New Qualitative Features in Intramolecular Dynamics: Simple Examples

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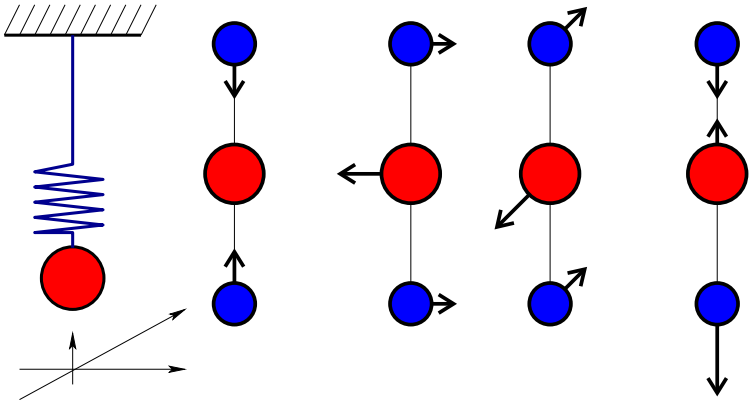
Monodromy of *swing-spring* with 1:1:2 resonance - model of Fermi resonance in CO_2



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

CO_2 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

$$L = \frac{1}{2}(z_2\bar{z}_3 - \bar{z}_2 z_3)\mathrm{i}, \tag{1}$$

$$N = \bar{z}_1 z_1 + \frac{1}{2}\bar{z}_2 z_2 + \frac{1}{2}\bar{z}_3 z_3, \tag{2}$$

$$H = aS + bR + cR^2 + E(N, L). \tag{3}$$

written in terms of invariant polynomials

$$R = \tfrac{1}{2}\bar{z}_2 z_2 + \tfrac{1}{2}\bar{z}_3 z_3 = (n_2 + n_3), \tag{4}$$

$$S = \tfrac{1}{4}(\bar{z}_1 z_3^2 + z_1\bar{z}_3^2 + z_1\bar{z}_2^2 + \bar{z}_1 z_2^2), \tag{5}$$

$$T = \tfrac{1}{4}(\bar{z}_1 z_3^2 - z_1\bar{z}_3^2 - z_1\bar{z}_2^2 + \bar{z}_1 z_2^2)\mathrm{i}, \tag{6}$$

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

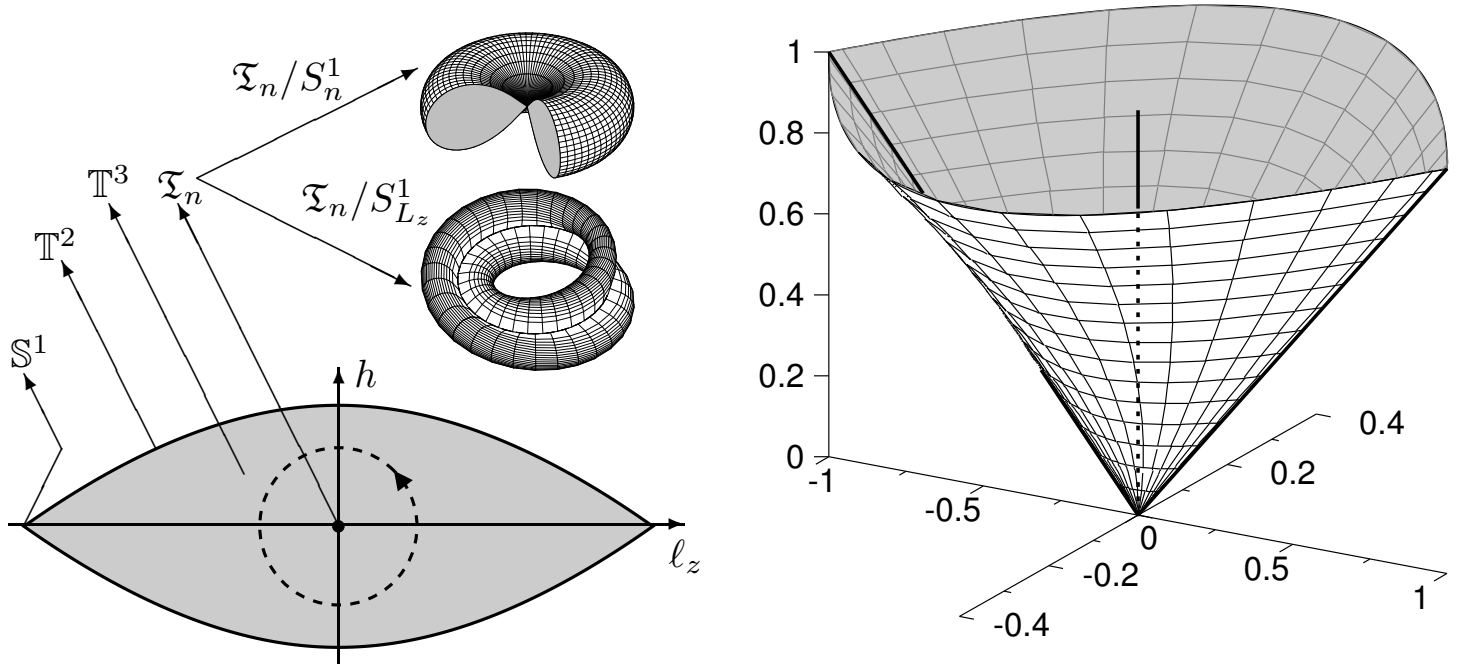
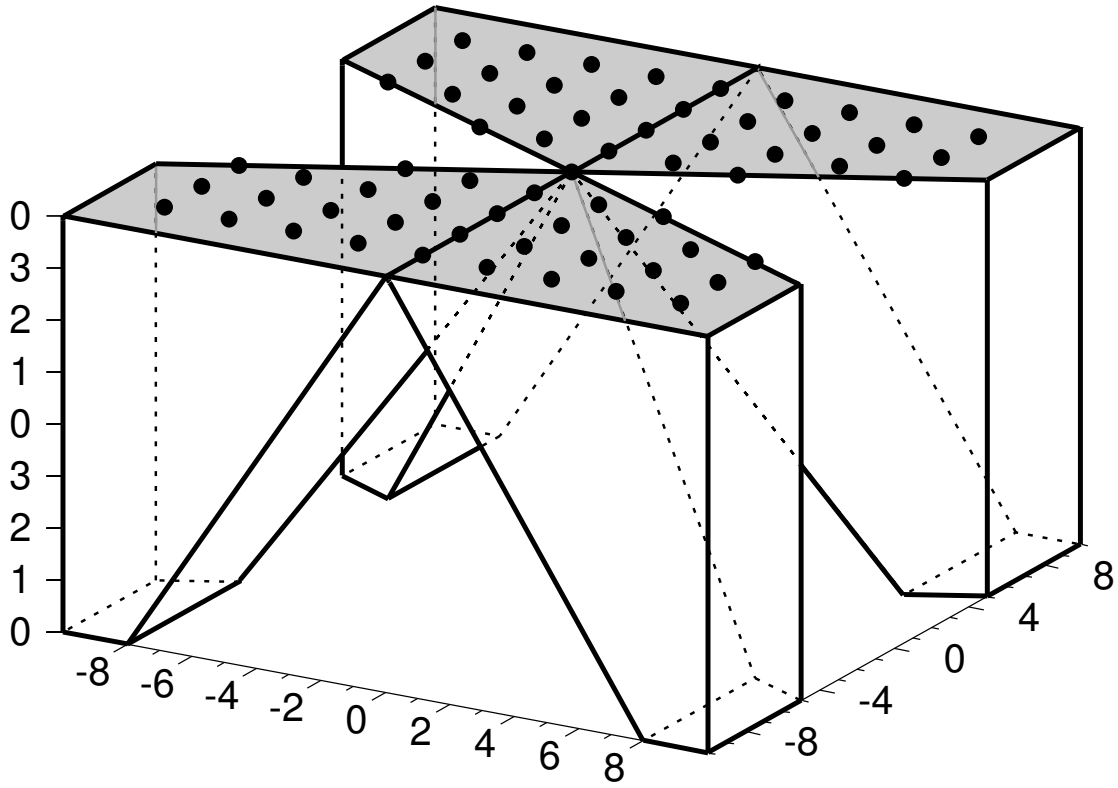
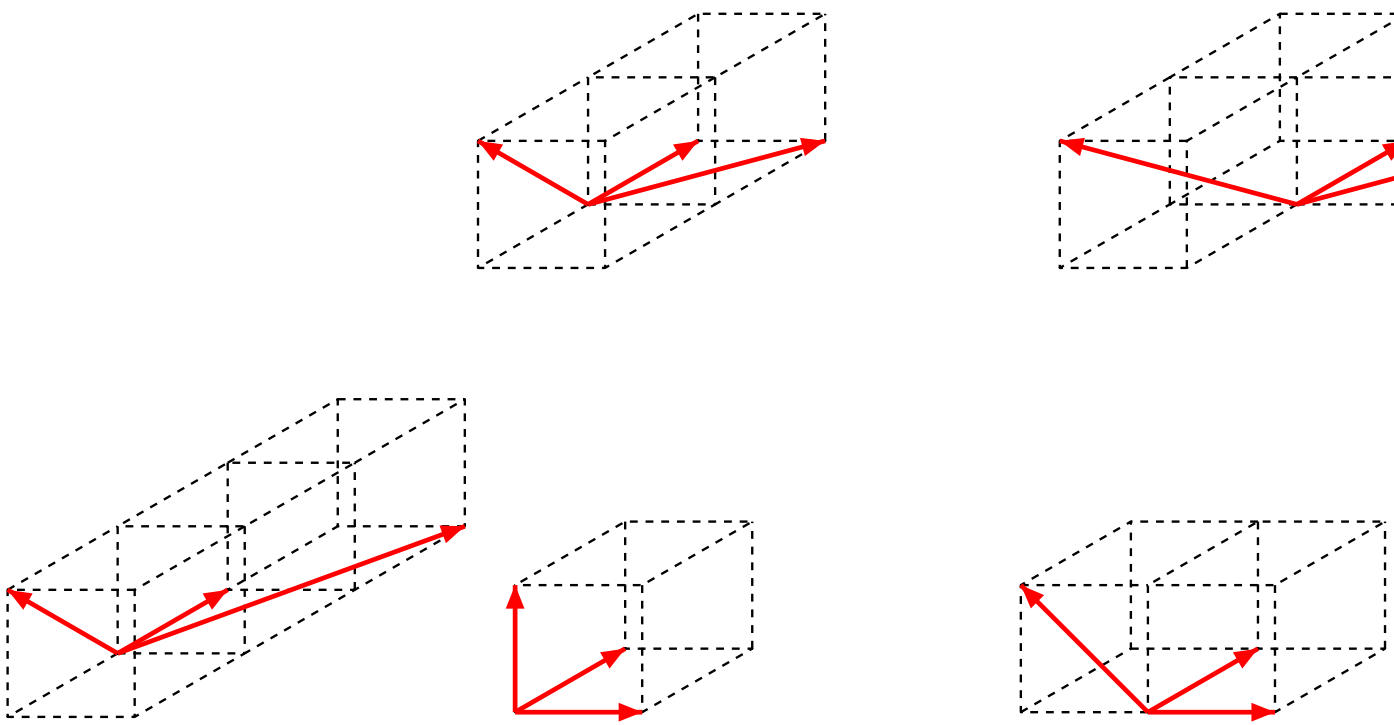


Image of the energy momentum map for the $1:1:2$ resonant oscillator system with axial symmetry (*and without detuning*). Full 3D-image, typical constant-n section and fibers.

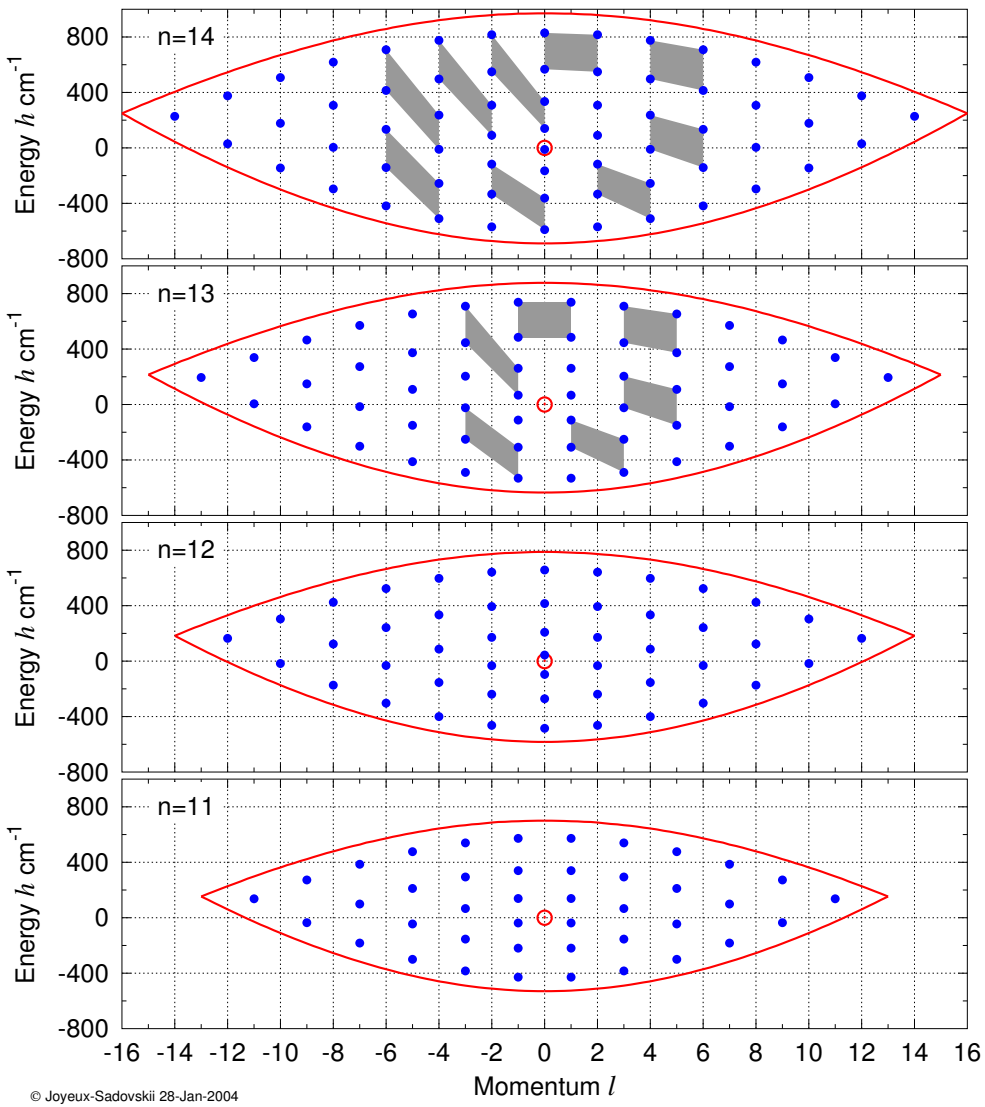

0
3
2
1
0
3
2
1
0
-8
-6
-4
-2
0
2
4
6
8
-8
-4
0
4
8

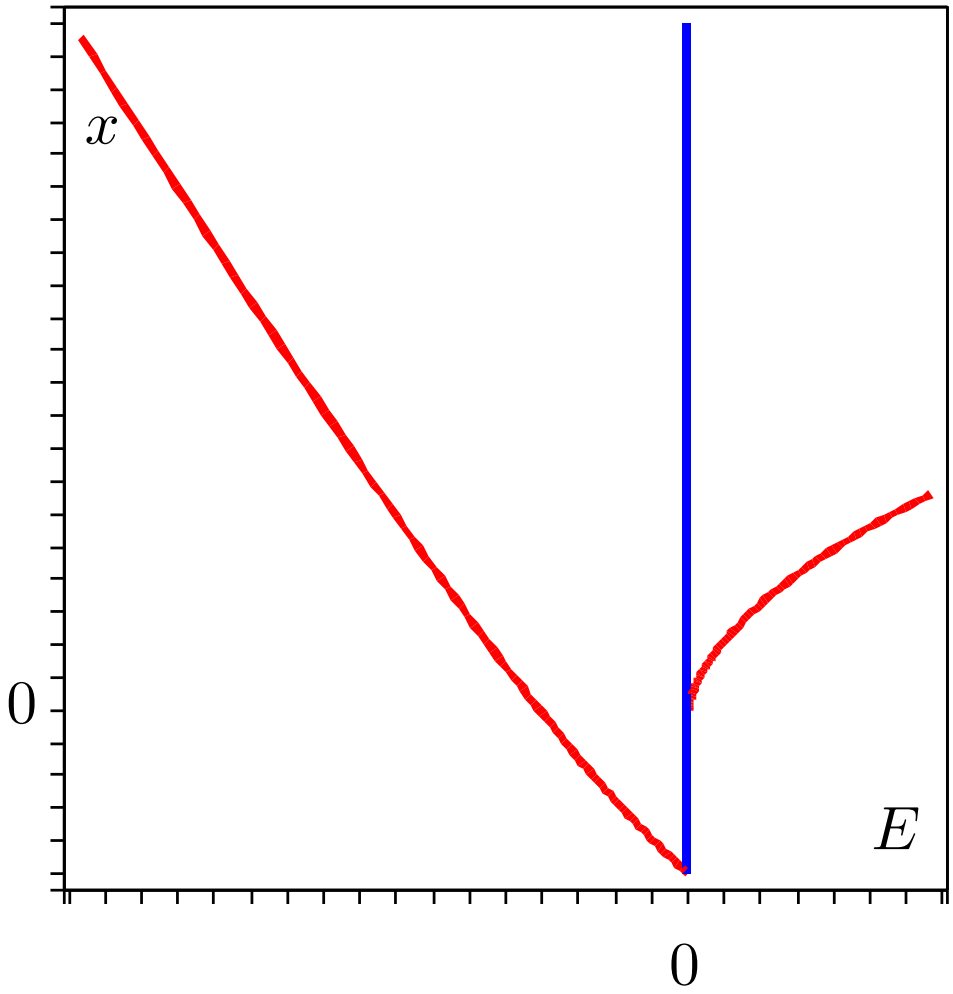


Matrix representation of monodromy for model with $1:1:2$ resonance

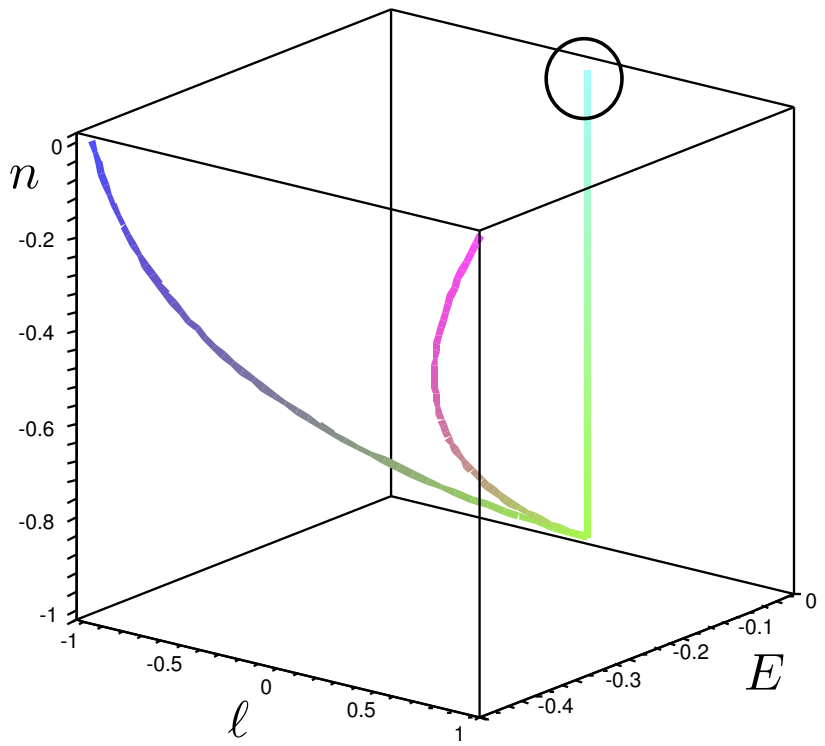
$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \sim \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7}$$

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

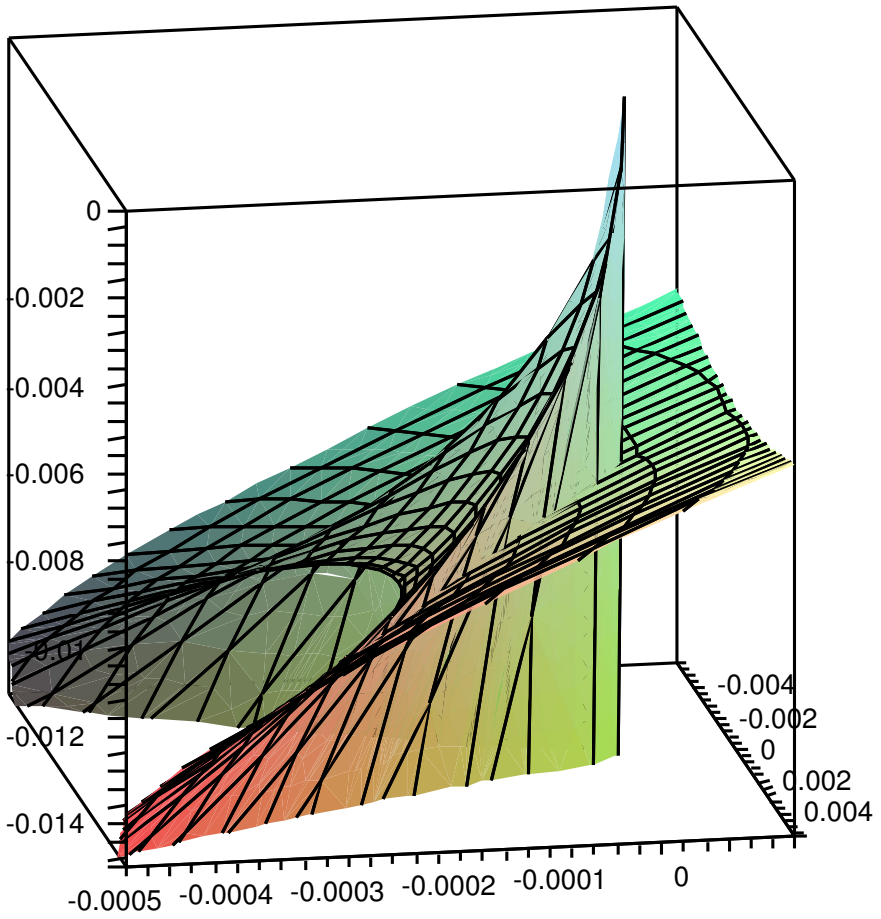

n=14
n=13
n=12
n=11
Energy h cm^{-1}
800
400
0
-400
-800
-16 -14 -12 -10 -8 -6 -4 -2 0 2 4 6 8 10 12 14 16
Momentum l
© Joyeux-Sadovskii 28-Jan-2004

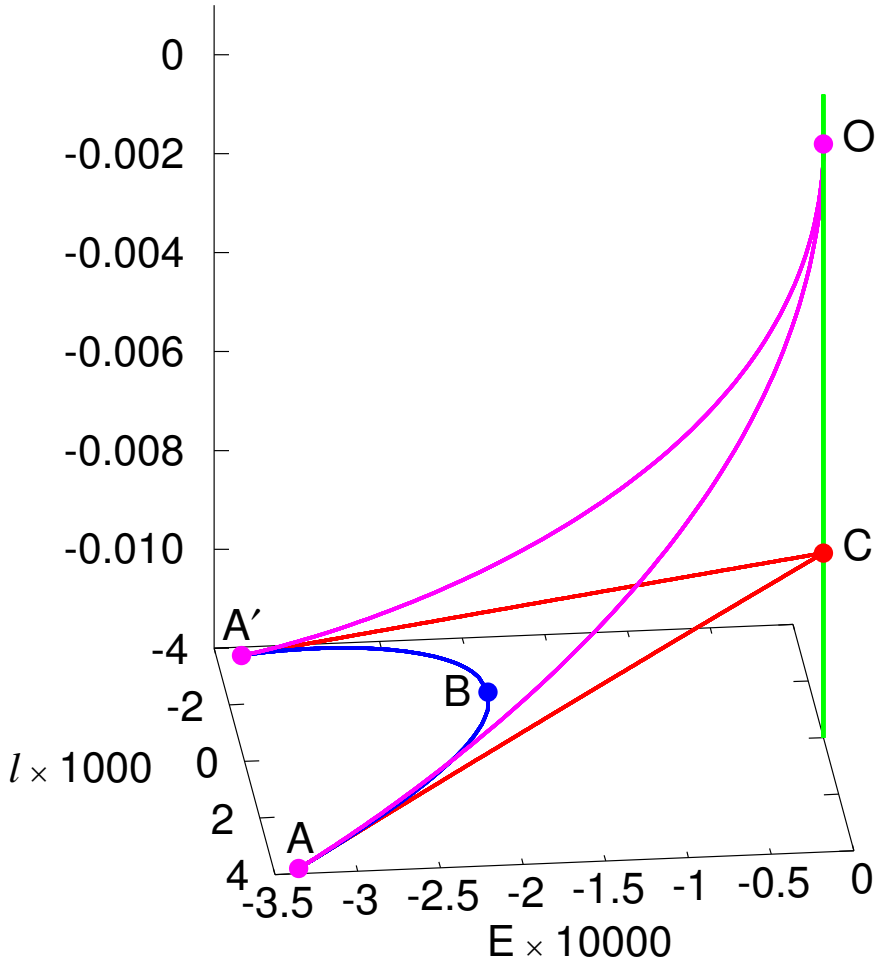


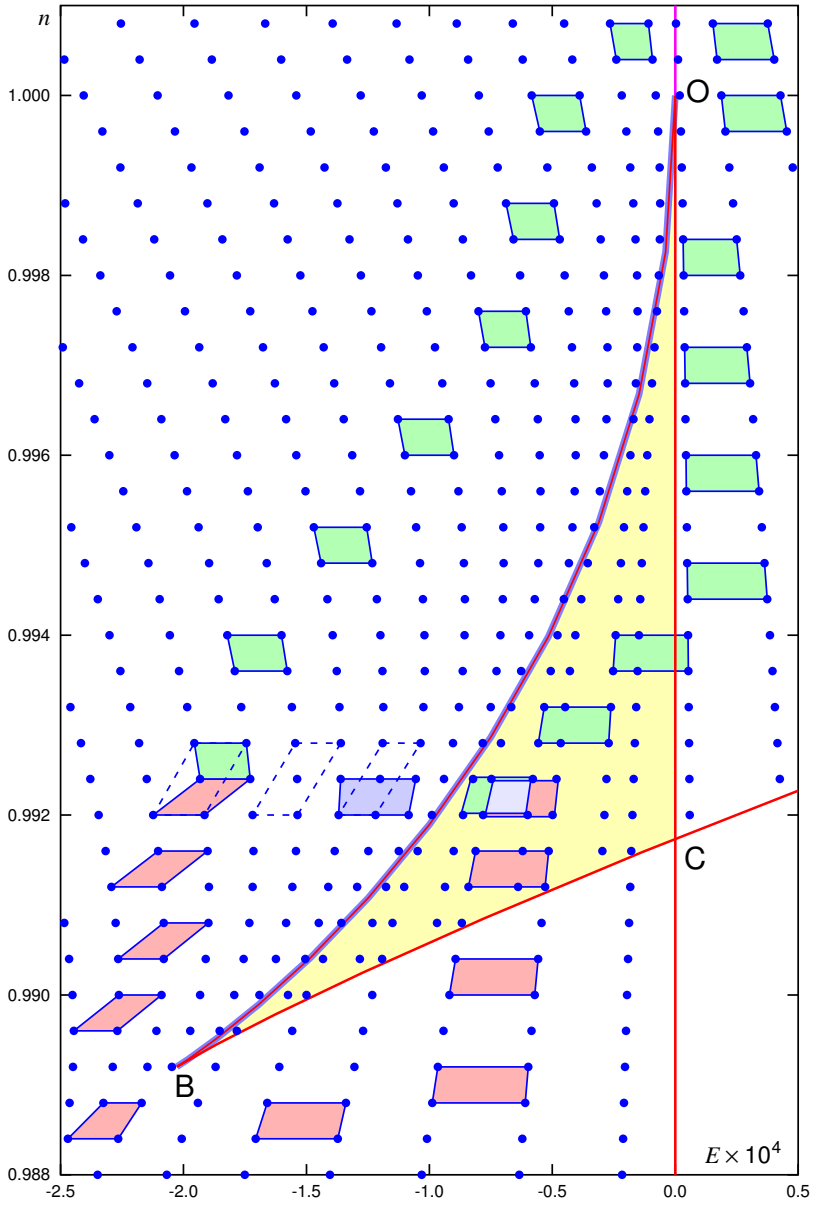
Global view of the image of energy-momentum map for $L^2 = 0$ with small detuning.



Singular lines on the boundary of the image of the energy momentum map. The detailed representation of the boundary within the region near $E = x = \ell = 0$ indicated by a big circle is given in the next figure.

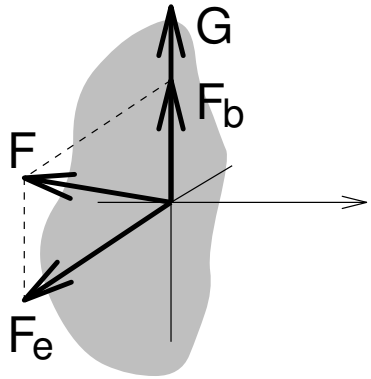

0
-0.002
-0.004
-0.006
-0.008
-0.01
-0.012
-0.014
-0.0005
-0.0004
-0.0003
-0.0002
-0.0001
0
-0.004
-0.002
0
0.002
0.004

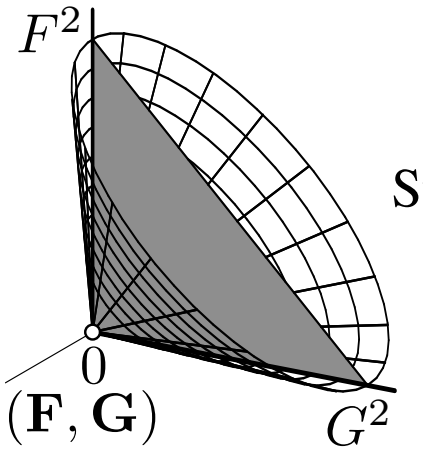

0
-0.002
-0.004
-0.006
-0.008
-0.010
O
C
A′
B
A
-4
-2
0
2
4
$l \times 1000$
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0
E × 10000

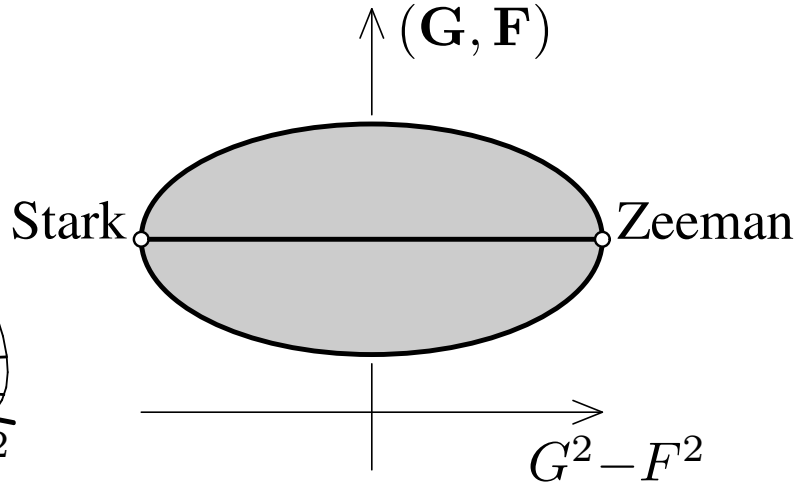

n
1.000
0.998
0.996
0.994
0.992
0.990
0.988
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
0.5
O
C
B
$E \times 10^4$

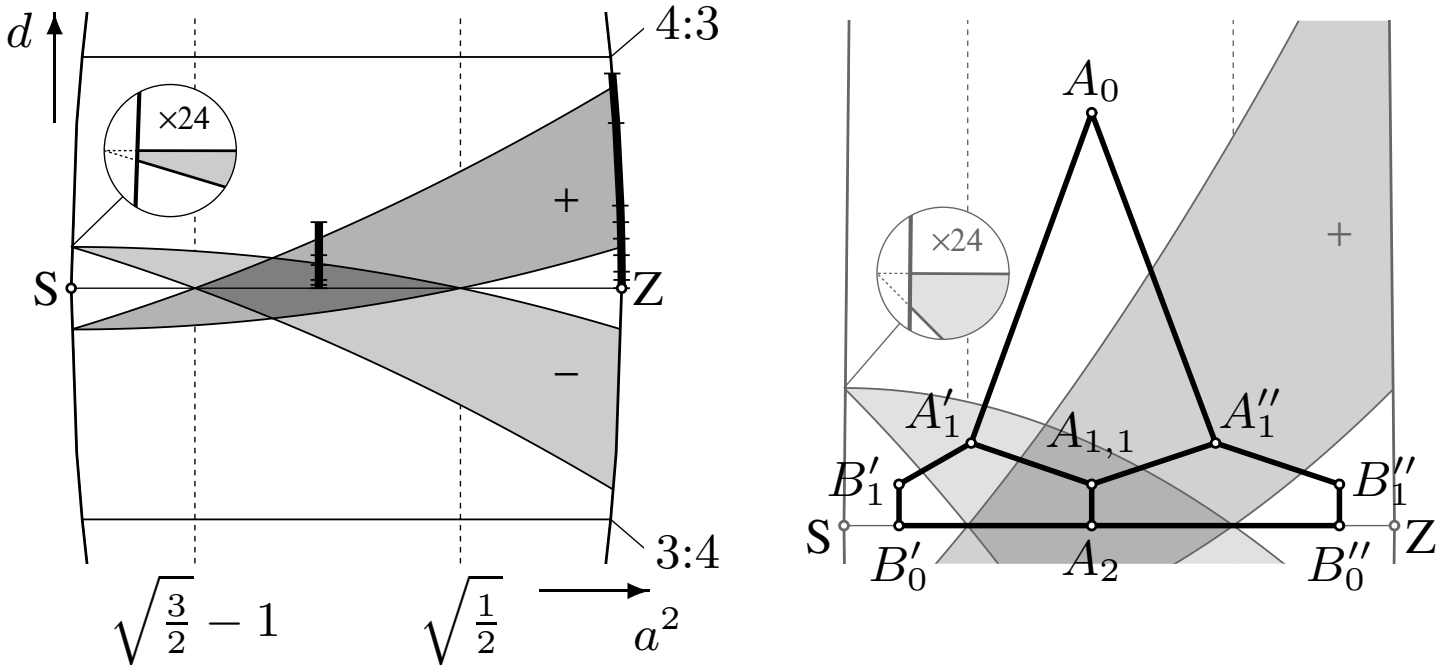
Hydrogen atom in external electric and magnetic fields

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



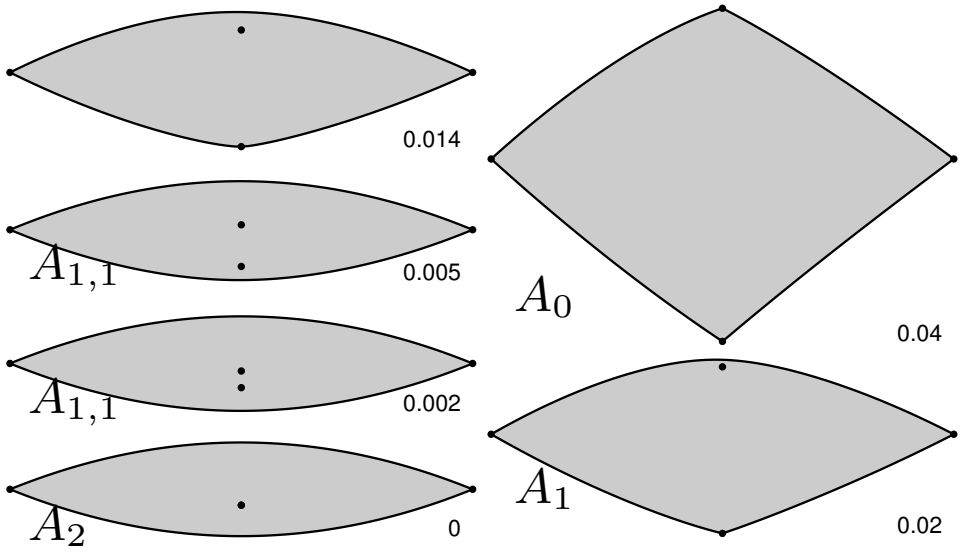




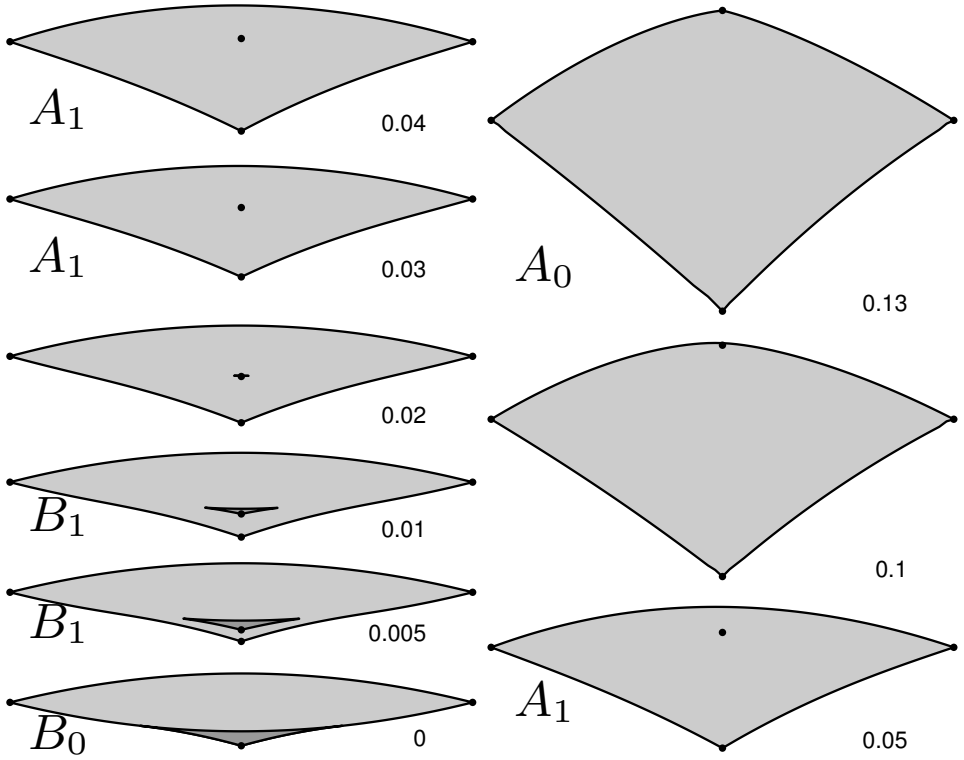


Structure of the 1:1 zone. Different dynamical strata of the zone (left) correspond to vertices of the genealogy graph (right).

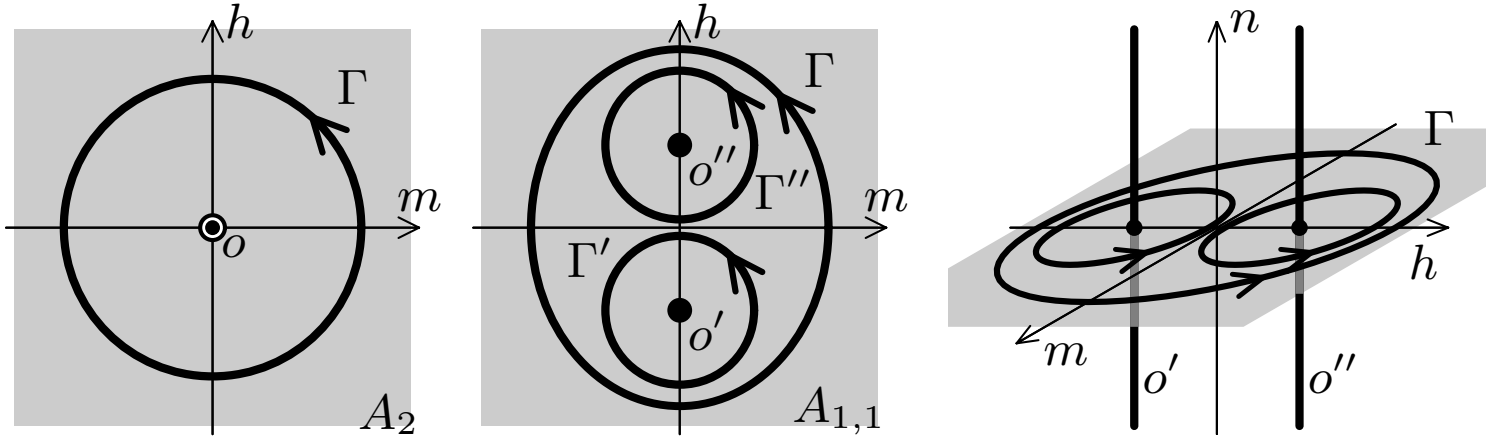
path $A_2 A_{11} A_1'' A_0$ with fixed $a^2 = 0.45$



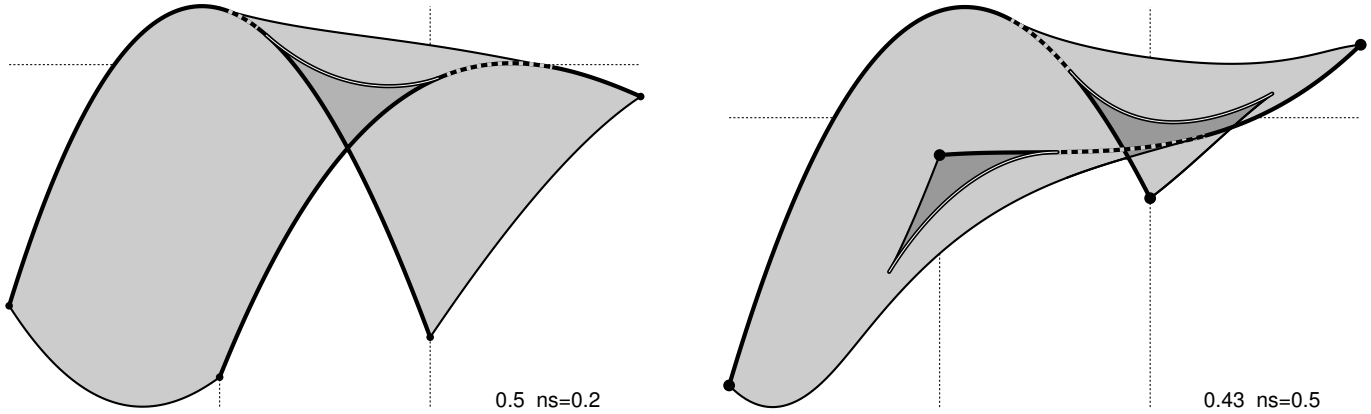
path $B_0'' B_1'' A_1'' A_0$ for parallel fields near Z



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).

References

Phys. Rep. **341**, 11, 85, 173 (2001) *[Reviews "for physicists"]*

Proc. R. Soc. A **463** 1771-1790 (2007) *H atom in fields*

Phys. Rev. Lett. **93** 024302 (2004); J. Math. Phys. **45** 5076-5100 (2004); Ann. Phys (N.Y.) **322** 164-200 (2007) CO_2

SIAM J. Appl. Dyn. Syst. **3** 261-351 (2004); Eur. Phys. J D **42** 61-72 (2007); *tetrahedral molecules* A_4, AB_4

Spectrochim. Acta A **61** 2867-2885 (2005) O_3

Chem. Phys. Lett. **89** 439 (2003); Phys.Rev. A **69** 032504 (2004) *LiCN, HCN*