

**Modèles qualitatifs de systèmes quantiques:
Symétrie et topologie.**

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19 mai 2011

JDM 2011, Ambleteuse, France

Plan

1. Molecular preliminaries. Qualitative reasoning.
2. General scheme of qualitative analysis.
3. Examples.

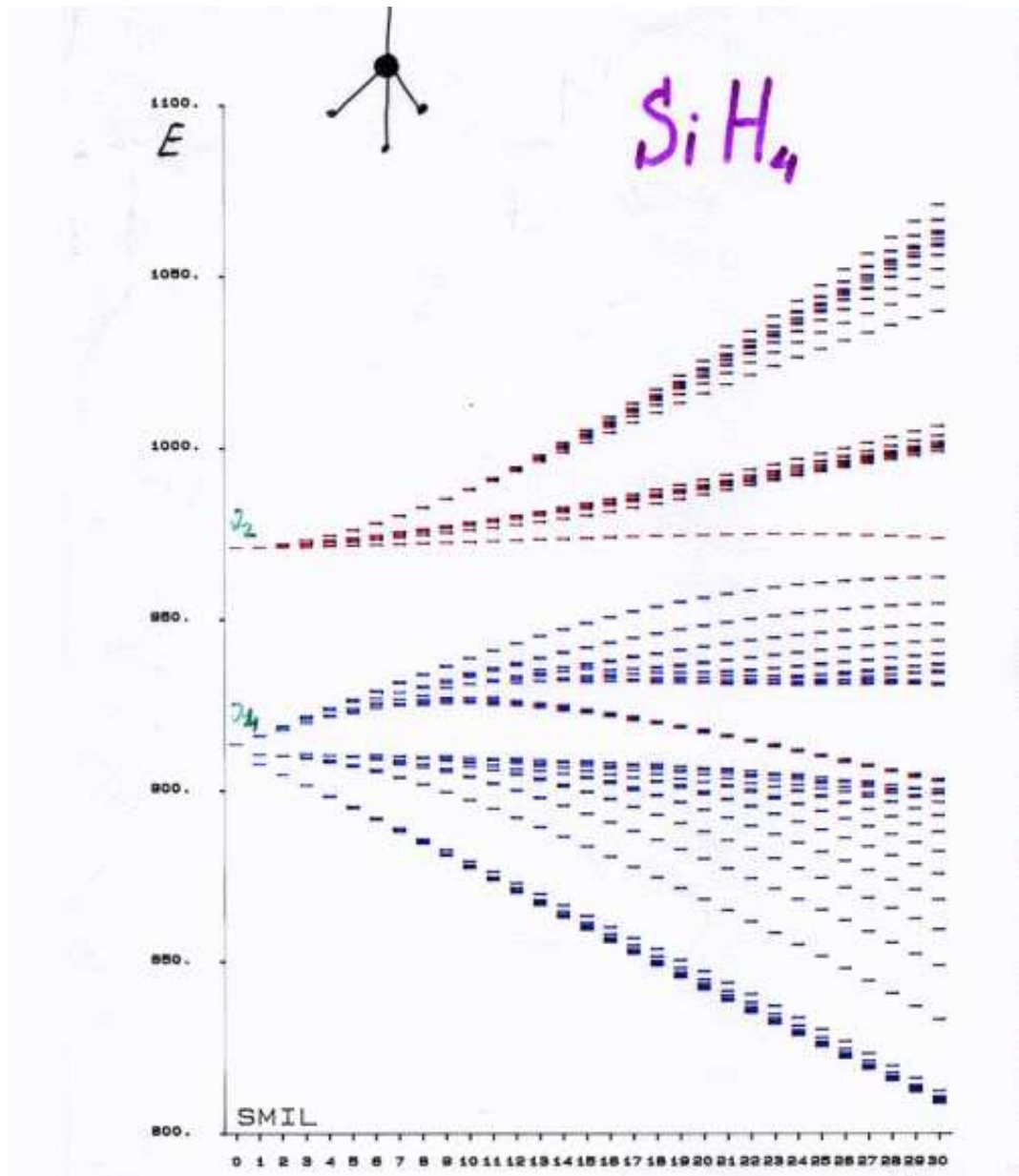
Rotational clusters and bifurcations.

Resonant vibrations, non-linear modes, state counting

H atom in fields. Energy-momentum map evolution.

Rearrangement of bands, Chern classes.

4. Conclusions.



Energy level representation in

Energy (E) - Angular momentum (J)

coordinates corrected with the scalar function $E(J)$ to see better the band structure and the evolution of internal structure of bands as a function of a strict integral of motion J .

Qualitative features to explain:

- i) Rotational clusters (6-fold, 8-fold, 12-fold quasidegenerate)
- ii) Modification of cluster structure (appearance of 12-fold cluster as J increases).
- iii) Number of energy levels in a band:
 $2J + 1 + \Delta$, ??? Δ ???
- iv) Rules for redistribution of energy levels between branches.

Typical rovibrational spectrum of a small molecule



Equilibrium configuration - tetrahedron - T_d point group.

Internal degrees of freedom:

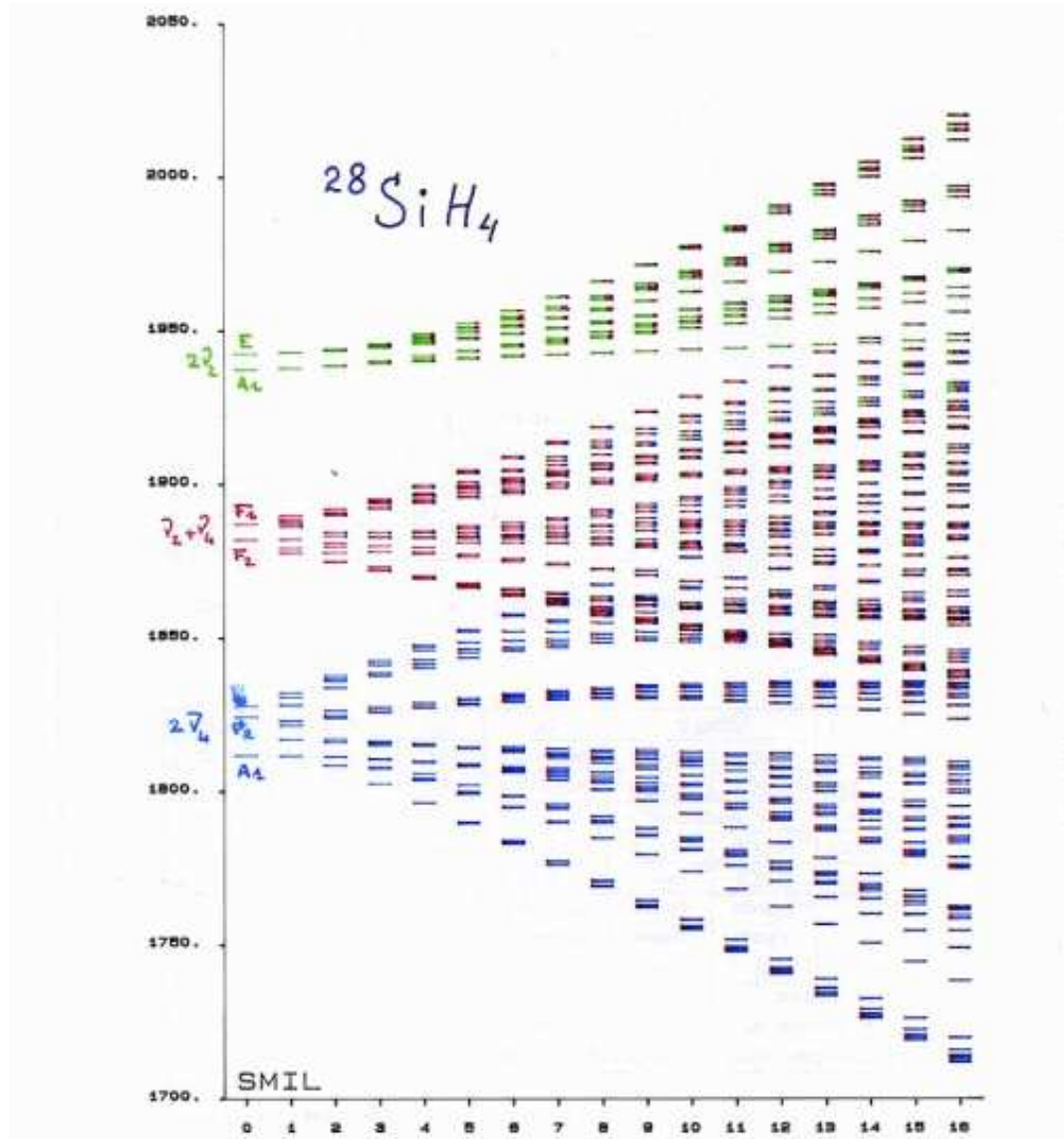
Rotation (non-rigid spherical top) + nine vibrations

ν_1 - nondegenerate, A_1 irrep,

ν_2 - doubly degenerate, E irrep,

ν_3 - triply degenerate, F_2 irrep,

ν_4 - triply degenerate, F_2 irrep.



General scheme of qualitative analysis.

Classical limit of effective quantum Hamiltonians.

Symmetry group action analysis.

Simplest Morse type functions.

Qualitative modifications (bifurcations, redistribution, ...)

Topological quantum numbers.

Examples of *classical limit manifolds* for effective quantum Hamiltonians.

Hamiltonian	Phase space
Rotational	S_2
Vib. polyads	CP_{n-1}
Rot-vib. polyads	$S_2 \times CP_{n-1}$
Rydberg	$S_2 \times S_2$

n being the number of degenerate (or quasi-degenerate) vibrational modes.

Qualitative tools

One degree of freedom dynamical (reduced) systems.

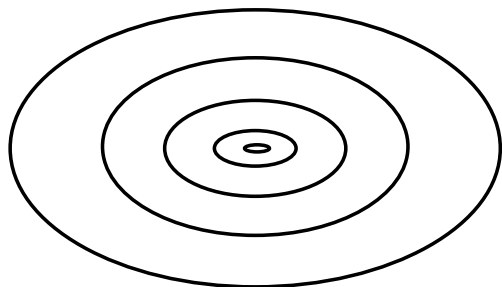
Classical phase portraits.

Reeb diagrams.

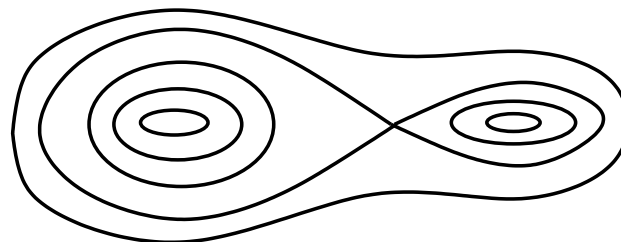
Singularities of classical integrable toric fibrations

Lattices of quantum states and their defects.

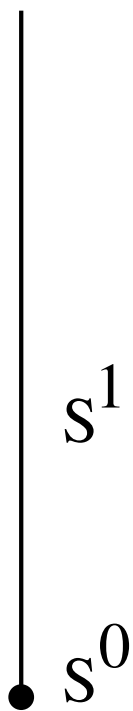
Simplest examples of symmetry and topology manifestations.



e



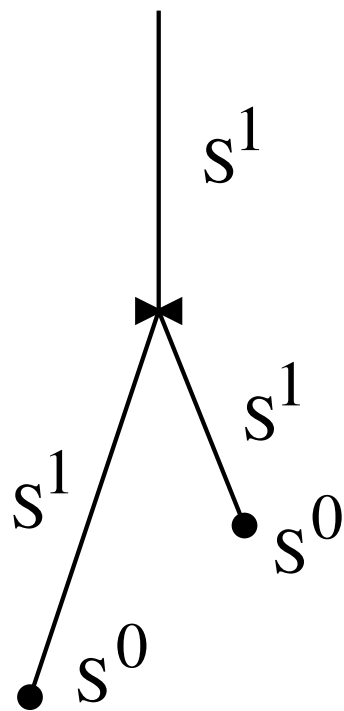
f



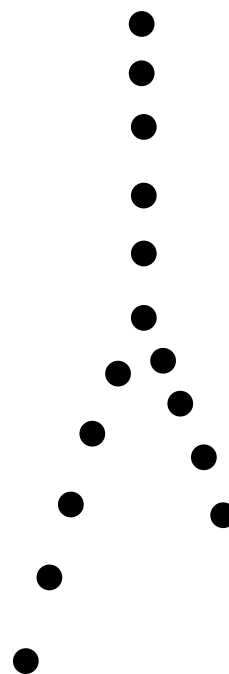
a



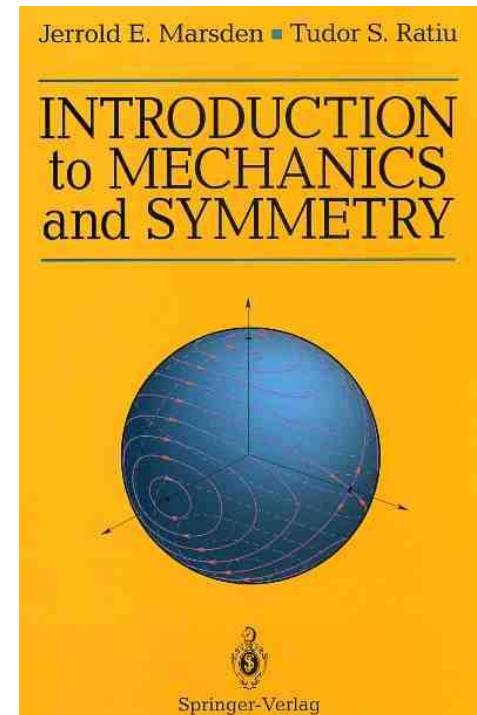
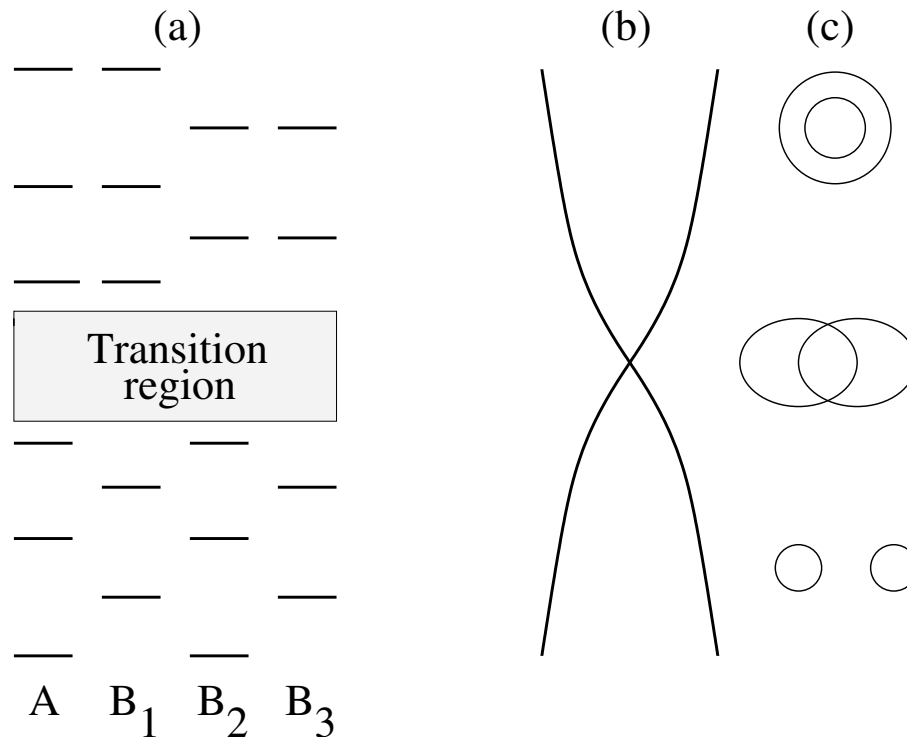
b



c



d



- (a) Schematic representation of the energy level structure for asymmetric top molecule.
- (b) Foliation of the classical phase space (S^2 sphere)
- (c) Geometric representation of the constant energy sections.

Examples of **symmetry group action** on classical limit manifolds.

Images rather than group themselves are important.

Many stationary points are defined by the *group action*.

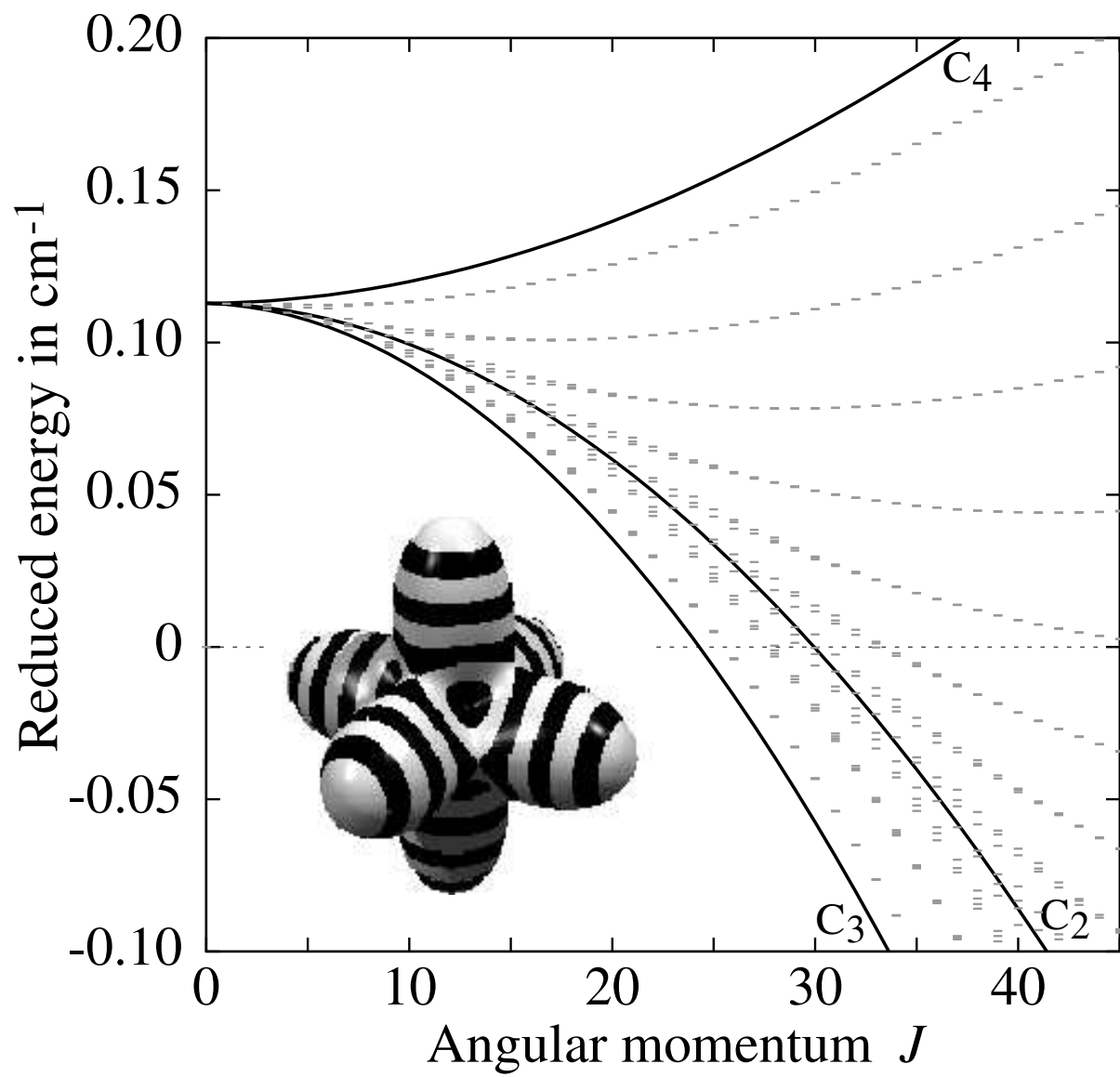
Orbits of the group action, isolated in their strata, are **critical**.

For CF_4 molecule the symmetry group is

$$T_d \times \mathcal{T} \sim O_h$$

T_d point group extended by time reversal \mathcal{T} .

O_h group action on CP_1 phase space for vibrational E polyads is equivalent to natural D_{3h} action on a S_2 sphere.



Simplest Morse type functions:

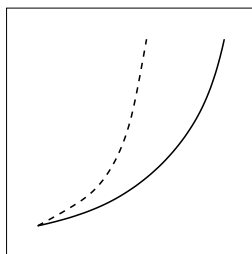
Rotational energy surface for asymmetrical, symmetrical and spherical top molecules at low excitation.

(There are two simplest Morse type functions for the rotational energy surface of AB_4 (or AB_6 , ...) molecule.

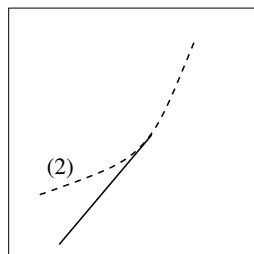
As J increases the rotational energy surfaces become typically more complicated (of non-simplest Morse type). Additional stationary points appear through bifurcations.

1 degree of freedom; 1 control parameter

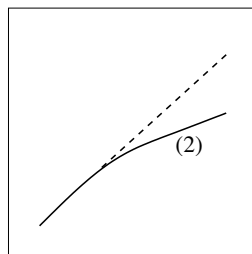
Table 1: Bifurcations in the presence of symmetry. Solid lines denote stable stationary points. Dash lines - unstable stationary points. Numbers in parenthesis indicate the multiplicity of stationary points.



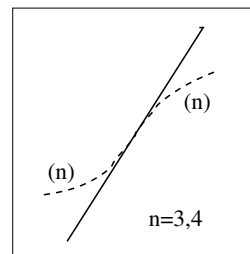
C_1^\pm



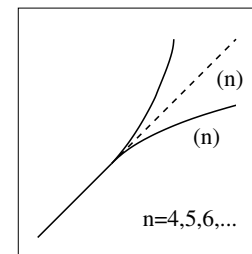
$C_2^{N\pm}$



$C_2^{L\pm}$



$C_n^N, n = 3, 4$



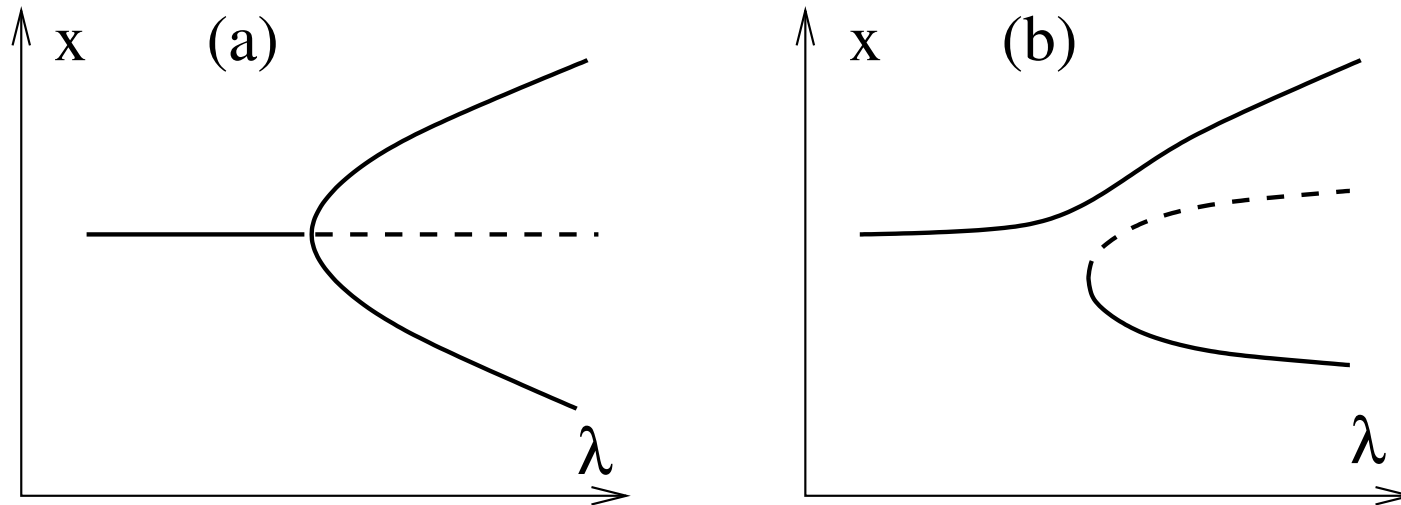
$C_n^{L\pm}, n \geq 4$

I.M. Pavlichenkov, B.Zhilinskii. Critical phenomena in rotational spectra.

Ann. Phys. **184**, 1-32 (1988)

Table 2: Molecular examples of quantum bifurcations in the rotational structure of individual vibrational components under the variation of the absolute value of angular momentum, J . J_c is the critical value corresponding to bifurcation.

Molecule	Component	J_c	Bifurcation type
SiH ₄	$\nu_2(+)$	12	C_2^{N+}
SnH ₄	$\nu_2(-)$	10	$C_2^{N+}, C_3^N, C_4^N, C_2^{N-}$
CF ₄	$\nu_2(+)$	50	C_4^{L+}
H ₂ Se	$ 0\rangle$	20	C_2^{L+}



Imperfect bifurcations.

(a) Position x of stationary points as a function of control parameter λ during a pitchfork bifurcation in the presence of C_2 local symmetry.

(b) Modifications induced by small symmetry perturbation of lower symmetry.

Solid line - stable stationary points. Dash lines - unstable stationary points.

[B. Zhilinskii, I. Kozin, S. Petrov, Spectrochim Acta A **55**, 1471-84 (1999)]

Semi-quantum approach:

One part of variables (rotational) is treated as classical whereas another (vibrational) as quantum.

Symbol of the Hamiltonian is a matrix defined over classical limit manifold.

Example: (rotational Hamiltonian for three vibrational states).

$$H = \begin{pmatrix} H_{11}^J(\theta, \varphi) & H_{12}^J(\theta, \varphi) & H_{13}^J(\theta, \varphi) \\ H_{21}^J(\theta, \varphi) & H_{22}^J(\theta, \varphi) & H_{23}^J(\theta, \varphi) \\ H_{31}^J(\theta, \varphi) & H_{32}^J(\theta, \varphi) & H_{33}^J(\theta, \varphi) \end{pmatrix}$$

θ, φ are the angles characterizing the orientation of the angular momentum \mathbf{J} .

Eigenvalues of matrix Hamiltonian play the role of rotational energy surfaces for different vibrational quantum states.

Presence or absence of *degeneracy* is extremely important.

Alternative complete classical description of the same model can be done by a Hamiltonian function defined over classical limit manifold

$$S_2 \times CP_2$$

for the complete rotation-vibration problem.

Vibrational quasi-modes.

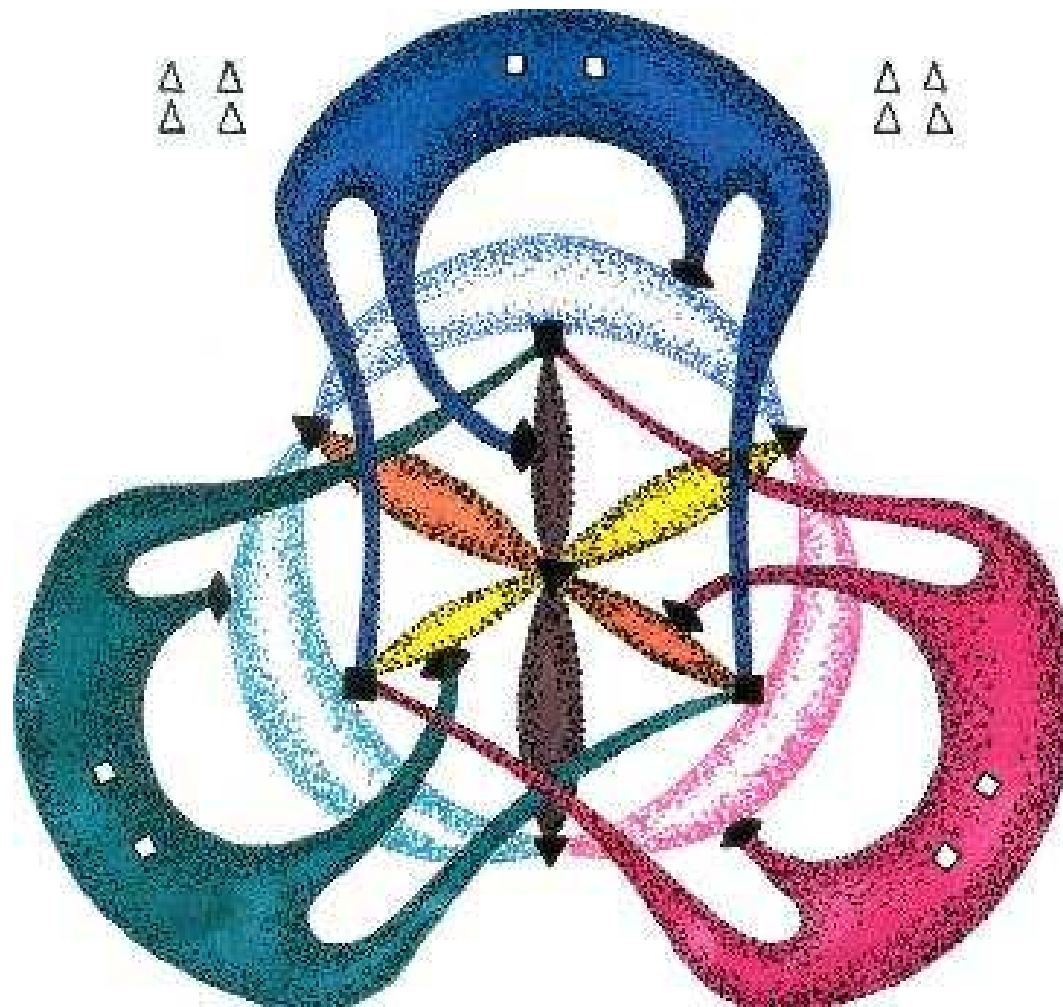
27 nonlinear normal modes for triply degenerate vibrational polyads correspond to 27 relative equilibria on the reduced phase space of the triply degenerate oscillator (reduced phase space is topologically CP_2).

For vibrational $n\nu_2^{(E)}$ polyads (reduced space is topologically $CP_1 \sim S^2$ with D_{3h} action) there are 8 nonlinear normal modes.

CH_4 molecule has 63 nonlinear normal modes (one for ν_1 , 8 for ν_2 , 27 for ν_3 , 27 for ν_4).

Montaldi J., Roberts R., Stewart I., *Philos. Trans. Roy. Soc. London*, A 325, 237–293 (1988);

Zhilinskii B., *Chem. Phys.* 137, 1-13 (1989).



$T_d (O, O_h)$ group action on CP_2 . Five critical orbits include 27 points.

Qualitative models:

N –degree of freedom reduced systems

Integrable Hamiltonian models

Energy-momentum map images (singular and regular parts)

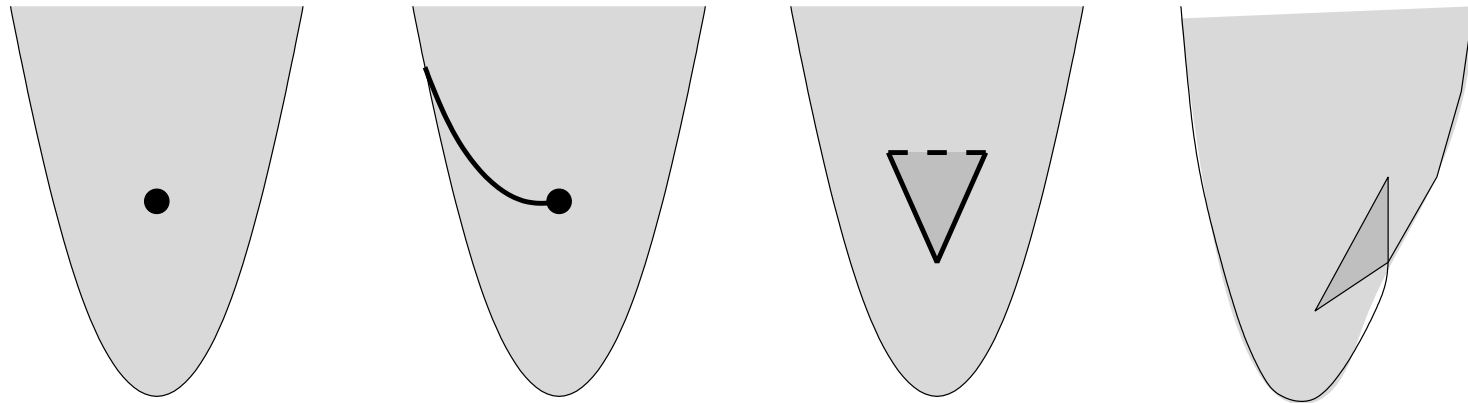
Toric fibrations with singularities.

Cushman R., Bates L. *Global aspects of classical integrable systems*. Birkhäuser, Basel, 1997

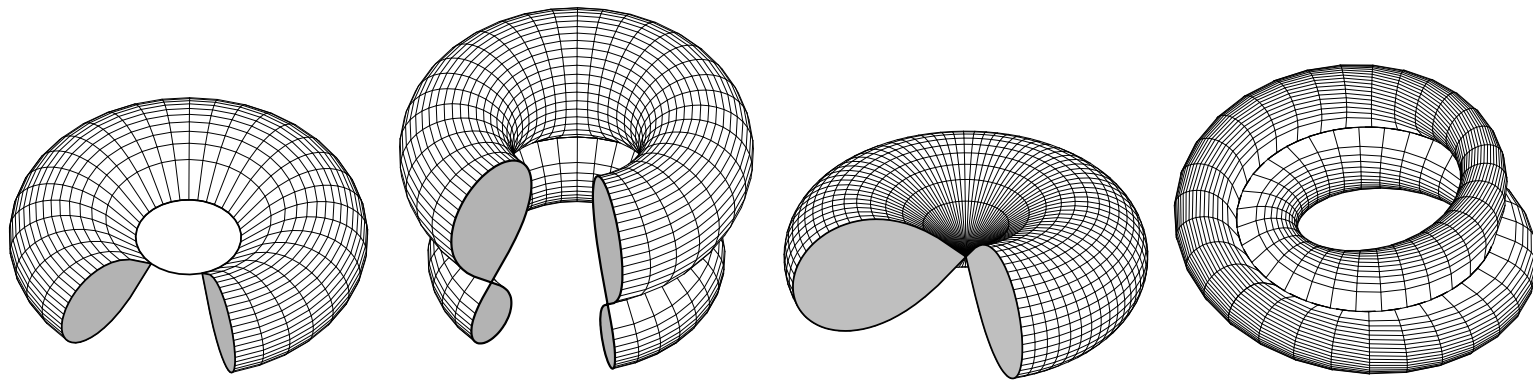
Duistermaat J.J. *On global action angle coordinates*. *Comm. Pure Appl. Math.* **33**, 687-706 (1980)

Nekhoroshev N.N. *Action-angle variables and their generalizations*. *Trans. Moscow Math. Soc.* **26**, 180-198 (1972)

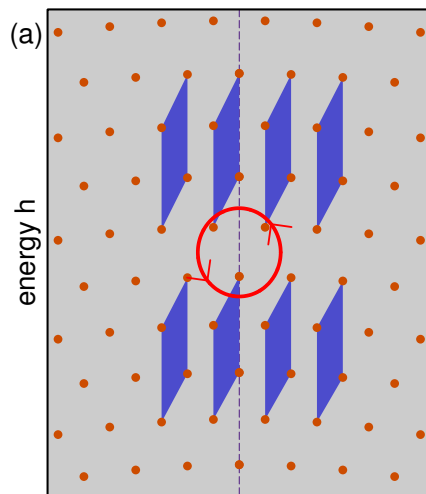
Bolsinov A.V., Fomenko A.T. *Integrable Hamiltonian Systems*. Chapman & Hall, 2004



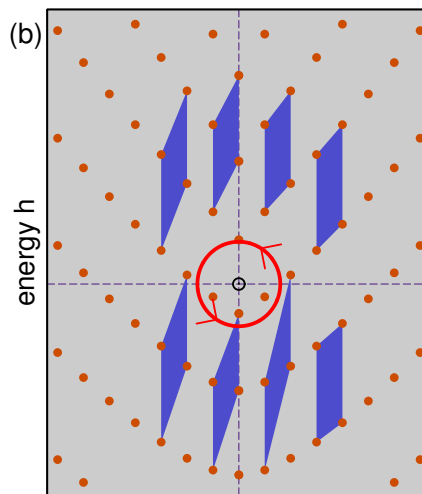
Typical images of the energy momentum map for completely integrable Hamiltonian systems with two degree of freedom in the case of integer monodromy, fractional monodromy, nonlocal monodromy, and bidromy. Values in light shaded area lift to single 2-tori; values in dark shaded area lift to two 2-tori.



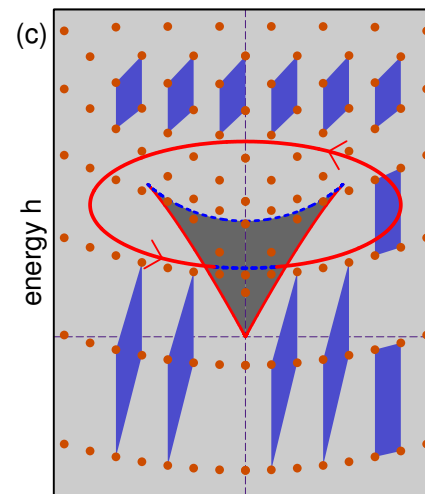
Two dimensional singular fibers in the case of integrable Hamiltonian systems with two degrees of freedom (left to right): singular torus, bitorus, pinched and curled tori.



value of the first action

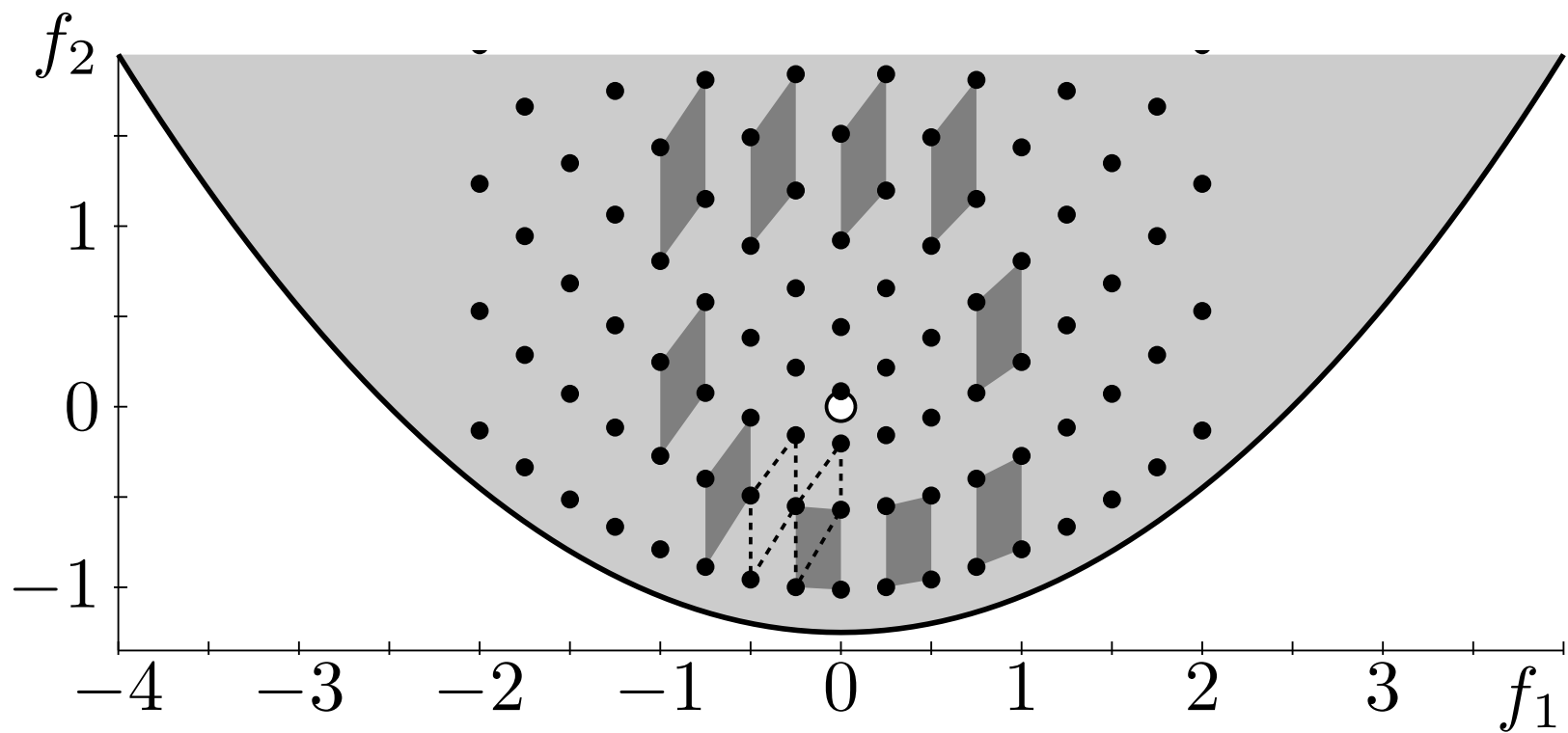


value of the first action

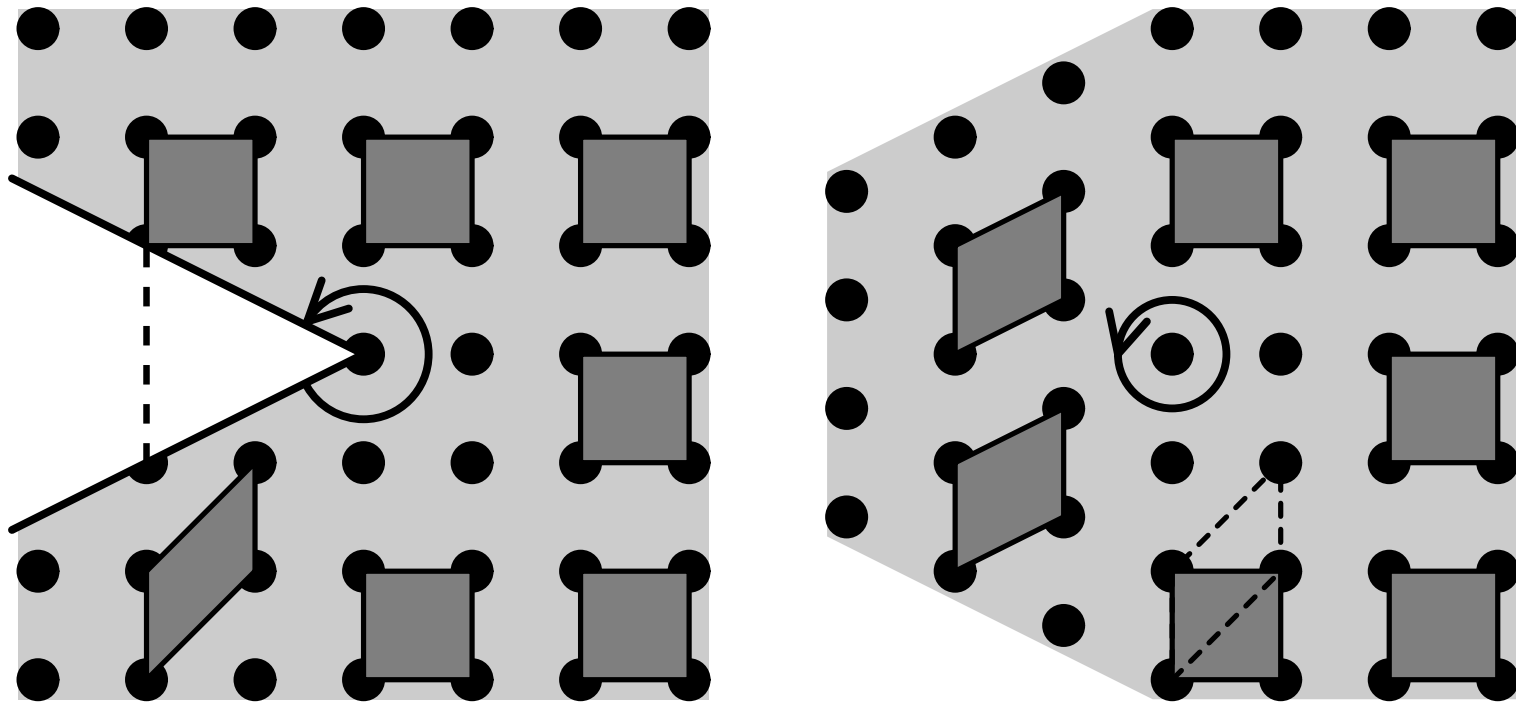


value of the first action

Quantum joint spectra for typical regions of the image of energy - momentum map for integrable problems.

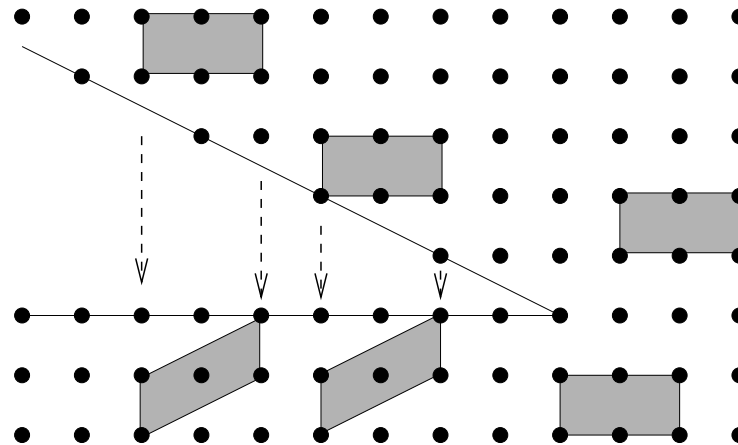
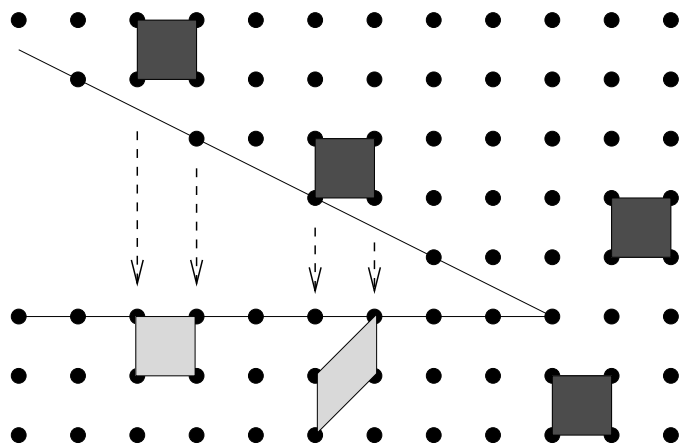


Quantum monodromy for 1 : (-1) resonant oscillator system.



Construction of the $1:(-1)$ lattice defect starting from the regular Z^2 lattice. Dark grey quadrangles show the evolution of an elementary lattice cell along a closed path around the defect point.

BZ, in "Topology in condensed matter", Springer series in solid state sciences, vol. 150, 165-186 (2006)



Construction of 1 : 2 rational lattice defect.

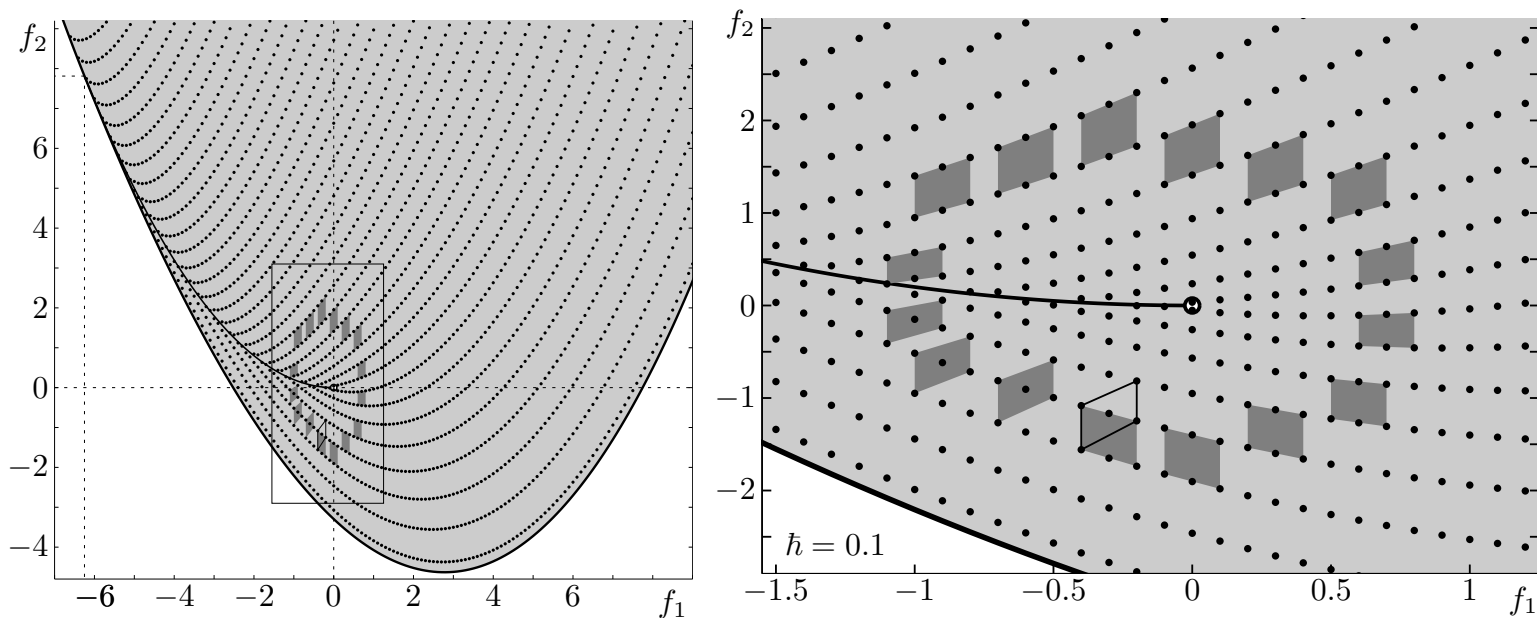
Left: Elementary cell does not pass

Right: Double cell passes.

unambiguously.

N.Nekhoroshev, D. Sadovskii, BZ, Fractional Hamiltonian monodromy. Ann. Henri Poincaré, 7, 1099-1211 (2006)

“Wall crossing“ example

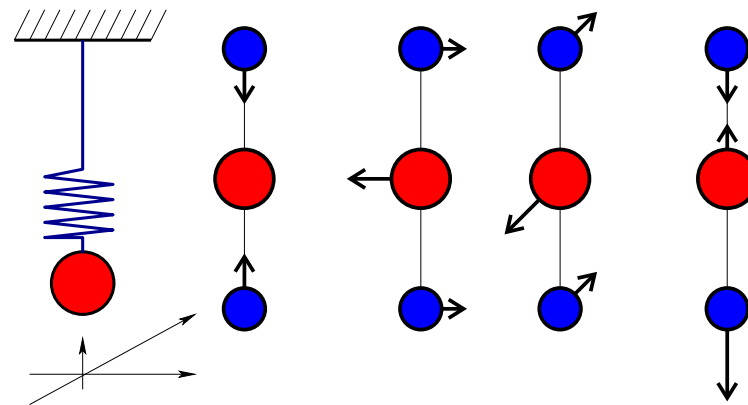


Quantum fractional monodromy for 1 : (−2) resonant oscillator system.

$$F_1 = \frac{\omega}{2}(p_1^2 + q_1^2) - \frac{2\omega}{2}(p_2^2 + q_2^2) + R_1(q, p), \quad (1)$$

$$F_2 = \text{Im}[(q_1 + ip_1)^2(q_2 + ip_2)] + R_2(q, p). \quad (2)$$

Monodromy of *swing-spring* with 1:1:2 resonance - model of Fermi resonance in CO₂



3D of freedom dynamical system - three resonant nonlinear oscillators - in the presence of axial symmetry.

CO₂ has four vibrational modes: symmetric and antisymmetric stretch and doubly degenerate bending. Antisymmetric vibration is out of resonance and can be “neglected” (averaged).

Integrable model

$$L = \frac{1}{2}(z_2\bar{z}_3 - \bar{z}_2z_3)i, \quad (3)$$

$$N = \bar{z}_1z_1 + \frac{1}{2}\bar{z}_2z_2 + \frac{1}{2}\bar{z}_3z_3, \quad (4)$$

$$H = aS + bR + cR^2 + E(N, L). \quad (5)$$

written in terms of invariant polynomials

$$R = \frac{1}{2}\bar{z}_2z_2 + \frac{1}{2}\bar{z}_3z_3 = (n_2 + n_3), \quad (6)$$

$$S = \frac{1}{4}(\bar{z}_1z_3^2 + z_1\bar{z}_3^2 + z_1\bar{z}_2^2 + \bar{z}_1z_2^2), \quad (7)$$

$$T = \frac{1}{4}(\bar{z}_1z_3^2 - z_1\bar{z}_3^2 - z_1\bar{z}_2^2 + \bar{z}_1z_2^2)i, \quad (8)$$

with $z = q - ip$, $\bar{z} = q + ip$, $\{z, \bar{z}\} = 2i$

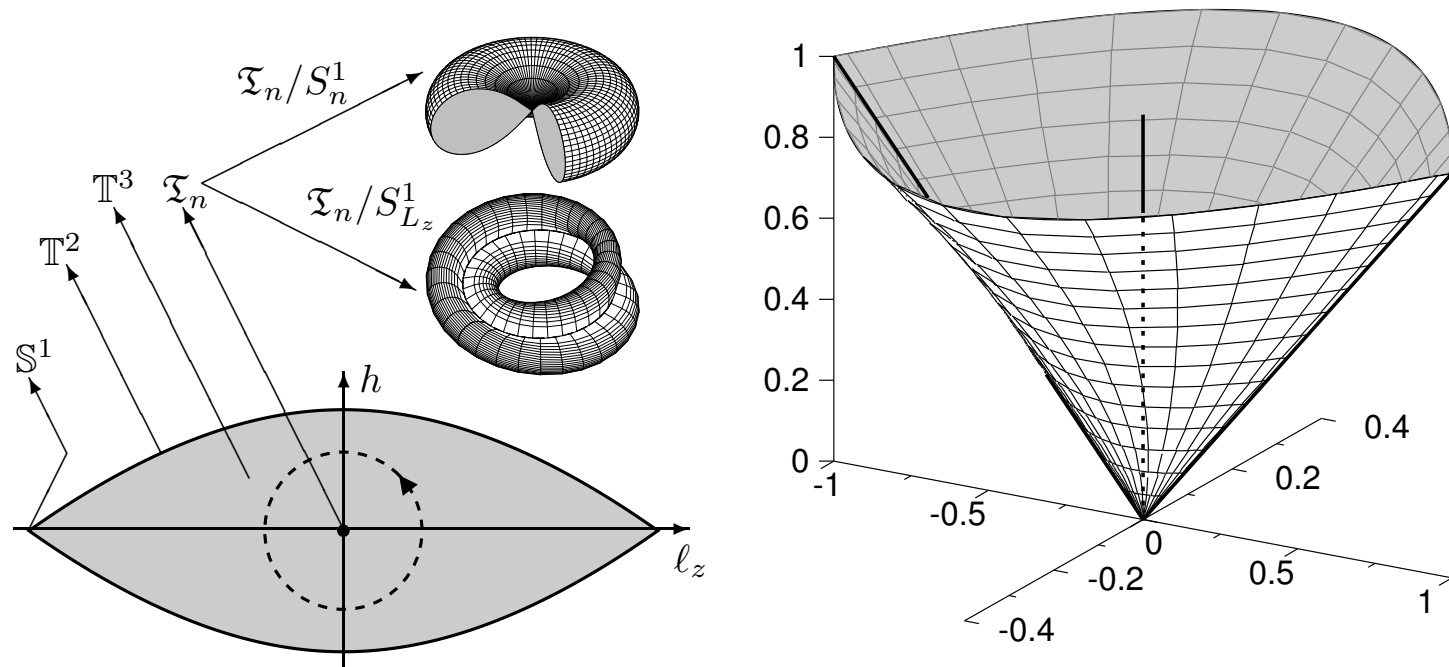
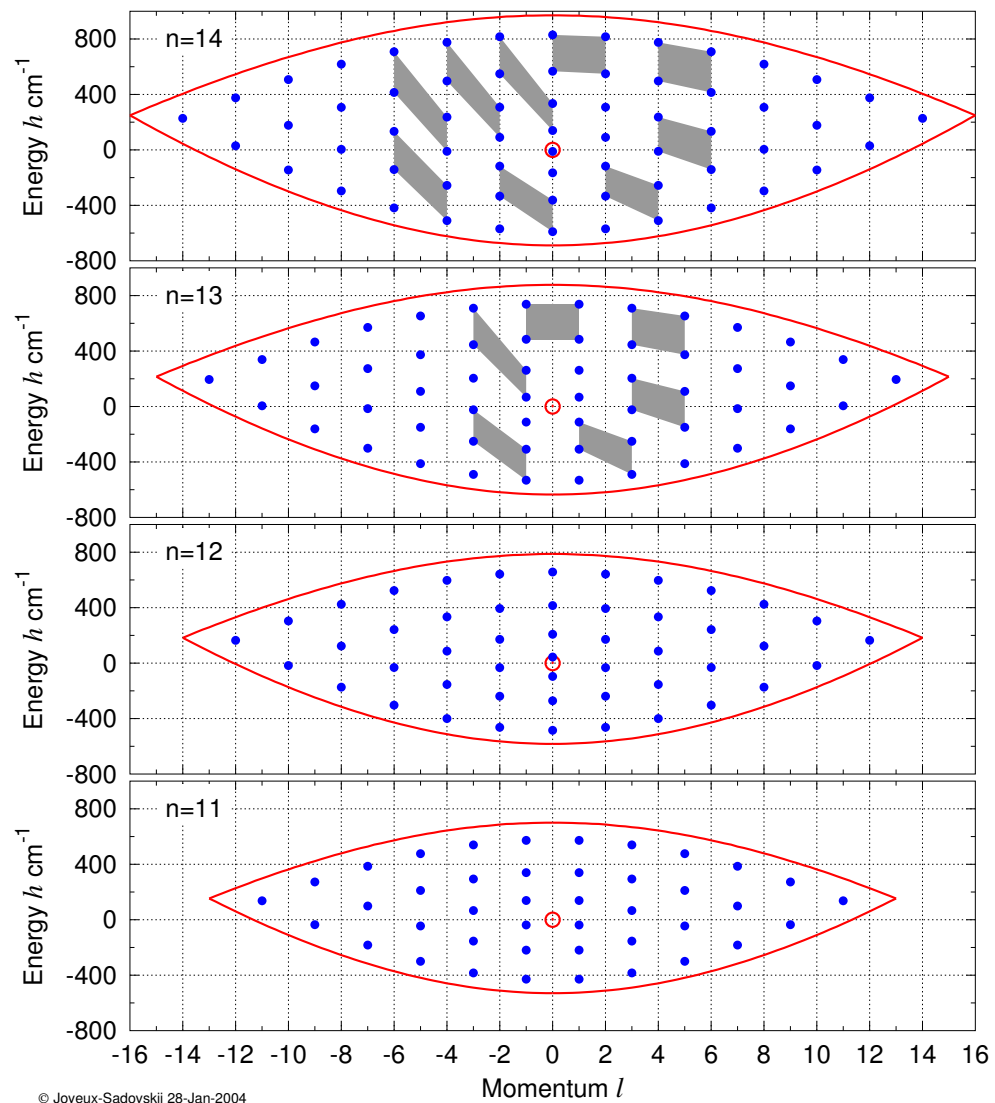
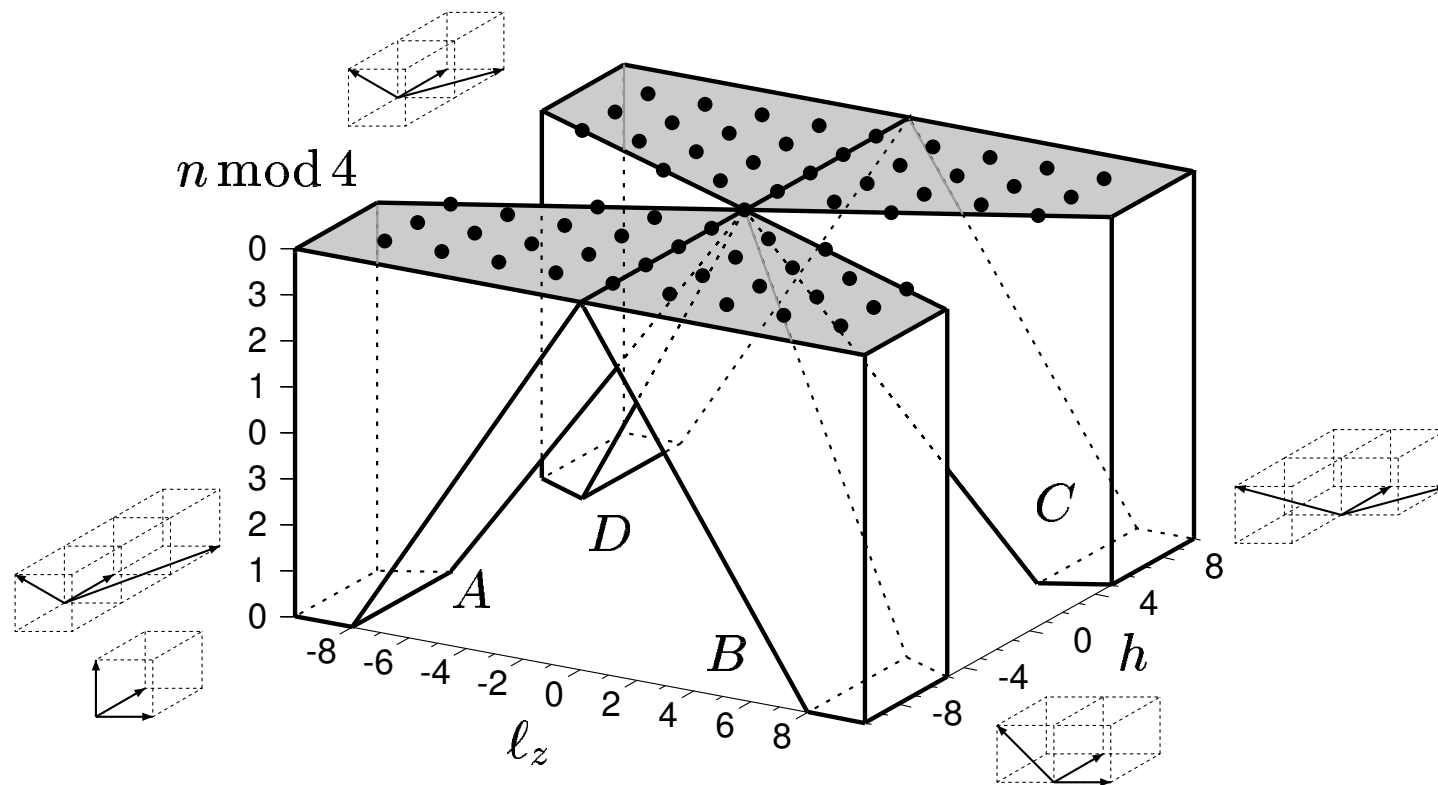


Image of the energy momentum map for the 1 : 1 : 2 resonant oscillator system with axial symmetry (*and without detuning*). Full 3D-image, typical constant- n section and fibers.

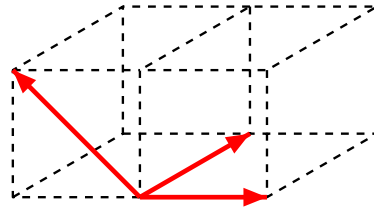
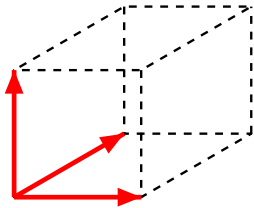
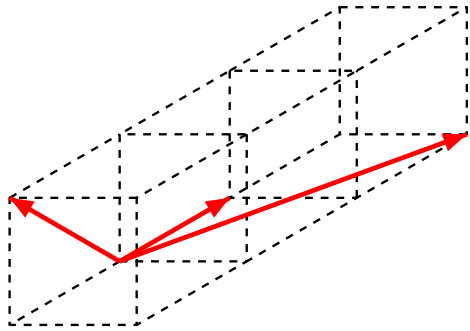
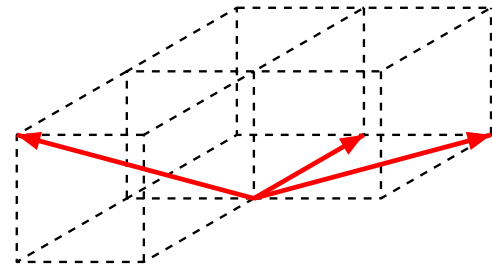
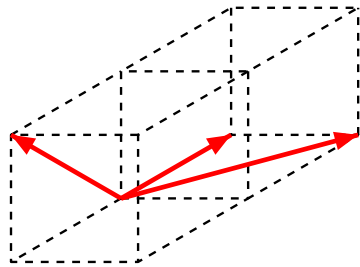
R.H. Cushman *et al*, *Phys.Rev.Lett.* **93**, 024302, 2004



© Joyeux-Sadovskii 28-Jan-2004



Quantum lattice with several elementary monodromy defects.



Matrix representation of monodromy for model with 1 : 1 : 2 resonance

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (9)$$

The monodromy matrix is defined up to similarity transformation $M \sim AMA^{-1}$ with $A \in SL(3, Z)$.

Rearrangement of bands. Topology aspects.

Semi-quantum model.

Slow variables (classical) - a compact phase space M

Fast variables (quantum) - k quantum states at each point of M , i.e. we have (k bands).

Global construction - *complex vector bundle* of rank k .

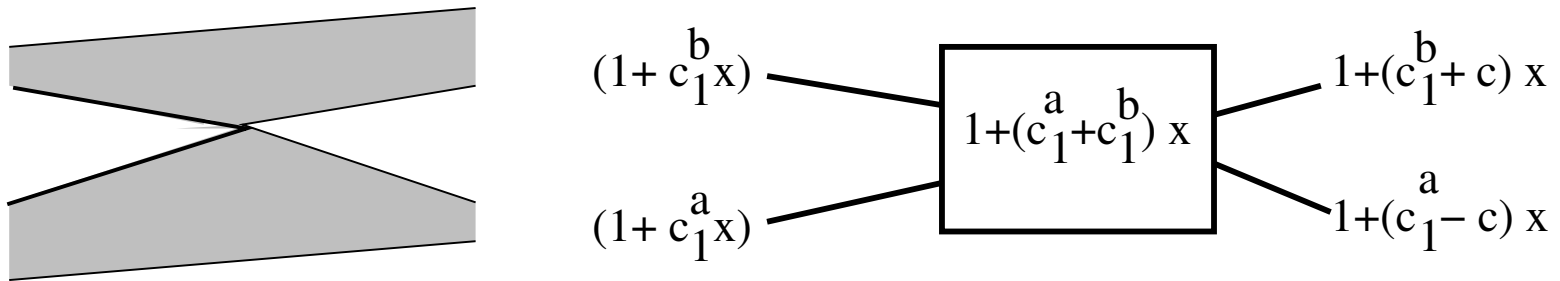
Topological non-triviality is given by *Chern classes*.

Chern polynomial:

$$1 + c_1x + c_2x^2 + \cdots ,$$

A *trivial rank 2* vector bundle over CP_1 can be rearranged into two nontrivial line bundles: $1 = (1 + c_1 x)(1 - c_1 x)$.

Possible rearrangement:



Here c gives the number of states transferred from one band to another. PRL, 85, 960 (2000).

A *trivial rank 2* vector bundle over CP_2 cannot be rearranged into two nontrivial line bundles because

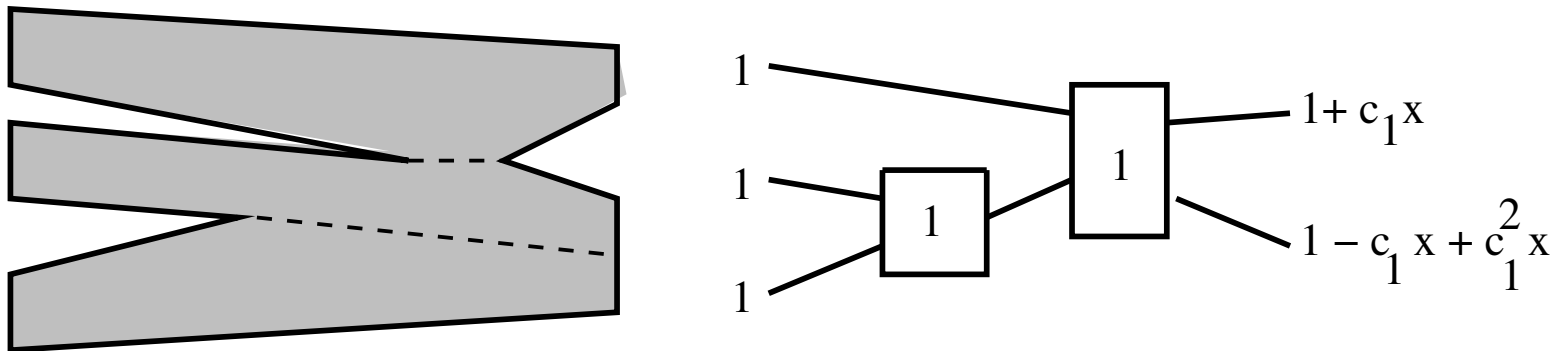
$$1 = (1 + c_1 x)(1 + c'_1 x) = 1 + (c_1 + c'_1)x + c_1 c'_1 x^2 \quad (10)$$

relation (10) implies that $c_1 = c'_1 = 0$

The redistribution of energy levels between *three bands over CP_2* classical phase space is *possible*

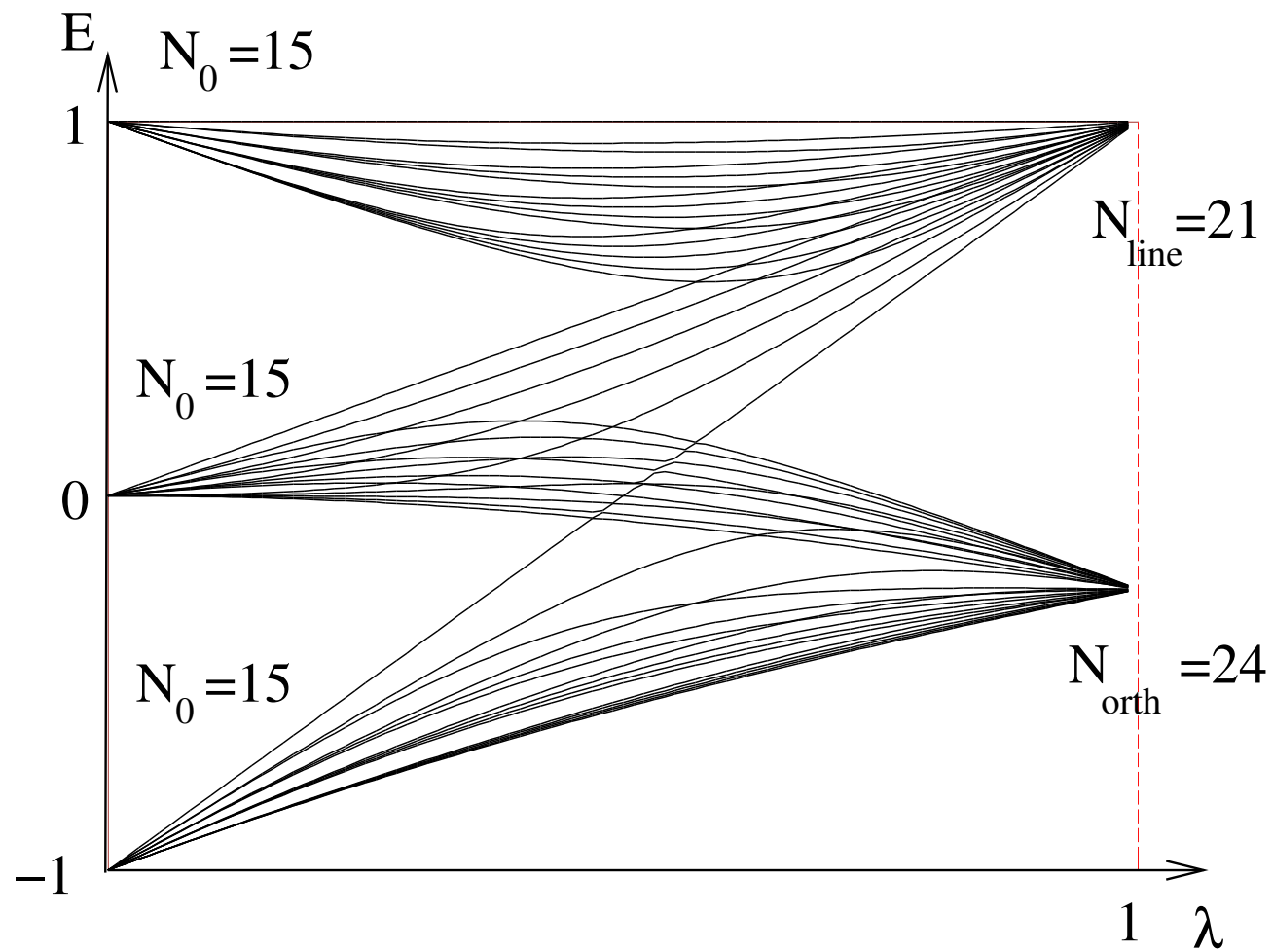
$$1 = (1 + c_1 x)(1 - c_1 x + c_1^2 x^2). \quad (11)$$

The first Chern class for the line bundle can be arbitrary, but the first and the second Chern classes for the complementary rank 2 vector bundle are non-trivial.



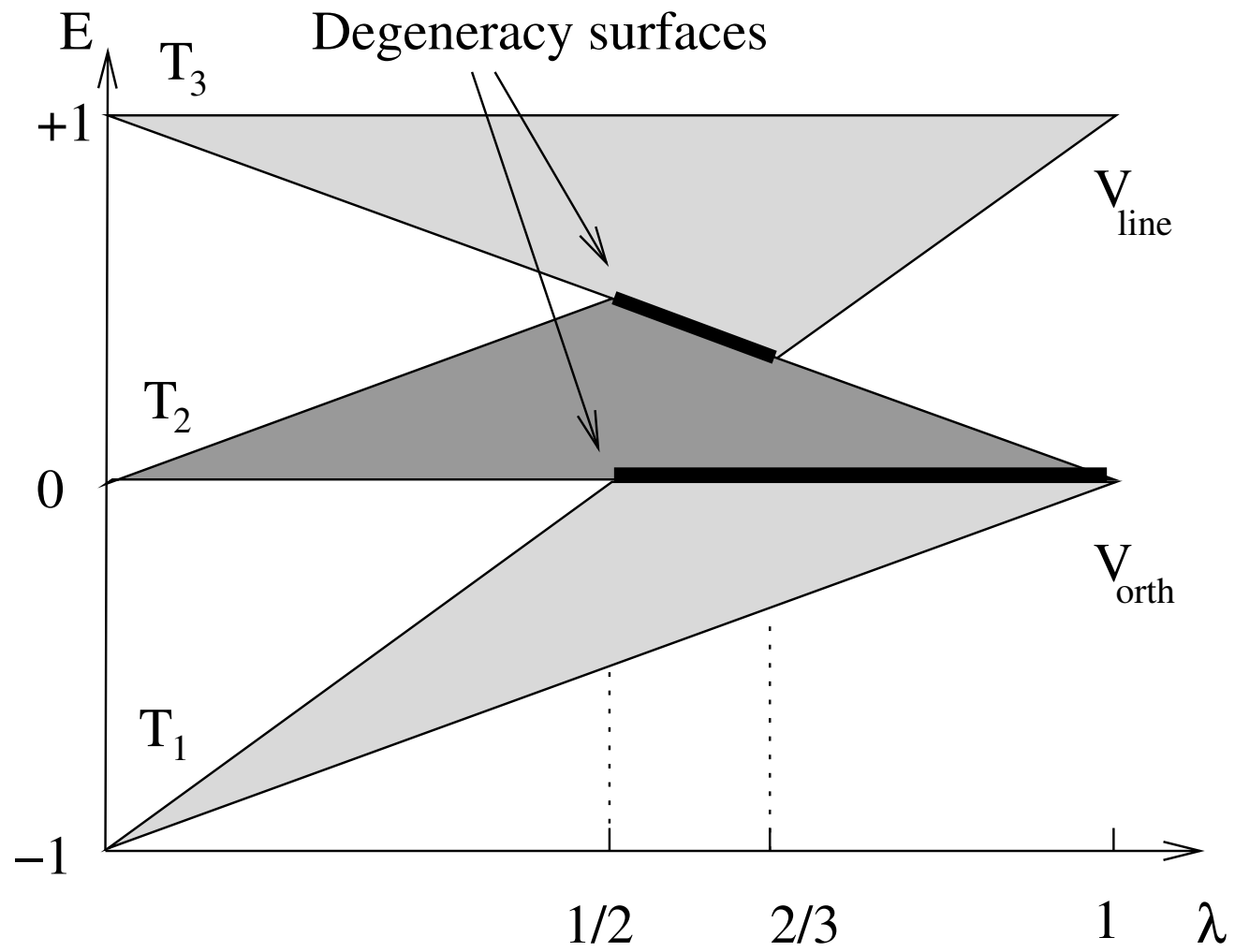
Rank 2 band cannot be decomposed without “touching” an extra band.

“topological entanglement”



(a)

F. Faure B.Zh., *Topologically coupled energy bands in molecules*. Phys. Lett. A 302, 242-252 (2002).



(b)

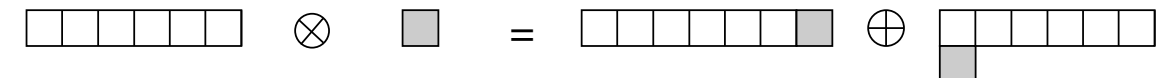
Classical limit for rearrangement of three bands over CP_2 space.

Three electronic states (H_0) with vibronic coupling (H_1).

$$H_\lambda ([Z]) = (1 - \lambda) H_0 + \lambda H_1 ([Z]), \quad (12)$$

with $H_0 = \text{Diag}(-1, 0, 1)$.

$$(H_1 ([Z]))_{i,j=1,2,3} = \overline{Z}_i Z_j / \left(\sum_{k=1,2,3} |Z_k|^2 \right) = (|Z\rangle\langle Z|)_{i,j}.$$

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


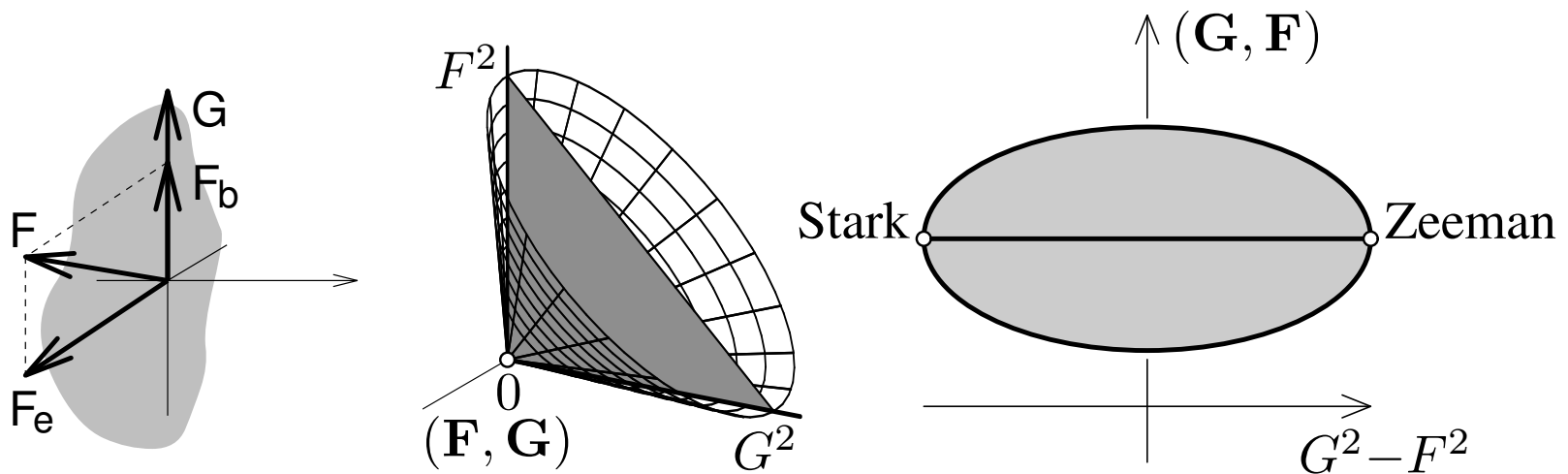
Numbers of states in bands:

$$\mathcal{N}_{\text{Line}} = (N + 2)(N + 3)/2 \sim N^2/2,$$

$$\mathcal{N}_{\text{Orth}} = N(N + 2) \sim N^2.$$

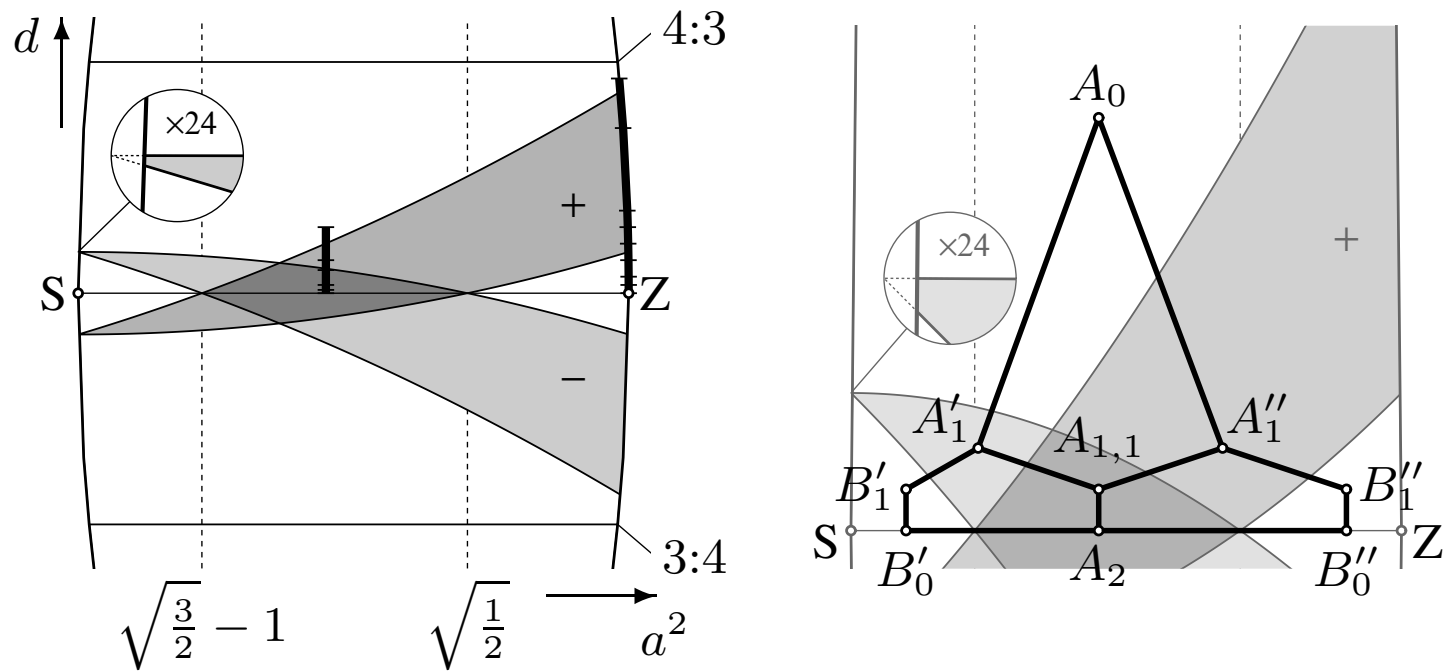
Hydrogen atom in external electric and magnetic fields

$$H = \frac{1}{2}\mathbf{P}^2 - \frac{1}{|\mathbf{Q}|} + F_e Q_2 + F_b Q_1 + \frac{G}{2}(Q_2 P_3 - Q_3 P_2) + \frac{G^2}{8}(Q_2^2 + Q_3^2) = E,$$



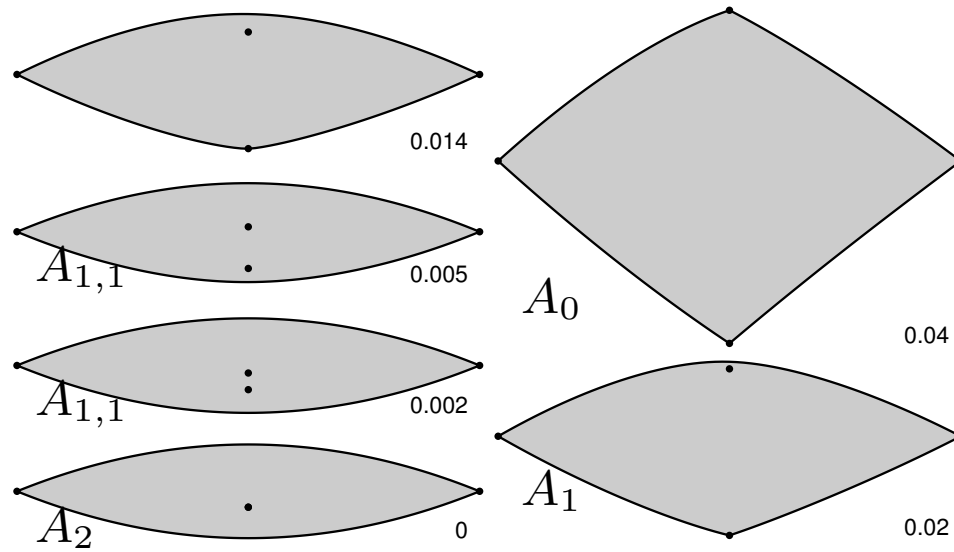
L.Michel,B.Zh. Phys.Rep. 341, 175-264 (2001);

K.Efstathiou, D. Sadovskii Rev.Mod.Phys. **82**, 2100 (2010).

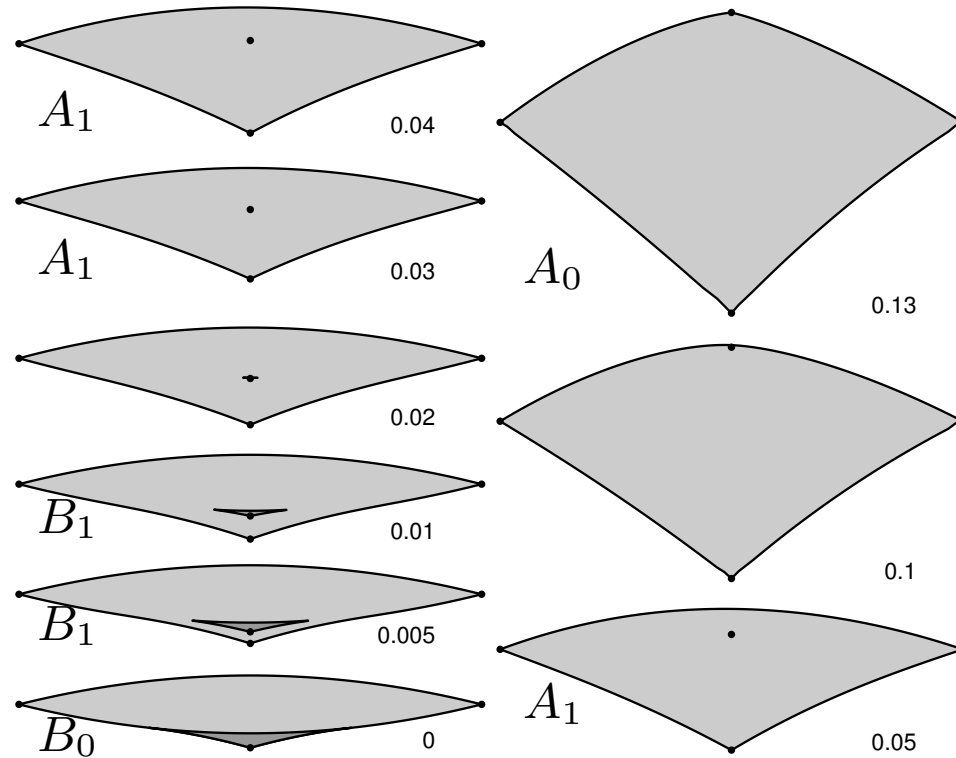


Structure of the 1:1 zone. Different dynamical strata of the zone (left) correspond to vertices of the genealogy graph (right).

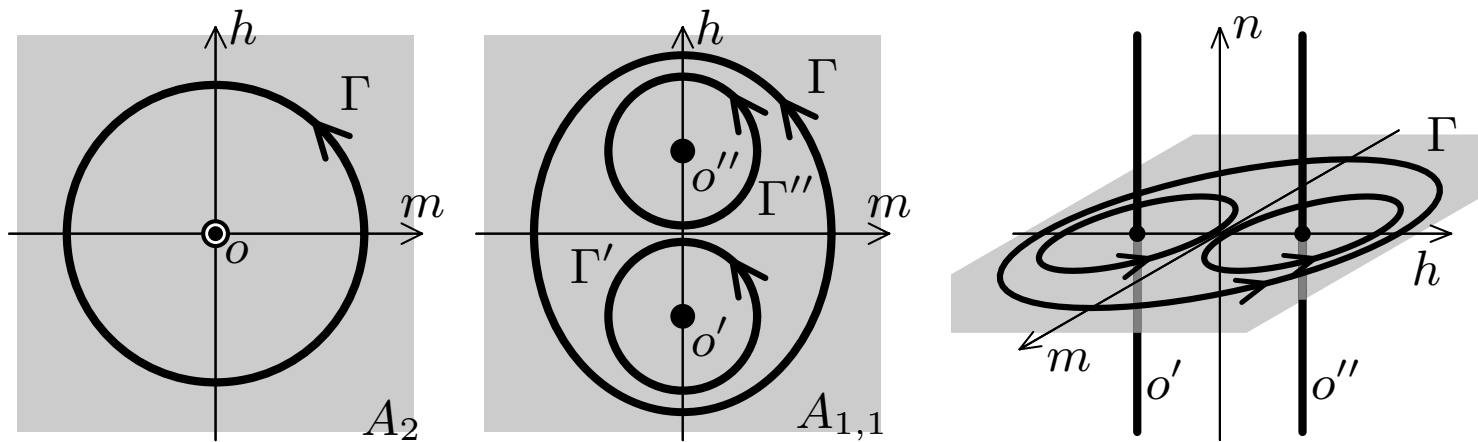
path $A_2 A_{11} A_1'' A_0$ with fixed $a^2 = 0.45$



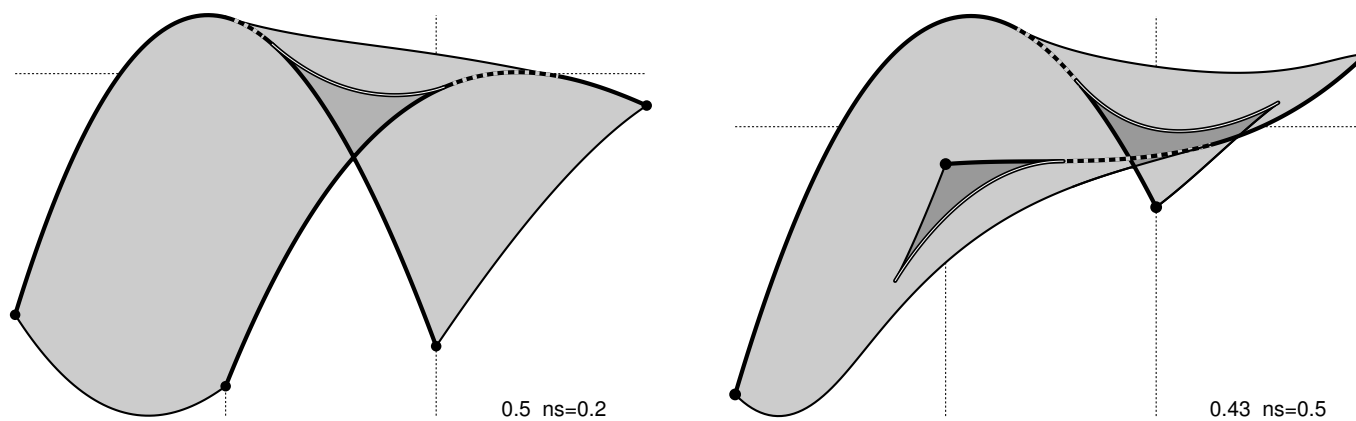
path $B_0'' B_1'' A_1'' A_0$ for parallel fields near Z



Changes (of the constant n section) of the stratified images of the energy-momentum map for detuned 1:1 systems.



Contours in the stratified range of the energy-momentum map in the 1:1 zone which encircle isolated critical values o and o' and o'' .



1:2 systems with fractional bidromy (left) and fractional monodromy (right).

Conclusions

Universal qualitative features observed in the behavior of different systems stimulated appearance of new mathematical concepts:

fractional monodromy, bidromy, ...

Qualitative mathematical description reveals universal behavior of different physical, chemical, biological, ... systems.

Spiral phyllotaxis for sunflower - Hamiltonian monodromy.

