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

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

Additivity of the indices: $\sum_i C_i = \sum_i c_1(L_i) = c_1(\oplus_i L_i) = c_1(\mathcal{H}_{fast}) = 0.$

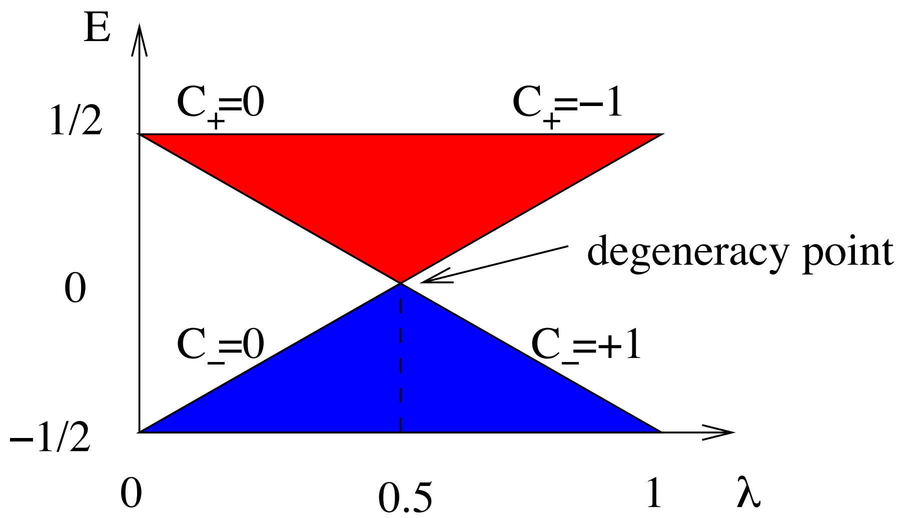
Simple Example of : **(**$n = 2$**) the** Spin-Orbit **coupling:**

$$\hat{H}_{fast}\left(\vec{J}\right) = (1-\lambda)\,\hat{S}_z + \lambda\vec{J}.\hat{\vec{S}}, \qquad \lambda \in [0,1]$$

– For $\lambda = 0$, $\hat{H}_{fast}\left(\vec{J}\right) = \hat{S}_z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}$. $E_\pm\left(\vec{J}\right) = \pm 1/2$, $C_\pm = 0$.

– For $\lambda = 1$, $\hat{H}_{fast}\left(\vec{J}\right) = \vec{J}.\hat{\vec{S}}$. $E_\pm\left(\vec{J}\right) = \pm 1/2$, $C_\pm = \mp 1$.

– At $\lambda = 1/2$, $\vec{J} = (0,0,-1)$, gives $H = 0$; an **isolated degeneracy** between the two bands.



Quantum model: (rotation $\vec{J}$ is quantized)

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

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

Construct ***projectors in*** $\mathcal{H}_{tot}$**,** $\hat{P}_1, \hat{P}_2, \hat{P}_3, \ldots \hat{P}_n$ *associated with bands* $1, 2, 3, \ldots, n$**,** *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 on level n°i of $\hat{H}_0\left(\vec{J}\right)$.)

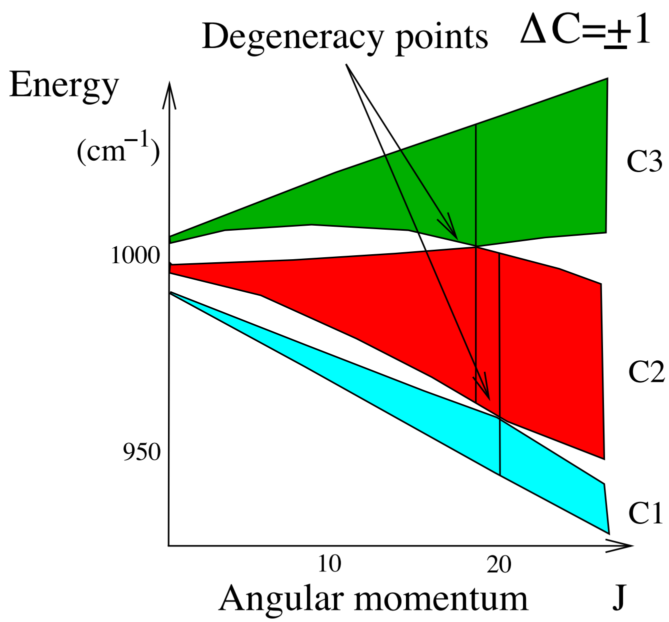
So define: $\mathcal{N}_i = Rank\left(\hat{P}_i\right)$: number of levels in band i

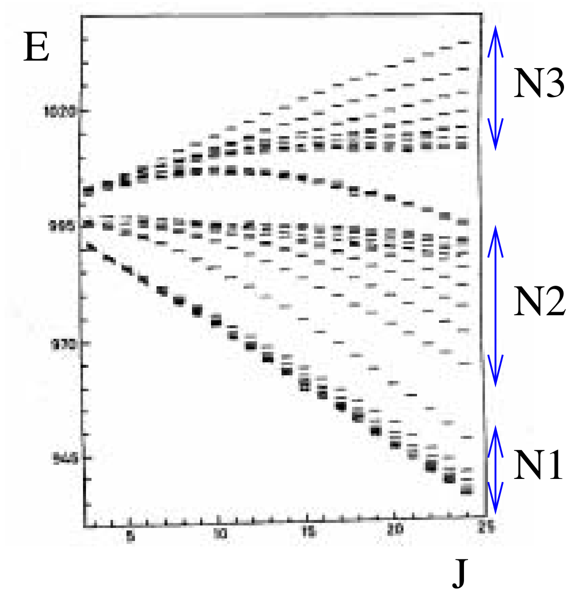
Remarks:

- This result is no so obvious **if bands overlap** in energy; (figure above).
- Corrections are due to possible **tunnelling effect** between bands.

Summary:

1/2 Quantum (Born.Opp.)	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: $\mathcal{N}_i$





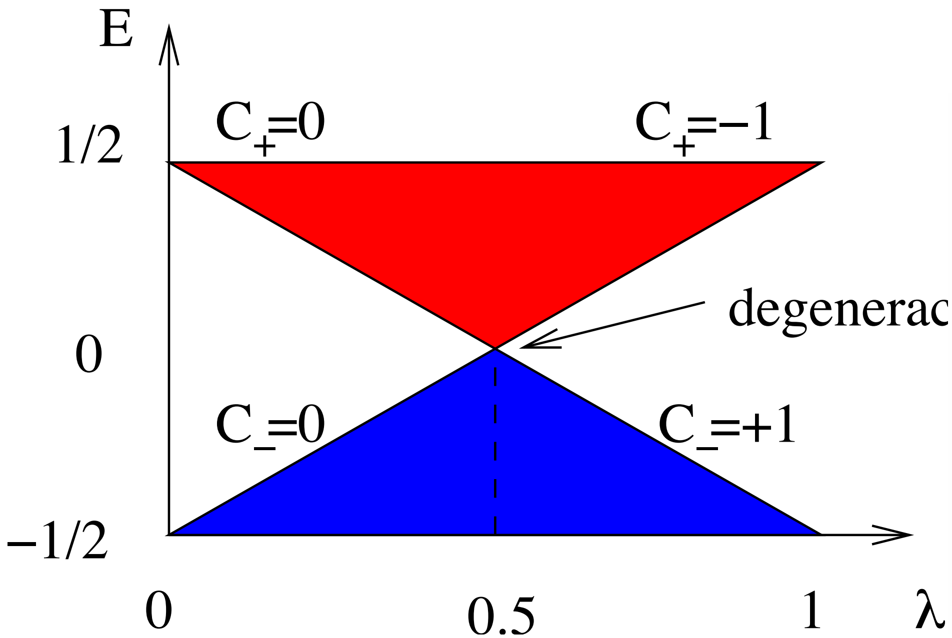
Question: relation between band topology C_i and $\mathcal{N}_i$?

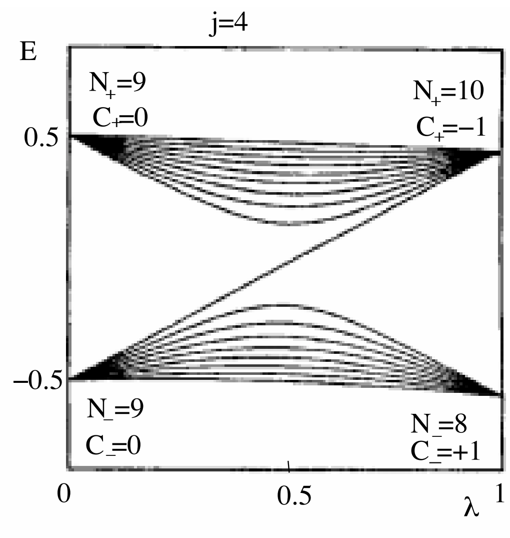
Simple Example of : **($n=2$) the** Spin-Orbit **coupling:**

$$\hat{H}_{fast}\left(\vec{J}\right) = (1-\lambda)\,\hat{S}_z + \lambda \vec{J}.\hat{\vec{S}}, \qquad \lambda \in [0,1].$$

– For $\lambda = 0$, $H = S_z$: $\quad \mathcal{N}_{\pm} = (2j+1)$ levels.

– For $\lambda = 1$, $H = \vec{J}.\vec{S}$: $\quad \mathcal{N}_{\pm} = (2j+1) \pm 1$ levels.





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

$$\mathcal{N}_i = (2j+1) - C_i \quad \Leftrightarrow \quad \Delta\mathcal{N}_i = -\Delta C_i :$$ **at degeneracies**

This is a simple case of the Index formula for the sphere (angular momentum)

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

Introduce

$$\begin{aligned} Ch(F^*) &= 1 - Cx && : \text{Chern Character of the band} \\ Ch(Quant_j) &= \exp((2j)x) = 1 + 2j\,x && : \text{coherent states line bundle} \\ Todd(TS^2) &= 1 + (1-g)x && : \text{Base space, genre g} = 0 \end{aligned}$$

Index formula:

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

gives

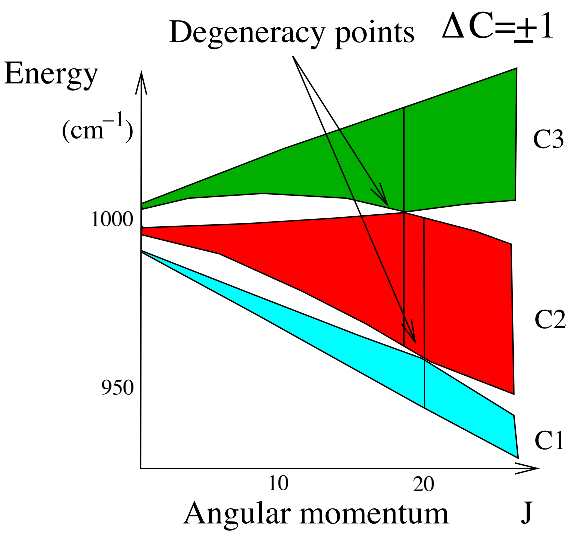
$$\begin{aligned} \mathcal{N}(F) = [(1 - Cx) \wedge (1 + (2j)x) \wedge (1 + (1-g)x)]_{/x} &= (2j) + (1-g) - C \\ &= (2j+1) - C \end{aligned}$$

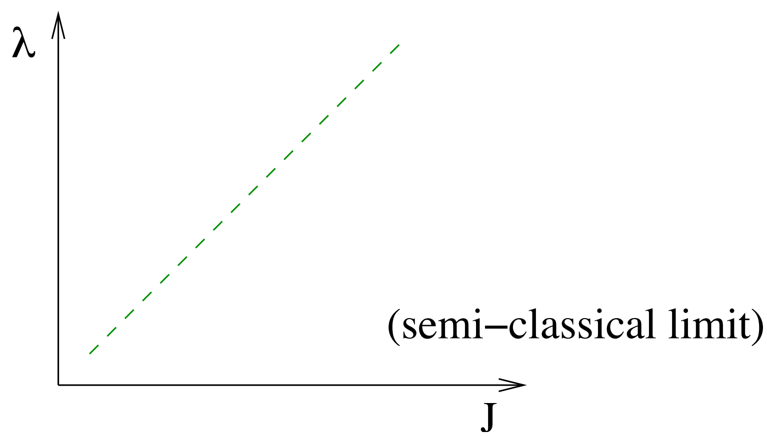
Modifications of bands by an external parameter λ. Proof of the formula $\mathcal{N}_i = (2j+1) - C_i$.

Remark: for molecules $\lambda = \left|\vec{J}\right|$,

the external parameters are:

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

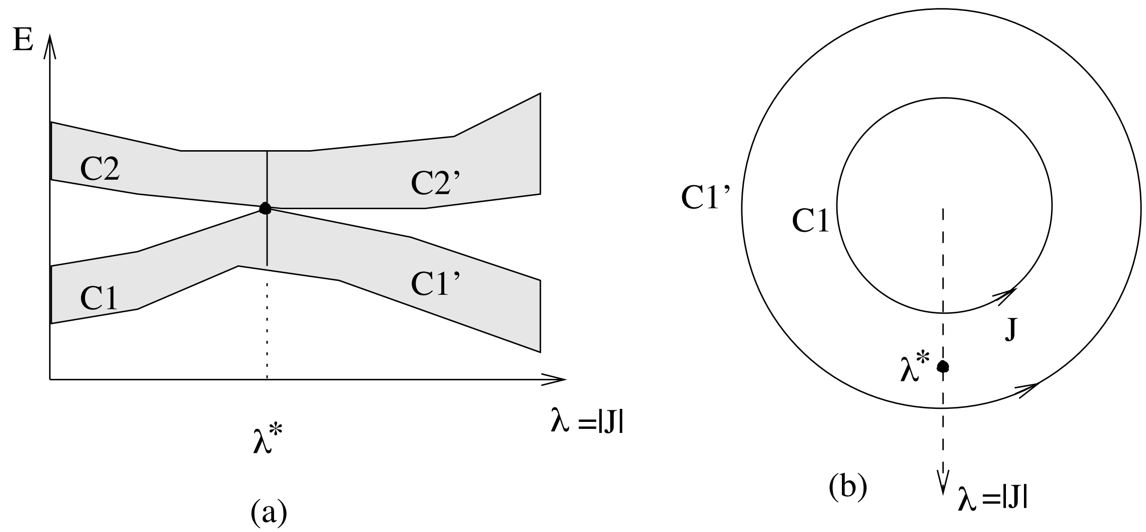


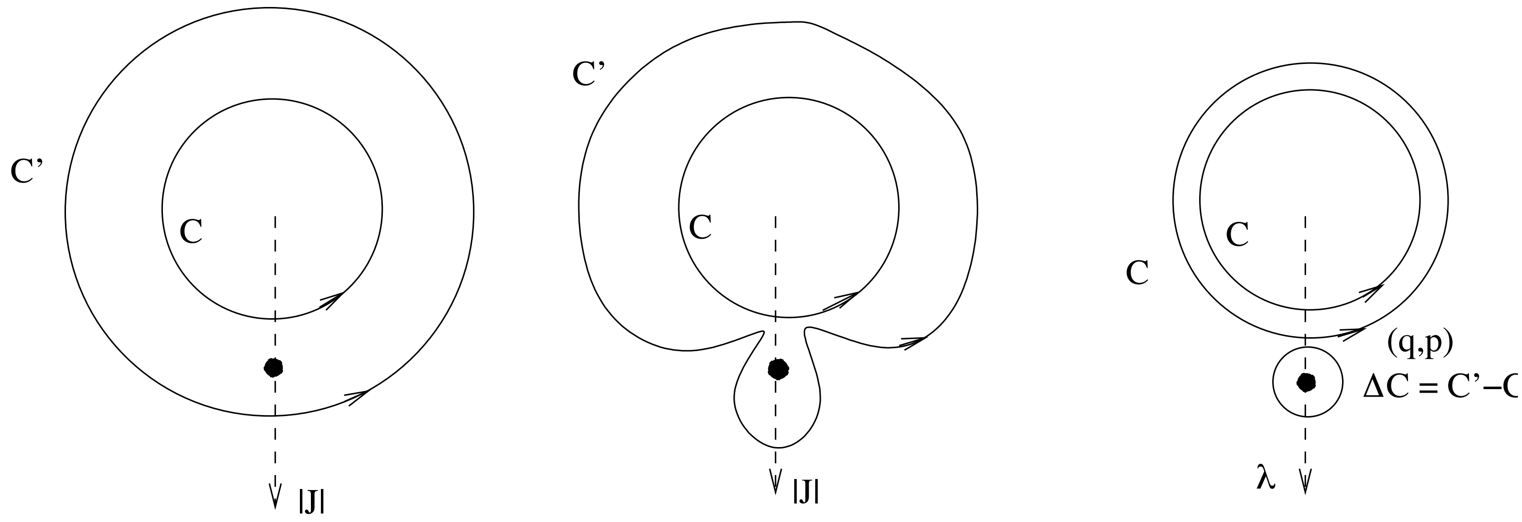


Modification of Chern index at a generic degeneracy:

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

Proof: in $\left(\frac{\vec{J}}{|\vec{J}|}, \lambda\right) \subset \mathbb{R}^3$ space,





Local model near an isolated degeneracy:

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

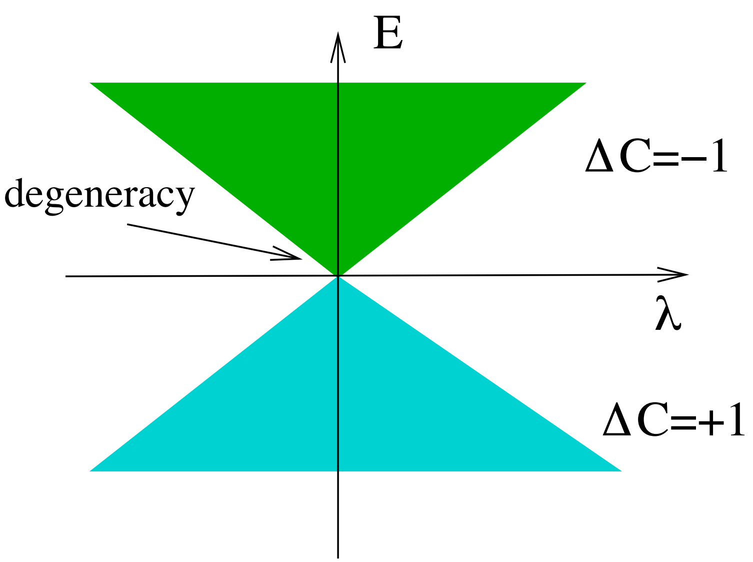
giving (Berry 84)

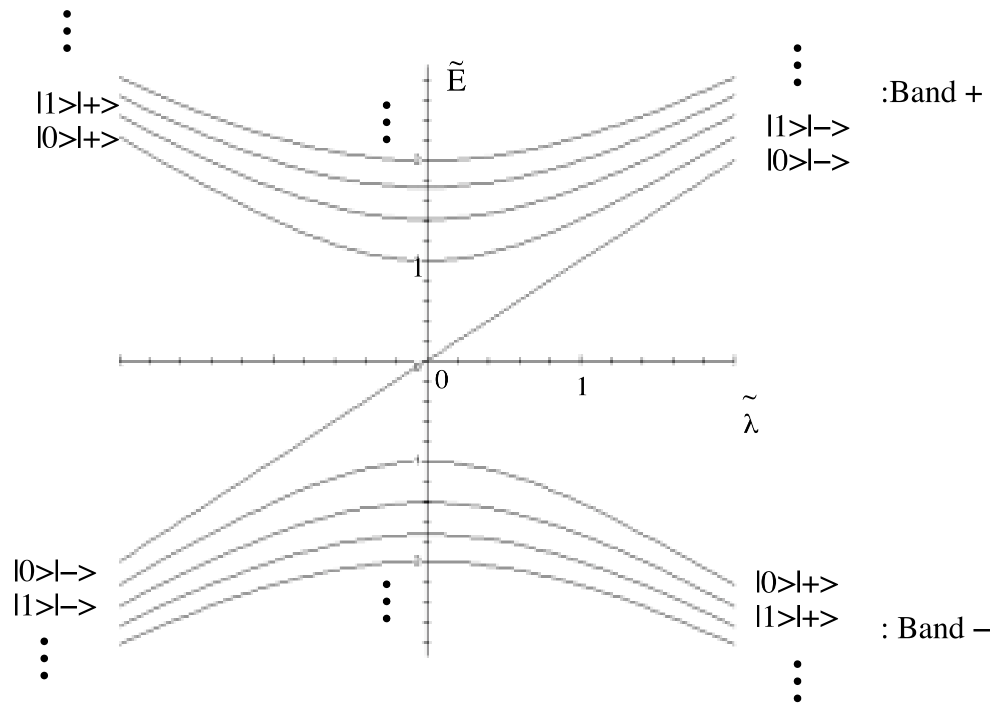
$$\boxed{\Delta C = \mp 1}$$

Its quantization:

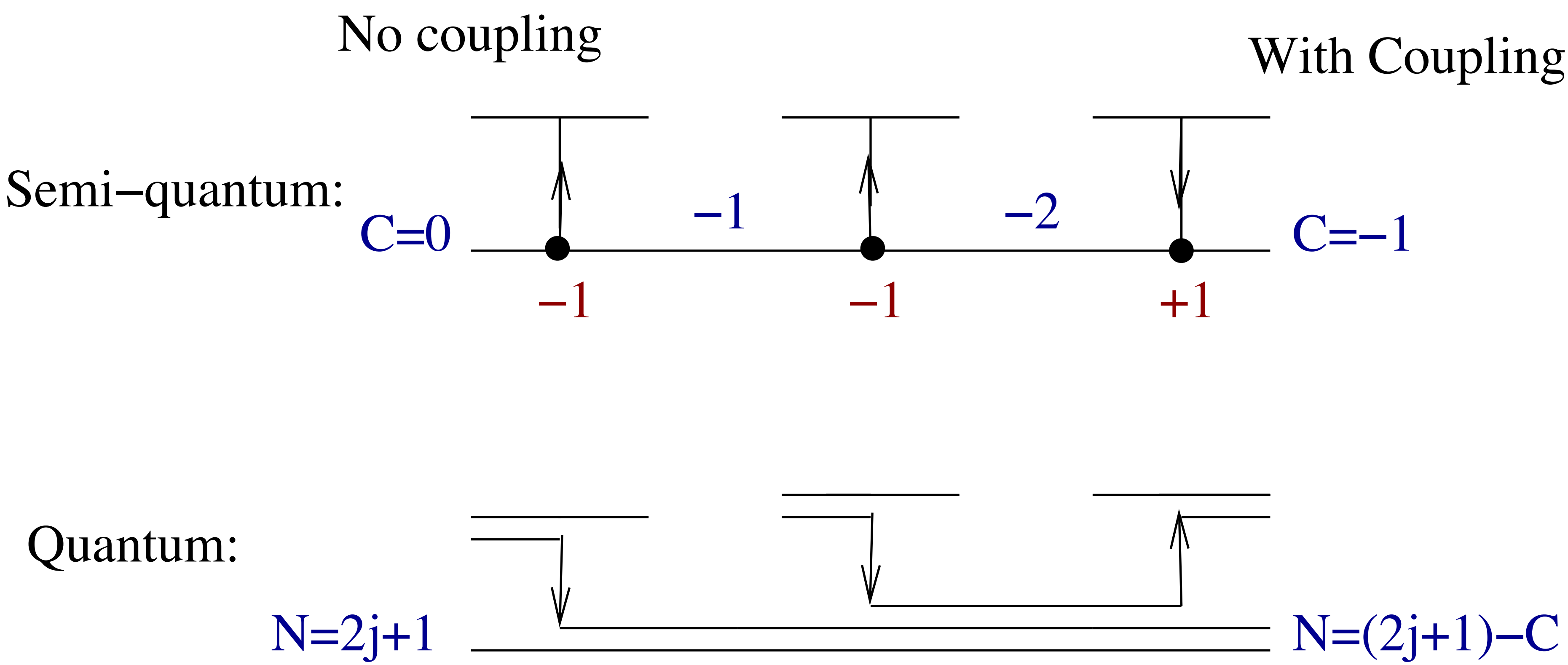
$$\hat{H}_\lambda = \begin{pmatrix} \pm\lambda & \hat{q} + i\hat{p} \\ \hat{q} - i\hat{p} & \mp\lambda \end{pmatrix}, \qquad \text{gives } \Delta\mathcal{N} = \pm 1$$

So $\Delta\mathcal{N}_i = -\Delta C_i$.





Generic deformation of the given symbol $\hat{H}\left(\vec{J}\right)$
from the trivial (uncoupled) situation $\hat{H}_0 = \hat{S}_z$,
where $\mathcal{N}_i = (2j+1)$, $C_i = 0$:



What is particular here:

•Dim(*phase space* S^2)=2 $<$ Codim(*degeneracies*)=3.

So Vector bundles have **rank 1.**

An external parameter $\lambda \in \mathbb{R}$, gives isolated degeneracies;

a unique local model (sign ± 1).

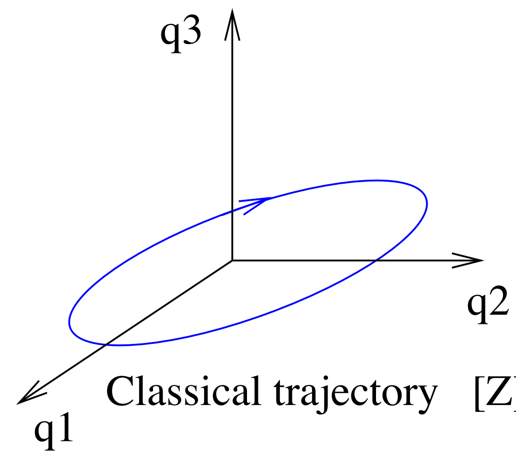
•Rank 1 vector bundles over S^2 are characterized by

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

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

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

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



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

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)**

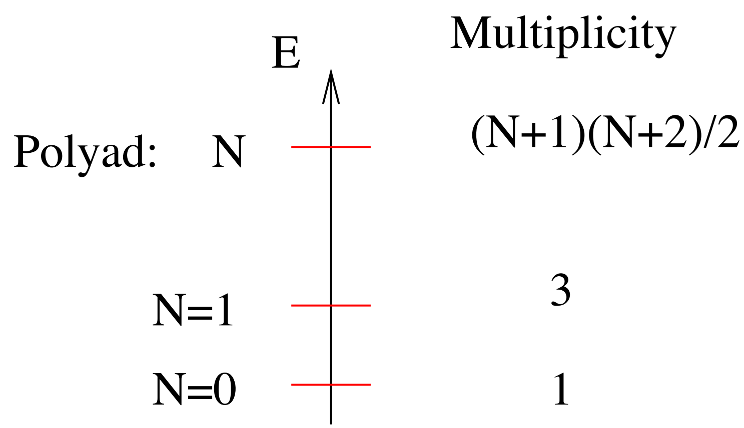
$$\mathbb{C}P^2 = \left(\mathbb{C}^3 \setminus \{0\}\right) / \sim, \qquad with\, Z \sim \lambda Z, \quad \lambda \in \mathbb{C}$$

Quantum mechanics: on $L^2\left(\mathbb{R}^3\right)$,

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:



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

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

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

Semi-classical limit: $\hbar_{eff} = 1/N \to 0$

Slow Vibrations coupled with 3 electronic states:

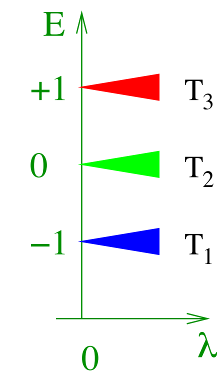
Matrix symbol: with parameter $\lambda \in [0,1]$ "*:magnetic field*",

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

•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.

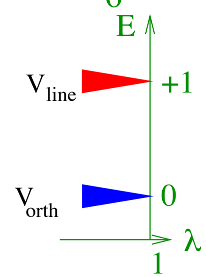


•For $\lambda = 1$,

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

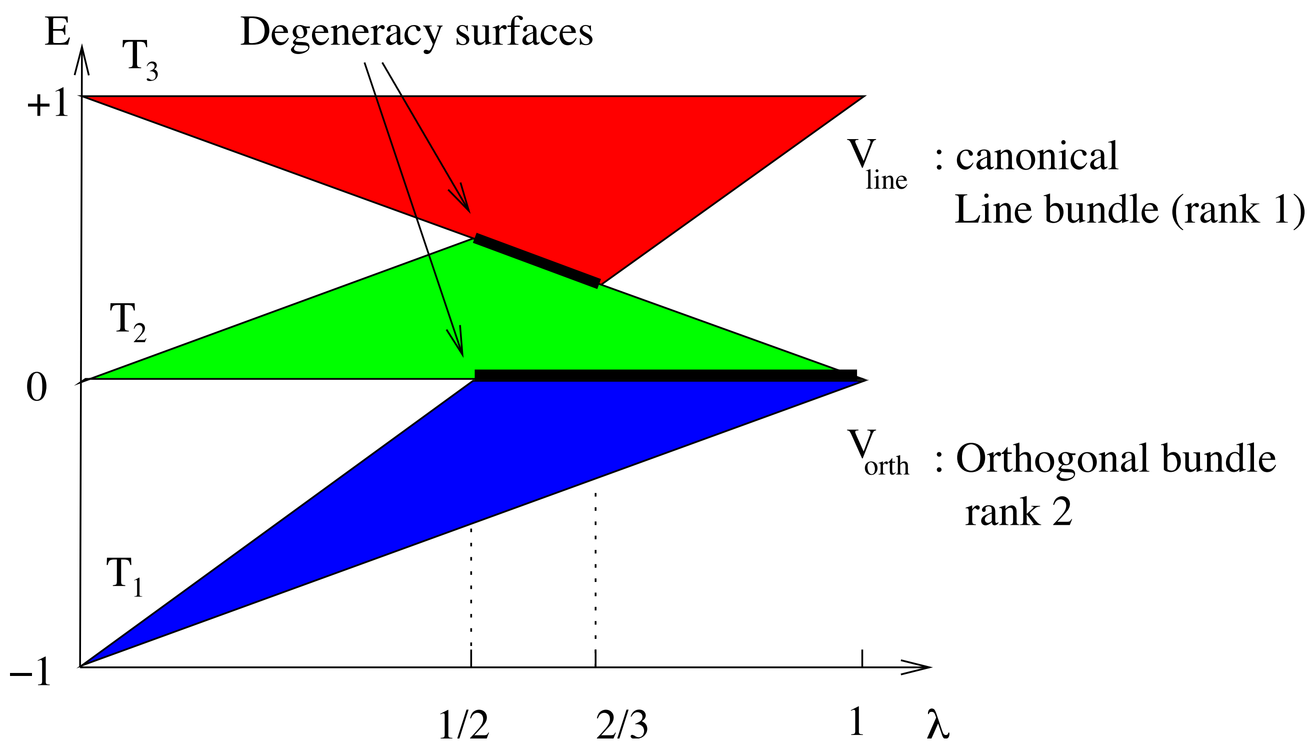
Eigenvalue ($E_3 = 1$): **rank 1 fiber bundle** V_{line} **:"the canonical bundle"**

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



Band spectrum in the Semi-quantum description

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



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

$$T_1 \oplus T_2 \oplus T_3 \quad = \quad \mathbb{C}^3 \quad = \quad V_{line} \oplus V_{orth}$$

$$Rank\,1,\ trivial \ = Rank\,3,\ trivial = \ Rank\,1 \oplus Rank\,2$$

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**: $r \in \mathbb{N}^*$, $\quad (B = 0 \text{ if } r = 1)$.

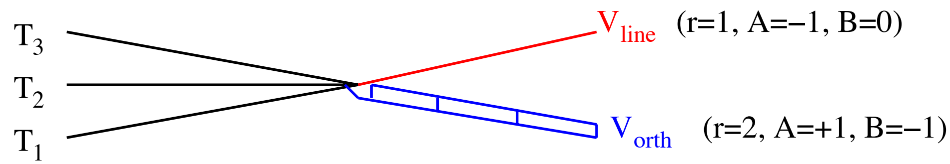
(x is symplectic two form on $\mathbb{C}P^2$).

•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:*

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

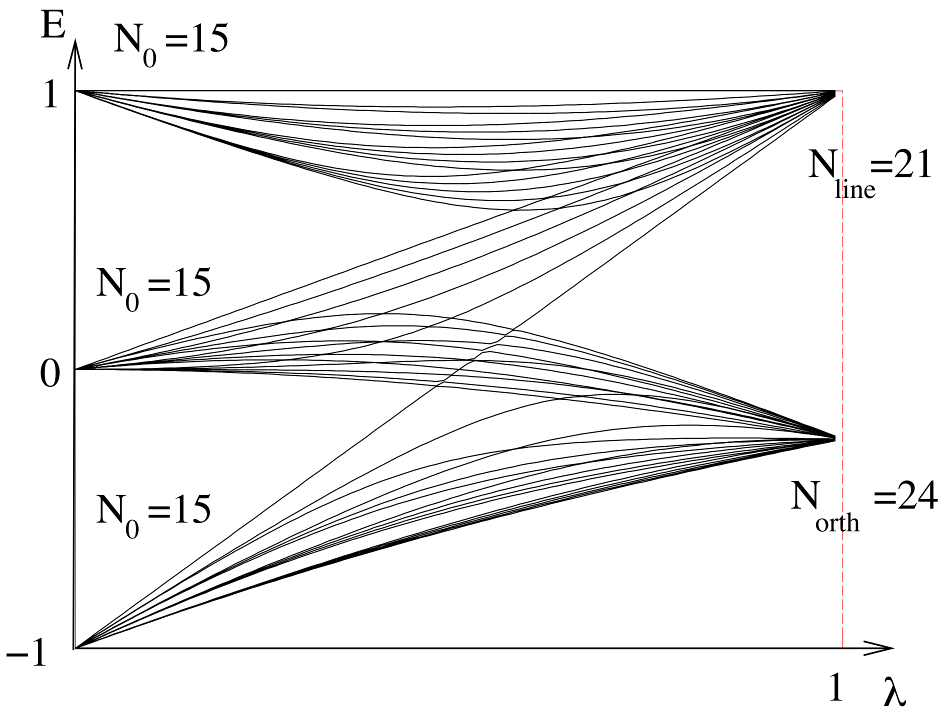
Quantization of vibrations:

$\mathbb{C}P^2 \rightarrow$ 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: $\mathcal{H}_{tot} = \mathcal{H}_{Polyad\,N} \otimes \mathbb{C}^3_{Electronics}$

For $N = 4$:



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)

relating Analysis (number of levels) and topology of bundles:

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

with

$$Ch(F^*) = r - Ax + \frac{1}{2}\left(A^2 + 2B\right)x^2 \quad : \text{Band topology}$$

$$Ch(Polyad_N) = \exp(Nx) \quad : \text{geometric quantization of } \mathbb{C}P^2$$

$$Todd(T\mathbb{C}P^2) = 1 + \frac{3}{2}x + x^2 \quad : \text{Base space}$$

Our model:

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

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

Important physical remarks:

the Index formula is more precise than just giving the total number of states.

From Levi-Civita connection in Hilbert space or Berry's connection, one has differential forms:

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

- 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.

3) Correspondances between the Classical and Semi-quantum descriptions

3.1) A simple class of classical 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 **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: $S^1_{fast}\times S^1_{slow}$).

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

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

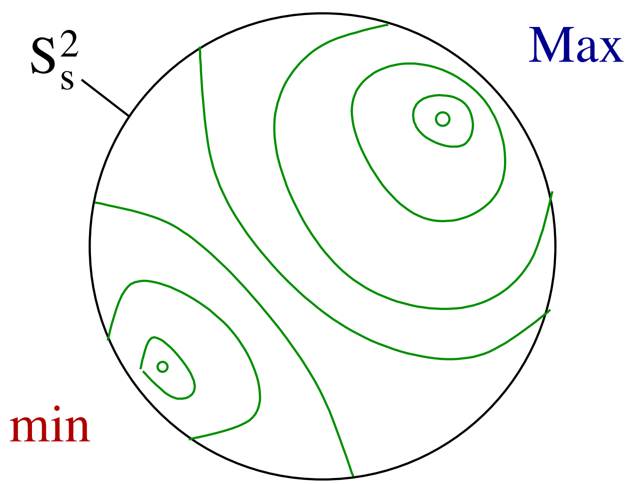
•**Summary:**

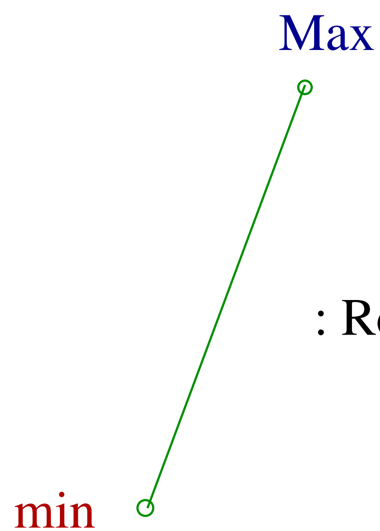
Slow $\vec{J}$ \ Fast $\vec{S}$	Classical in $P_{Fast}=S^2_s$	Quantum in $\mathcal{H}_{Fast}=\mathcal{H}_s$
Classical in $P_{Slow}=S^2_j$	Function $H_{tot}(\vec{J},\vec{S})$ (***Classical***, phase space $S^2_j\times S^2_s$)	Operator Symbol $\vec{J}\to\hat{H}_{fast}(\vec{J})$ (***Semi-Quantum***)
Quantum 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.





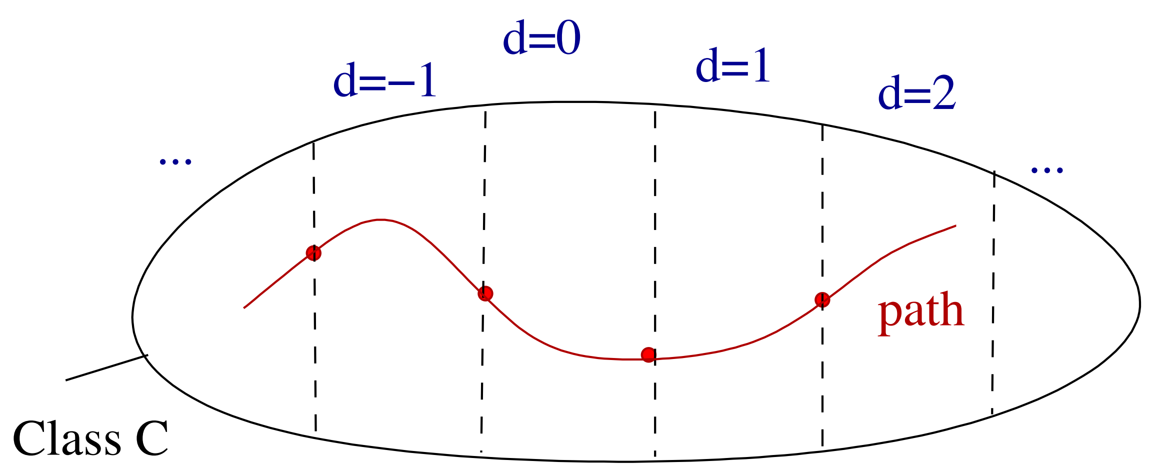
: Reeb graph

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

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

So Topological subclass of models

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



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

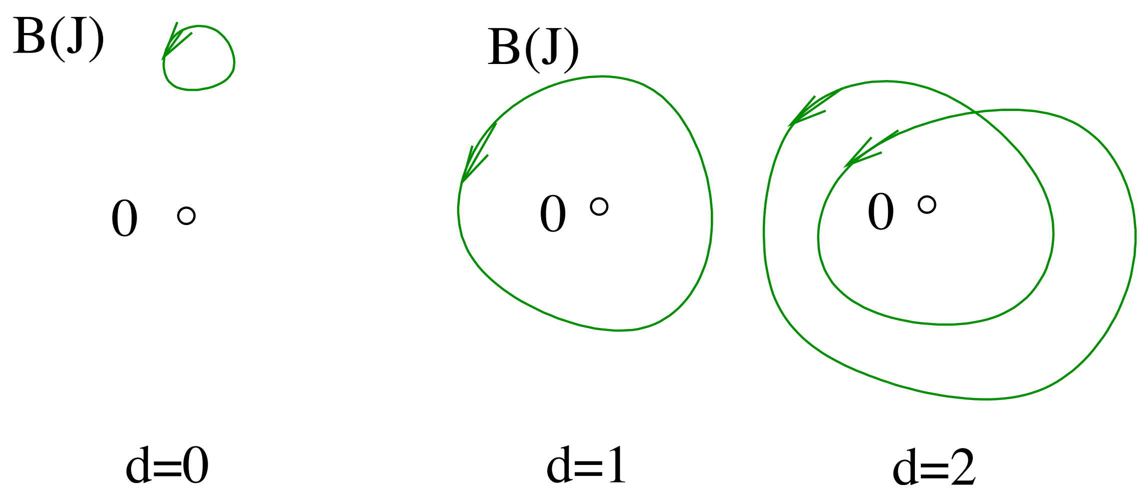
$$Chern_{Hannay} = 2\,d$$

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:

- $d = 1$, $\quad \vec{B} = \vec{J}$, $\quad H = \vec{J}.\vec{S}$ $\quad C_{Hannay} = 2$
- $d = 0$, $\quad \vec{B} = (0, 0, 1)$ $\quad H = S_z$, $\quad C_{Hannay} = 0$
- $d \neq 0$, $\quad \vec{B}(\theta' = \theta, \varphi' = d\varphi)$ $\quad H = \vec{B}(\vec{J})\vec{S}$, $\quad C_{Hannay} = 2d$



3.2) Semi-quantum model;

Energy Bands and their topology by semi-classical calculation

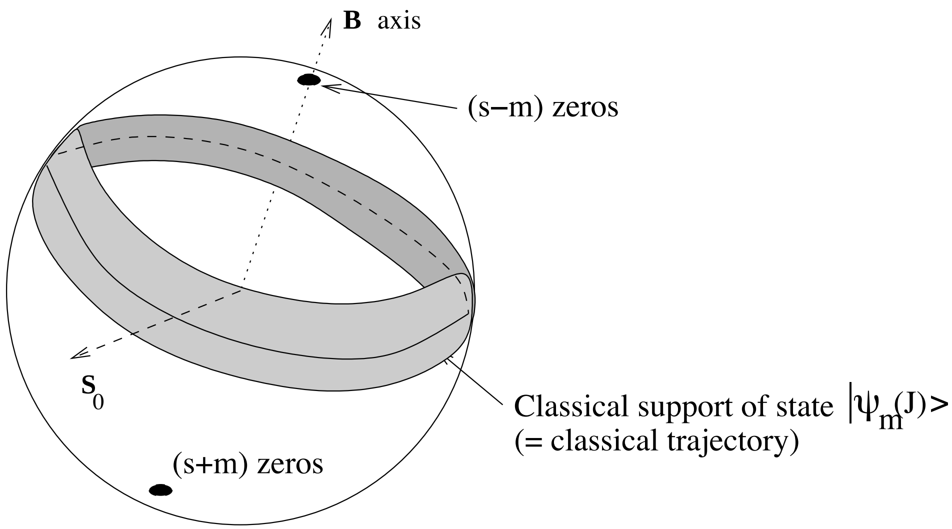
there are $dim\mathcal{H}_{fast} = 2s + 1$ isolated bands,
with Chern index $C_{Berry,m}$, $m = -s \to +s$.

Property: For $\mathcal{H} \in \mathcal{C}_d$,

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

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,

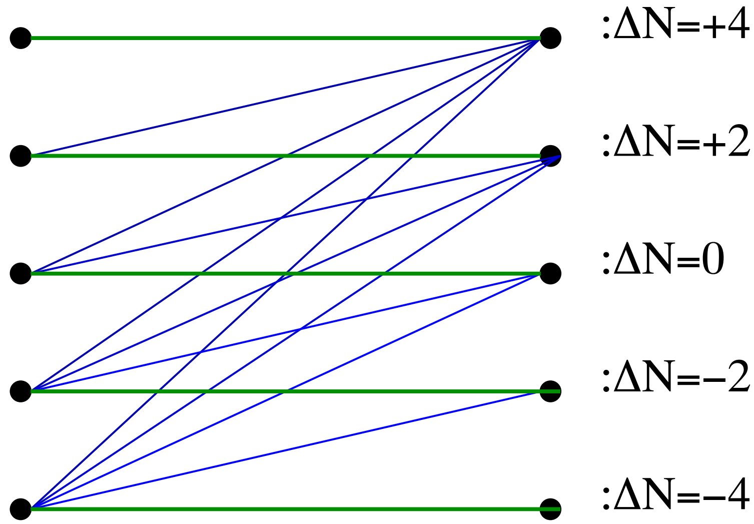
$$d = 1, \qquad C_{-2} = +4,\;\; C_{-1} = +2,\;\; C_0 = 0,\;\; C_1 = -2,\;\; C_2 = -4,$$

$$d = 2, \qquad C_{-2} = +8,\;\; C_{-1} = +4,\;\; C_0 = 0,\;\; C_1 = -4,\;\; C_2 = -8,$$

Remember in the *Quantum model* : $\mathcal{N}_m = (2j+1) - C_{Berry,m}$

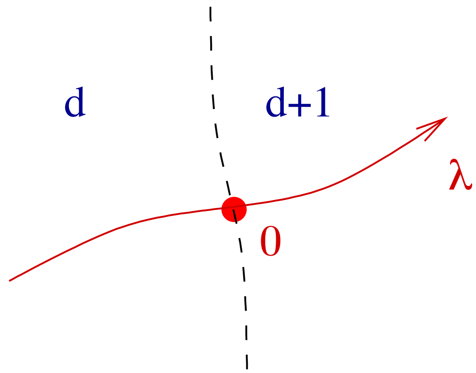
So transition $d \to d+1$ gives a **redistribution of levels** $\Delta\mathcal{N}_m = 2m$**.**

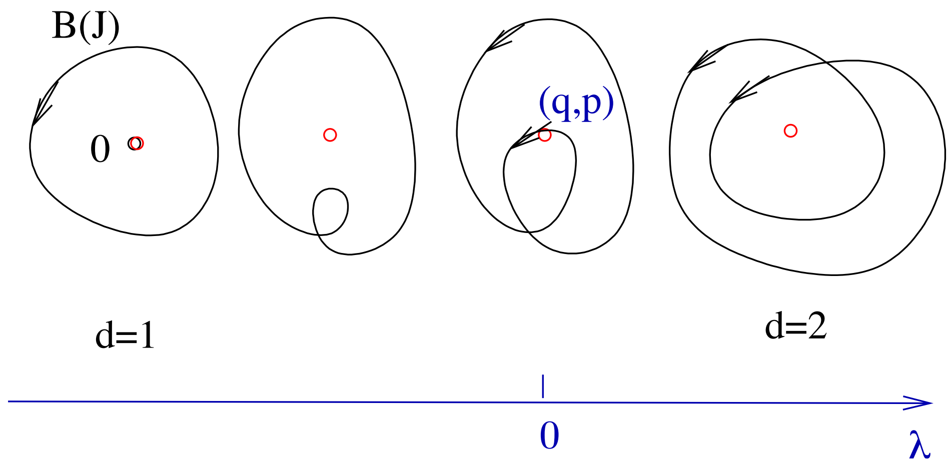
$$\Delta\mathcal{N}_{-2} = -4,\;\; \Delta\mathcal{N}_{-1} = -2,\;\; \Delta\mathcal{N}_0 = 0,\;\; \Delta\mathcal{N}_1 = +2,\;\; \Delta\mathcal{N}_2 = +4,$$



3.3) 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:

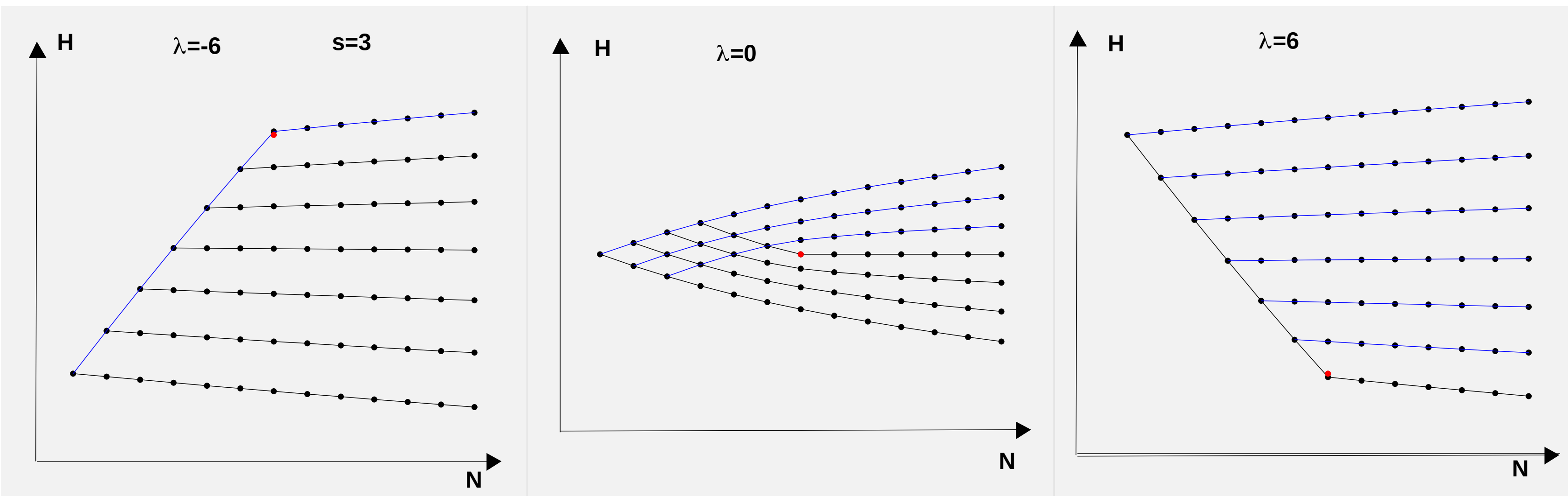
$$\hat{H}_{loc} = \begin{pmatrix} -\lambda & p + iq \\ p - iq & \lambda \end{pmatrix}$$

•This local model is **integrable**:

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

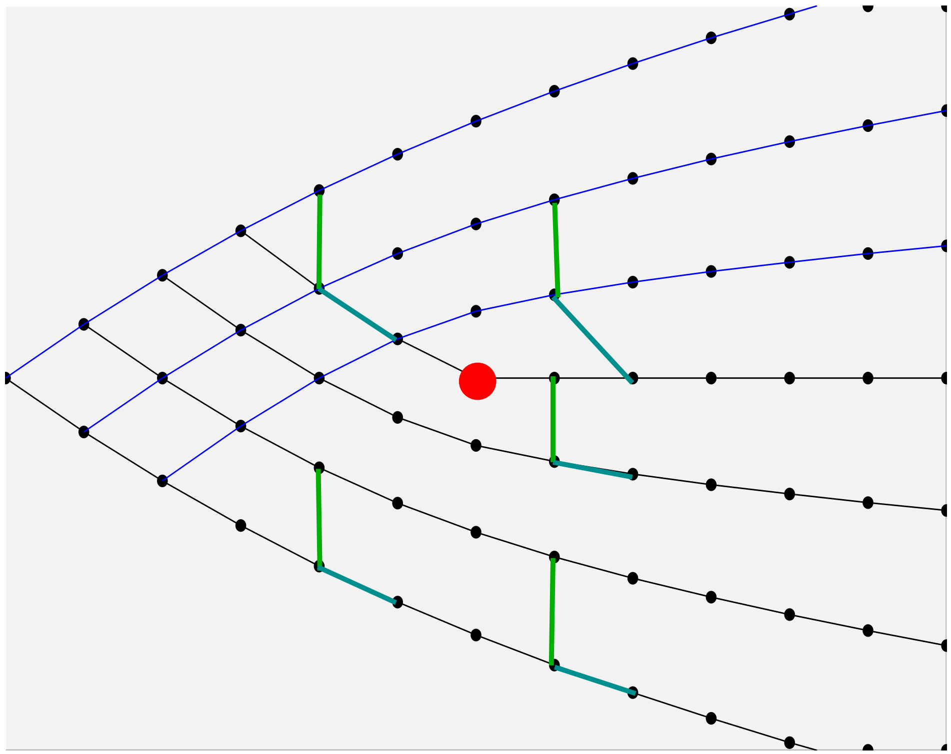
This local integrable model has a generic (classical and quantum) monodromy defect

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



See **Movie monodromie.gif.**

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.

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.

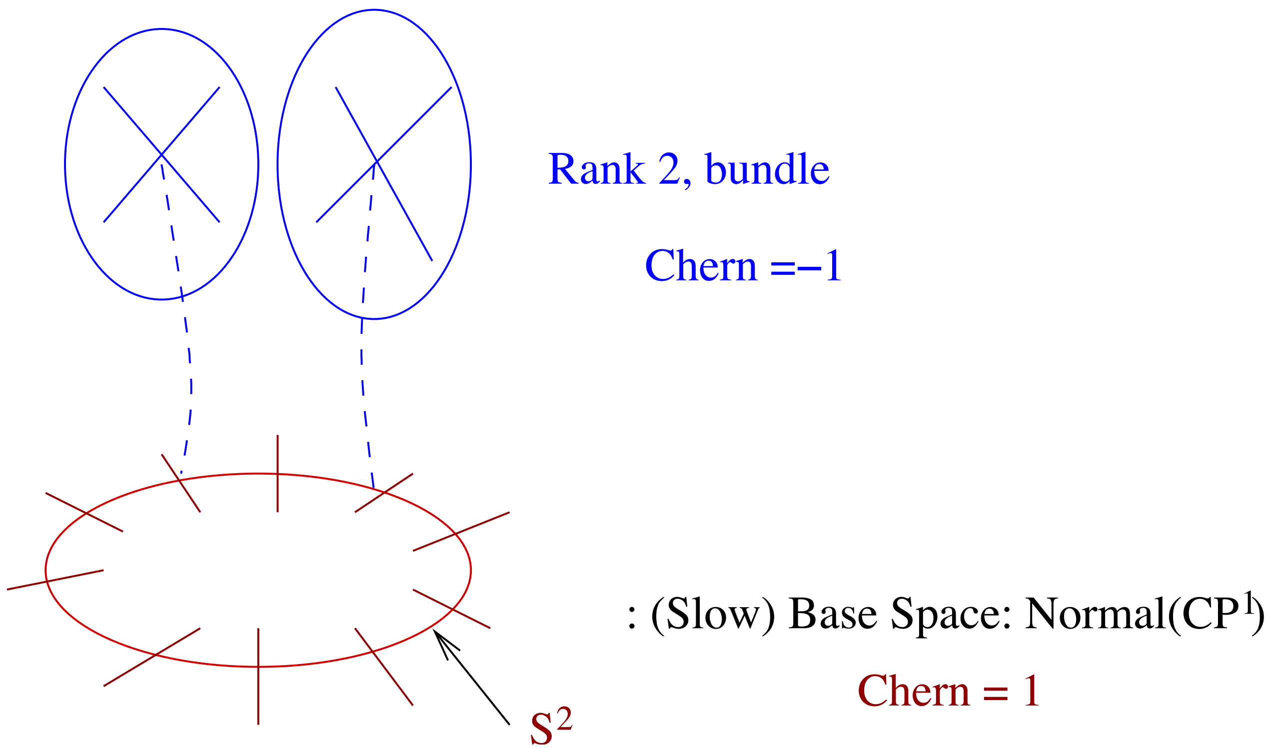
also related with **monodromie** in the Classical description.

•Perspectives : extend this topological approach for infinite dimensional degrees of freedom systems (spins on lattice ...) ?

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:

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

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:

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

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

So

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

Remark on "Naturality" of index formula

•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:

$$\mathcal{N}\left((F_1 \otimes F_2) \to (M_1 \times M_2)\right) = \mathcal{N}\left(F_1 \to M_1\right)\mathcal{N}\left(F_2 \to M_2\right) \; : \text{product of Hilbert spaces}$$

$$\mathcal{N}\left((F_1 \oplus F_2) \to M\right) = \mathcal{N}\left(F_1 \to M\right) + \mathcal{N}\left(F_2 \to M\right) \qquad : \text{Sum of bands}$$

This comes from

$$Ch(F_1 \otimes F_2) = Ch(F_1) \wedge Ch(F_2)$$
$$Ch(F_1 \oplus F_2) = Ch(F_1) + Ch(F_2)$$
$$Todd\,(T\,(M_1 \times M_2)) = Todd\,(TM_1) \wedge Todd\,(TM_2)$$

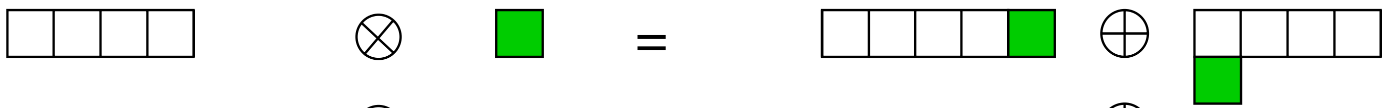
So the index formula is an expected formula:

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

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

Index theorem and group theory:

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



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

$$15 \quad * \quad 3 \quad = \quad 21 \quad + \quad 24$$

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:

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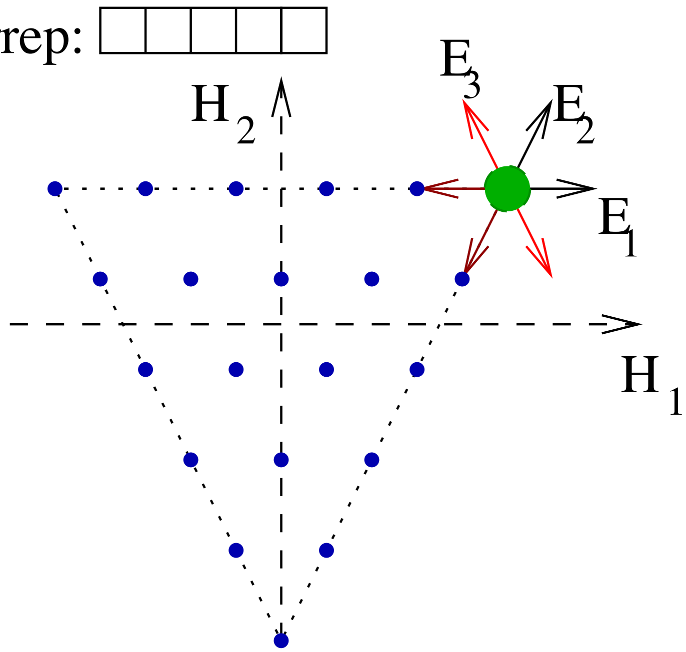

Orbit of ●:

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

(Perelomov coherent states)

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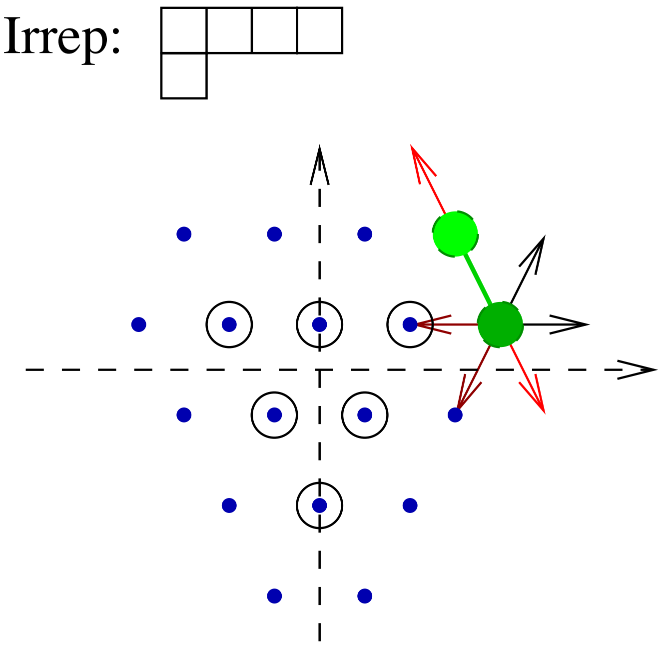

Orbit of ●:

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

Orbit of ●—●:

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

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*** $p \in P_{slow} \rightarrow \hat{H}(p) \in Herm(\mathcal{H}_{fast})$ *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* $\hat{\pi}_0(p)$.
- $E \rightarrow P_{slow}$ *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:

$$\hat{\pi}_{tot}^2 = \hat{\pi}_{tot} + \mathcal{O}(\hbar^{k+1}) \quad : \textit{quasi} - \textit{projector}, \tag{2}$$

$$\left[\hat{H}_{tot}, \hat{\pi}_{tot}\right] = \mathcal{O}(\hbar^{k+1}) \quad : \textit{almost commute}. \tag{3}$$

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* $\hat{\text{Ker}}\,(\hat{\pi}(p))$.
- **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 $\hat{\text{Ker}}\,(\hat{\pi}(p))$., as it occurs usually in the **tunneling effect**.

<u>Indications for the proof :</u>

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

Hypothesis for a given k:

$$\pi * \pi - \pi = \hbar^{k+1} A + O\left(\hbar^{k+2}\right)$$

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

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:

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

and write in this basis:

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix}, \quad idem\ for\ F.$$

Lemme 1: $[A, \pi_0] = 0$, so $A = \begin{pmatrix} A_{00} & 0 \\ 0 & A_{11} \end{pmatrix}$.

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

Write:

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

with unknown $K = \begin{pmatrix} K_{00} & K_{01} \\ K_{10} & K_{11} \end{pmatrix}$ such that:

$$\tilde{\pi} * \tilde{\pi} - \tilde{\pi} = O\left(\hbar^{k+2}\right)$$

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

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.

■