Quantum and classical monodromy

Geometric analysis of perturbed hydrogen atom and similar systems

Dmitrií Sadovskií
sadovski@univ-littoral.fr
Université du Littoral, Dunkerque, France

with contributions by
Richard Cushman and *Boris Zhilinskií*

Abstract

We consider a class of perturbed Kepler problems such as hydrogen atom in external electric and magnetic fields where perturbations are assumed to be small enough to validate the use of Keplerian (first or n-shell) normalization. Using singular reduction we remove the additional S_1 symmetry which can either be strict (spatial) or approximate (dynamical) and obtain an integrable approximation to the original system. We give a complete classification of the dynamically invariant sets of this approximation by analyzing level sets of the second reduced Hamiltonian. We find a domain of parameters where the system of regular invariant tori has *monodromy* and where the introduction of global action-angle variables is impossible. We follow by analyzing the quantum analogue of this phenomenon and suggest generalizations.

Publications
http://pca3.univ-littoral.fr/~sadovski

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Monodromy in perturbed Kepler systems: hydrogen atom in crossed fields
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D. A. Sadovskií and B. I. Zhilinskií,
Monodromy, diabolic points, and angular momentum coupling
Phys. Lett. A **256**(4) 235–44 (1999)

D. A. Sadovskií and B. I. Zhilinskií,
Tuning the hydrogen atom in crossed fields between the Zeeman and Stark limits
Phys. Rev. A **57**(4) 2867–84 (1998)

D. A. Sadovskií, B. I. Zhilinskií and L. Michel
Collapse of the Zeeman structure of the hydrogen atom in the external electric field
Phys. Rev. A **53**(6) 4064–7 (1996)

Outline:

- Normalization of perturbed Kepler problems: n-shell approximation, first normal form, and first reduced space $S_2 \times S_2$
- Analysis of symmetries: group action, integrity basis, orbit space
- Examples: hydrogen atom in orthogonal (crossed) and parallel magnetic (G) and electric (F) fields
- Example of two coupled momenta.
- Relative equilibria and their evolution: tuning the nonlinear normal modes
- Second reduction. S_1 group action on $S_2 \times S_2$, second reduced phase space $P_{n,c}$, integrity basis and Poisson algebra.
- Qualitative analysis of the second reduced problem. The case with monodromy.
- What is quantum monodromy?
- Relation between monodromy and diabolic points.

History, anticipation, and theory:

E. A. Solov'ev, JETP Lett. **34** 265 (1981);
D. R. Herrick, Phys. Rev. A **26** 323 (1982).

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J. C. van der Meer and R. Cushman,
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R. H. Cushman and L. M. Bates, *Global Aspects of Classical Integrable Systems* (Birkhäuser, Basel, 1997).

Regularization of the Kepler problem
using Kustaanheimo-Stiefel transformation with matrix $M_{\mathrm{KS}}: R_4 \to R_4$ such that coordinates in the initial 3D space are

$$(q_b, q_e, q_p, 0)^T = M_{\mathrm{KS}}(q_1, q_2, q_3, q_4)^T,$$

$$r = q_b^2 + q_e^2 + q_p^2 = q_1^2 + q_2^2 + q_3^2 + q_4^2,$$

and momenta in the initial 3D space are

$$(p_b, p_e, p_p, \Pi)^T = \frac{1}{2r} M_{\mathrm{KS}}(p_1, p_2, p_3, p_4)^T,$$

where we impose an extra restriction

$$\zeta \stackrel{\mathrm{def}}{=} -2r\Pi = q_1p_4 - q_4p_1 + q_3p_2 - q_2p_3 = 0.$$

The unperturbed Kepler Hamiltonian

$$H_0 = \frac{1}{2}p^2 - \frac{1}{r}$$

becomes a 1:1:1:1 oscillator in the KS space

$$2n \stackrel{\mathrm{def}}{=} \frac{1}{2}(p_1^2 + p_2^2 + p_3^2 + p_4^2 + q_1^2 + q_2^2 + q_3^2 + q_4^2)$$

Keplerian reduction
first normal form in the KS space

consider n as an approximate integral and construct quadratic polynomials invariant under the combined flow of X_ζ and X_n

Angular momentum components:

$$\begin{aligned} L_b &= (q_2p_3 - q_3p_2 + q_1p_4 - q_4p_1)/2 \\ L_e &= (q_2p_4 + q_3p_1 - q_1p_3 - q_4p_2)/2 \\ L_p &= (q_1p_2 + q_3p_4 - q_2p_1 - q_4p_3)/2 \end{aligned}$$

Laplace-Runge-Lentz vector components:

$$\begin{aligned} K_b &= (p_2^2 + q_2^2 + q_3^2 + p_3^2 - q_1^2 - p_1^2 - q_4^2 - p_4^2)/4 \\ K_e &= (p_4p_3 - q_2q_1 - p_1p_2 + q_4q_3)/2 \\ K_p &= -(q_3q_1 + p_1p_3 + q_4q_2 + p_4p_2)/2 \end{aligned}$$

The two vectors $\mathbf{K}$ and $\mathbf{L}$ are related so that

$$n^2 = \mathbf{K}^2 + \mathbf{L}^2, \quad \mathbf{K} \cdot \mathbf{L} = 0$$

First reduced phase space Σ

is defined in the embedding space R_6 spanned by vectors $\mathbf{J}_{1,2} = (\mathbf{K} \pm \mathbf{L})/2$ such that

$$\mathbf{J}_1^2 = \mathbf{J}_2^2 = n^2/4 = \text{const}.$$

It follows that the topology of Σ is $S_2 \times S_2$.

The dynamics on Σ can be described in terms of the Poisson algebra so(4) of vectors $\mathbf{K}, \mathbf{L}$

$$\{L_b, L_e\} = L_p, \ \{K_b, K_e\} = L_p, \ \{L_b, K_e\} = K_p,$$

or the equivalent algebra su(2)×su(2) of

$$\{J_{ib}, J_{ie}\} = J_{ip}, \ i = 1, 2, \quad \{J_1, J_2\} = 0.$$

The above relations can be easily derived from the KS definitions of $\mathbf{K}$ and $\mathbf{L}$ restricting to $n = $ const and $\zeta = 0$.

Applications of invariant theory

Q. How to work with the space $S_2\times S_2$? How to study the Hamiltonian flow and the group actions and to express the reduced Hamiltonian H_{fnf} on it?

A. Use polynomial invariants $\mathbf{K}$, $\mathbf{L}$, n, and ζ.

Q. But these invariants are algebraically related, the ring generated by $\mathbf{K}$ and $\mathbf{L}$ (restricted to $\zeta=0$ and $n=$ const is *not* free!

A. Construct the *integrity basis* for this ring.

Molien generating function for invariants of the combined action of Keplerian (n) and KS (ζ) symmetry

$$g(\lambda)_{C_4/T_2} \;=\; \frac{1+2\lambda^2+\lambda^4}{(1-\lambda^2)^6}.$$

indicates that there are *six* main and *three* auxiliary (numerator) integrity basis polynomials which we can choose to be

auxiliary (ϕ) $\quad K_p,\quad L_p,\quad K_p^2-L_p^2,$

main (θ) $\quad K_e,\quad L_b,\quad K_b,\quad L_e,\quad n,\quad \zeta$.

We use integrity basis

1. to express any invariant polynomial and in particular the reduced Hamiltonian H_{fnf} in the form

$$H_{\text{fnf}} = \mathcal{P}(\theta) + \sum_i \phi_i \mathcal{P}_i(\theta)$$

with $\mathcal{P}(\theta)$ arbitrary polynomials in main invariants K_b, K_e, L_b, L_e, n, and ζ. We subsequently restrict to $\zeta=0$ and consider n as a constant.

2. to represent the reduced phase space $S_2\times S_2$ using its maps with coordinates K_b, K_e, L_b, L_e. The *signs* of auxiliary polynomials ϕ_i distinguish different maps.

3. to study the group action on $S_2\times S_2$ as action on the invariants and on the maps.

Hydrogen atom in crossed fields

F electric field along q_e
G magnetic field along q_b
C effective charge of the nucleus

Hamilton function in 3D (q_b, q_e, q_p)

$$H = \frac{1}{2}\mathbf{p}^2 - \frac{C}{r} + Fq_e + \frac{1}{2}GL_b + \frac{1}{8}G^2(q_e^2+q_p^2)$$

Hamilton function in the KS space

$$\begin{aligned} H &= \frac{1}{2}(p^2+q^2) \\ &\quad + \frac{1}{3}f(q_2q_1-q_4q_3)q^2 + \frac{1}{2}g(q_2p_3-q_3p_2)q^2 \\ &\quad + \frac{1}{8}g^2(q_2^2+q_3^2)(q_1^2+q_4^2)q^2 \\ &= \frac{4}{\omega}\,, \end{aligned}$$

Parameterization

4D oscillator frequency $\omega = \dfrac{2\sqrt{-2E}}{C}$

scaled field parameters:

$$g = G\left(\frac{2}{\omega C}\right)^2, \qquad f = 3F\left(\frac{2}{\omega C}\right)^3$$

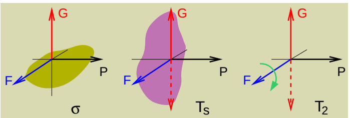
uniform field parameters:

$$F = \frac{1}{3}F_s\frac{S}{C}\left(\frac{\omega C}{2}\right)^4, \qquad G = G_s\frac{S}{C}\left(\frac{\omega C}{2}\right)^3$$

formal smallness parameters:

$$S = C\left(\frac{2}{\omega C}\right)^3\sqrt{G^2+\left(3F\frac{2}{\omega C}\right)^2} \approx \tau = n\frac{\omega}{2}S$$

Symmetry group $G_4 = Z_2 \times Z_2$
of the orthogonal field problem



$$G_4 = \{I, \sigma, T_s = T\circ\sigma', T_2 = T\circ C_2\}$$

σ reflection in the ep plane
T time reversal
C_2 rotation around axis e
σ' reflection in the eb plane

Molien generating function for invariants

$$g_{C_4/T_2\wedge G_4}(\lambda) = \frac{1+4\lambda^4+3\lambda^8}{(1-\lambda^2)^3(1-\lambda^4)^3}.$$

Action of G_4
on the generators of the polynomial ring

	I	$C_*\circ\sigma^{(eb)}$	$\sigma^{(ep)}$	$C_*\circ C_2^{(e)}$
n	+	+	+	+
ζ	+	+	−	−
K_e	+	+	+	+
K_b	+	+	−	−
K_p	+	−	+	−
L_e	+	+	−	−
L_b	+	+	+	+
L_p	+	−	−	+

Integrity basis polynomials

main $\quad K_e,\quad L_b,\quad K_b^2,\quad L_e^2$
$\quad n,\quad \zeta^2$

auxiliary $\quad K_bL_e,\quad K_p^2-L_p^2,\quad K_bL_e(K_p^2-L_p^2),$
$\quad \zeta K_b,\quad \zeta L_e,$
$\quad \zeta K_b(K_p^2-L_p^2),\quad \zeta L_e(K_p^2-L_p^2)$

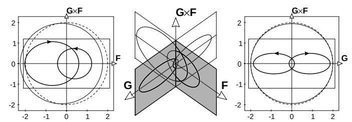
Keplerian (first) normal form
for the orthogonal fields problem

$$\begin{aligned} H_{\text{fnf}} &= 4/\omega \\ H_{\text{fnf}} &= 2n\left(1+\frac{\tau}{2}H_1+\frac{\tau^2}{4}H_2+\frac{\tau^3}{32}H_3+\ldots\right) \end{aligned}$$

$$\begin{aligned} H_1 &= -G_sL_b - F_sK_e \\ H_2 &= -\left(3L_b^2-2K_e^2+3K_b^2+2L_e^2+2(L_p^2-K_p^2)-3\right)G_s^2/4 \\ &\quad -(7K_eL_b-L_eK_b)F_sG_s/3 \\ &\quad -(51K_e^2-9L_e^2+17)F_s^2/36 \\ H_3 &= -L_b(6L_e^2-6K_e^2+9K_b^2+5L_b^2+6(L_p^2-K_p^2)-9)G_s^3 \\ &\quad -K_e(125-43L_e^2+125K_e^2)F_s^3/9 \\ &\quad +(-45K_eL_e^2+45K_e^3-65K_eK_b^2+117K_e \\ &\quad -147L_b^2K_e-45K_e(L_p^2-K_p^2)+48L_b(L_eK_b))F_sG_s^2/6 \\ &\quad +(3K_b^2L_b+87L_e^2L_b-615K_e^2L_b-3L_b^3-232L_b \\ &\quad -3L_b(L_p^2-K_p^2)+108K_e(L_eK_b))F_s^2G_s/18 \end{aligned}$$

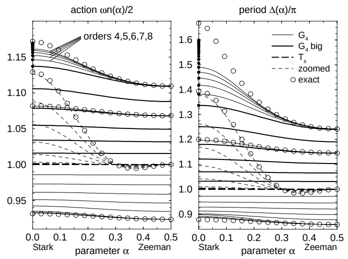
Relative equilibria
(stationary points of the first normal form)
in the crossed fields problem

3D image of the nonlinear normal modes
(also called the *Kepler ellipses*)
$S=0.2$ and $F_s=\cos(\pi/3)$ $(\alpha=1/3)$



normal form prediction of order ϵ^3

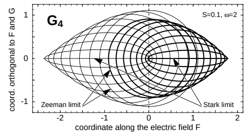
Action and period
of the nonlinear normal modes
of the Rydberg electron in the crossed fields



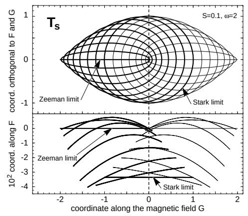
normal form prediction of order ϵ^3
for $S = 0.03$, 0.06, 0.09, 0.12, 0.15,0.18

nonlinear normal modes
of the crossed fields problem
$S = 0.1$ and $F_s = \cos(\alpha\pi)$ with $\alpha = 0 \ldots 1/2$

symmetry G_4



symmetry T_s



normal form prediction of order ϵ^3

Dynamical S_1 symmetry

of the first n. f. of the crossed fields system

Approximate integral of motion

$$T_1 = G_s L_b + F_s K_e = -\frac{1}{2} H_1 = c$$

Molien function for $C_4/S_1{\times}S_1{\times}S_1$

$$g(\lambda) = \frac{1+\lambda^4}{(1-\lambda^2)^4(1-\lambda^4)}$$

so(4) generators of the polynomial ring

$$\mathbf{T} = \begin{pmatrix} G_s L_b + F_s K_e \\ G_s L_e - F_s K_b \\ L_p \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} F_s L_e + G_s K_b \\ G_s K_e - F_s L_b \\ K_p \end{pmatrix}$$

Integrity basis polynomials

main $n,\ \zeta,\ T_1 = c,\ \pi_1 = V_1,$
$\pi_2 = T_2^2 + T_3^2 - V_2^2 - V_3^2$

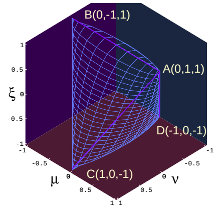
auxiliary $\pi_3 = 2(T_2 V_3 - T_3 V_2)$

Relation between invariants

$$\pi_2^2 + \pi_3^2 = [(n-c)^2 - \pi_1^2][(n+c)^2 - \pi_1^2] \geq 0$$

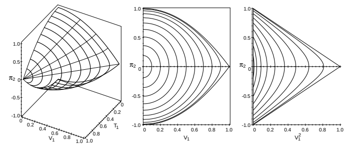
Orbit space

of the S_1 action on $S_2 \otimes S_2$



$$\begin{aligned} \pi_3 &\geq 0 \\ \xi &= \mathbf{T}^2 - \mathbf{V}^2 \\ \mu &= T_1 \\ \nu &= V_1 \\ |\xi| &\leq 1, \\ |\mu| &\leq 1, \\ |\nu| &\leq 1 \\ n &\to 1 \end{aligned}$$

$T_1 = c$ sections of the orbit space are images
of the second reduced phase spaces $P_{n,c}$

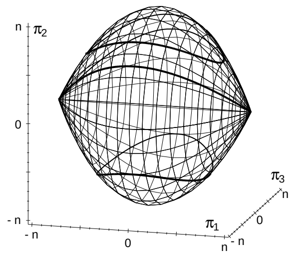


Second reduced phase space $P_{n,c}$

is defined in the ambient space R_3 by

$$\pi_2^2 + \pi_3^2 = [(n-c)^2 - \pi_1^2][(n+c)^2 - \pi_1^2]$$

for c=0 this is *not* a smooth sphere S_2 but a *singular* space with two conical points at $V_1 = \pm n$



Second reduced Hamiltonian

of the crossed fields system

Molien function for $Z_2 \times Z_2$-invariants

$$g(\lambda) = \frac{1+\lambda^4}{(1-\lambda^2)^2(1-\lambda^4)^3}$$

$Z_2 \times Z_2$-symmetrized integrity basis

main: $n,\quad c,\quad \zeta^2,\quad V_1^2,\quad \pi_2$
auxiliary: ζV_1

<u>Conclusion</u> : second normal form H_{snf} is a function of $V_1^2 = \pi_1^2$ and π_2.
To the lowest order this function is

$$H_{\text{snf}} = a\pi_2 - b\pi_1^2 = \text{const}(n, c, \tau)$$

where in our particular case

$$a = G_s^2, \quad b = \frac{1}{2} - G_s^2 - G_s^4$$

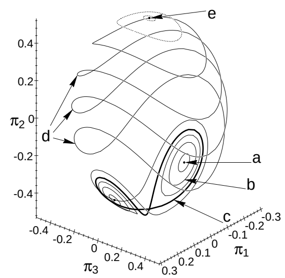
Dynamics on the second reduced space

of the crossed fields system

Poisson structure on the ambient space

$$\begin{aligned} \{\pi_1, \pi_2\} &= 4\pi_3 \\ \{\pi_3, \pi_1\} &= \pi_2 \\ \{\pi_2, \pi_3\} &= 2\pi_1(n^2 + \pi_2 + c^2 - \pi_1^2) \end{aligned}$$

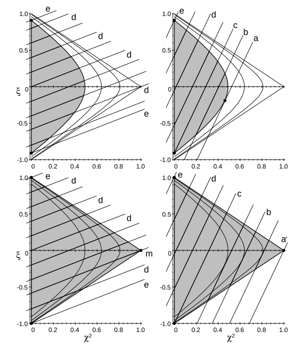
Constant energy level sets of H_{snf} for $c \neq 0$



Qualitative analysis of the second reduced Hamiltonian H_{snf}

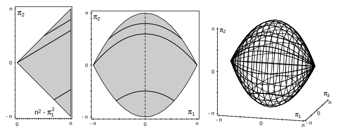
of the crossed fields system

orbit space representation
of the constant level sets

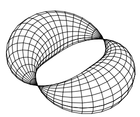


Reconstruction of the dynamically invariant sets in the case with monodromy
for the crossed fields system

from orbit space to $P_{n,c}$ and then to $S_2 \times S_2$



it follows that the singular fiber is a *doubly pinched torus* in $S_2 \times S_2$, a heteroclinic connection of stable and unstable manifolds of two fixed points

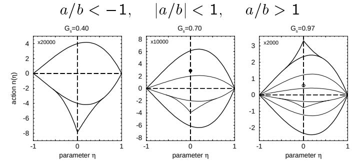


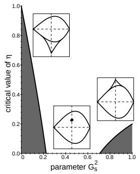
a system with such singular fiber has monodromy

Manifestation of monodromy in the energy momentum map
of the crossed fields system

three different dynamical regimes :

$$a/b < -1, \quad |a/b| < 1, \quad a/b > 1$$



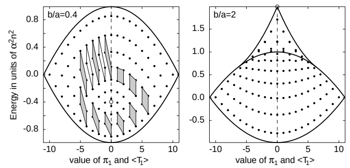


When $|a/b| < 1$, i.e., when

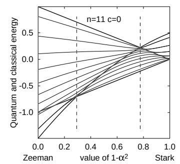
$$G_s^2 \in \left(\frac{\sqrt{6}}{2} - 1, \frac{\sqrt{2}}{2}\right)$$

the isolated critical point corresponds to the pinched torus and the system has monodromy.

Quantum monodromy
quantum levels form a regular *lattice* in the domain of the regular values of the energy momentum map



in the case with monodromy (left) this lattice has a point defect



we can now change the ratio of the two fields and "tune" the crossed fields system with $c = 0$ into the monodromy domain

Parallel fields system : a perturbed Keplerian system with cylindrical symmetry

Symmetry $S_1 \times Z_2$:

S_1 rotation around axis of the fields z

Z_2 reflection in any of the vertical planes containing axis z times time reversal

Invariants of the action of $S_1 \times Z_2$ and of the Keplerian and KS symmetries are described by the Molien function

$$g_{T_3 \times Z_2}(\lambda) = \frac{1}{(1-\lambda^2)^4(1-\lambda^4)}$$

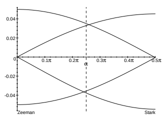
They form a free module generated by

$$n, \quad \zeta, \quad \mu = L_z, \quad \nu = K_z, \quad \xi = \mathbf{L}^2 - \mathbf{K}^2$$

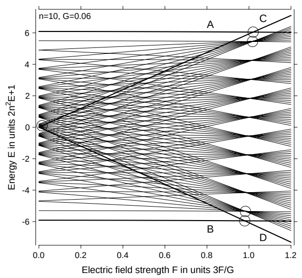
The normal form is a function of ν and ξ, and parameters $\mu = c$ and n

$$H_{\text{snf}} = 1 + \frac{1}{2}(F_s\nu + G_s\mu)\tau + \ldots = \frac{S}{\tau}$$

NB: in terms of the crossed fields system $\pi_1 = \nu$ and $\xi = \pi_2 + c^2 - \pi_1^2$, the second reduced phase space and the Poisson algebra are the *same*.

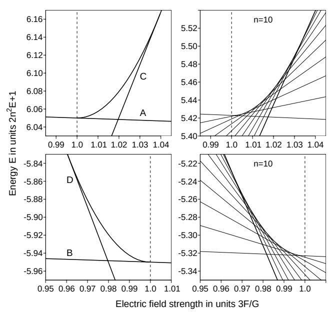


Crossover and relative equilibria of the parallel field system



changing the ratio of G_s and F_s we reach the point of *crossover* where the first order term in H_{snf} vanishes

Fine structure in the crossover region
calculated using second order normal form



classical relative equilibria (left) vs quantum solutions (right)

Monodromy, diabolic points, and coupling of angular momenta

Consider a simple generalization of systems on $S_2 \times S_2$ with cylindrical (S_1) symmetry

$$H = \frac{1-\gamma}{S} S_z + \frac{\gamma}{NS}(\mathbf{NS})$$

where $\mathbf{S}$ and $\mathbf{N}$ are two commuting sets of angular momentum components

$$\mathbf{S}^2 = S^2 = \text{const}, \quad \mathbf{N}^2 = N^2 = \text{const},$$

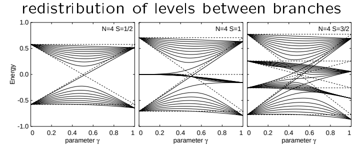
and γ is a *coupling constant*.

The momentum $J_z = N_z + S_z$ is conserved due to S_1 symmetry.

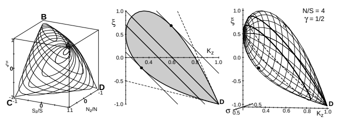
The symmetry $S_1 \times Z_2$, the integrity basis, the Poisson structure, and the orbit space are the *same* as in the case of parallel fields, but now $N \neq S$.

We show that in the limit $N \gg S$ monodromy and diabolic point coincide.

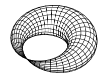
Quantum phenomenon of diabolic point : redistribution of levels between branches



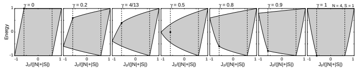
Orbit space, *singular* classical phase space, and constant level sets of H in the case with monodromy ($\gamma \approx 1/2$)



The singular fiber is a *singly pinched torus* in $S_2 \times S_2$



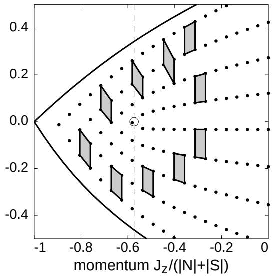
Evolution of the energy momentum map



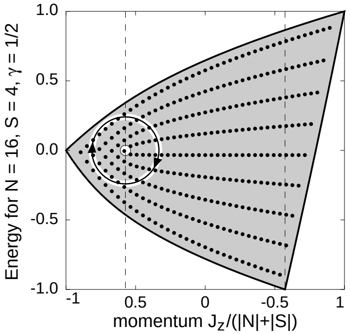
Monodromy interval :

$$\frac{N}{2N+S+2\sqrt{NS}} \leq \gamma \leq \frac{N}{2N+S-2\sqrt{NS}}$$

where an isolated critical point exists and global action-angle variables are *impossible*



The concept of monodromy and the energy momentum map



the torus bundle over a circle in the domain of regular values of the $\mathcal{EM}$ map is nontrivial (not a product $S_1 \times T_2$)

Conclusions

- We have demonstrated that monodromy exists in one of the most fundamental physical systems. Hopefully this phenomenon will finally be appreciated.
- Our study largely relies on the KAM picture and thus appeals for new mathematical foundations of monodromy in systems with "soft" chaos.
- We seem to know what quantum monodromy is and where and how to look for it. This calls for experiments.
- Our complete geometric treatement of perturbed Kepler problems retains a great potential of its own.
- Relation to many other systems, and to the phenomenon of diabolic points once again demonstrates the universality of monodromy.