SEMICLASSICAL DESCRIPTION OF THE DENSITY OF STATES IN THE CONTINUUM REGION OF THE HÉNON-HEILES SYSTEM

M. Brack, University of Regensburg

"Critical Stability of Few-Body Quantum Systems"

MPI-PKS Dresden, October 17 - 21, 2005

The Hénon-Heiles system:

- periodic orbits and bifurcation cascade
- classical escape over the barriers
- Gutzwiller's semiclassical trace formula
- density of states above barrier

Work done in collaboration with:

P. Winkler (University of Nevada, Reno, USA)
J. Kaidel (University of Regensburg, Germany)
S. Fedotkin (INR Kiev, Ukraine) (for partial results)

Motivation

- Simple few-body reactions with energy thresholds may be parameterized by the motion of a particle in a (multidimensional) potential landscape $V(x, y, \dots)$ with one or more saddles.

- Classical approach: look for classical trajectories (including complex paths for tunnelling); calculate phase-space flow through PODS; . . .

- Quantum-mechanical approach: density of states, scattering matrix, . . .

- Here: We consider the well-known 2-dimensional model potential $V(x, y)$ of Hénon and Heiles. Look for classical trajectories for escape; calculate density of states above the barriers in terms of periodic orbits using the semiclassical trace formula of Gutzwiller (generalized for bifurcations and symmetry breaking)

The Hénon-Heiles potential

$$\boxed{V(x,y) \;=\; \tfrac{1}{2}\,(x^2+y^2) + \alpha\,(x^2 y - \tfrac{1}{3}\,y^3)}$$

- Originally: gravitational potential of a galaxy, with possibility of escape for $E > E_{th} = 1/6\alpha^2$
  [M. Hénon and C. Heiles, Astron. J. **69**, 73 (1964)]

- Model for the deformation (vibrational) energy of triatomic molecules such as H_3^+, with possibility of dissociation

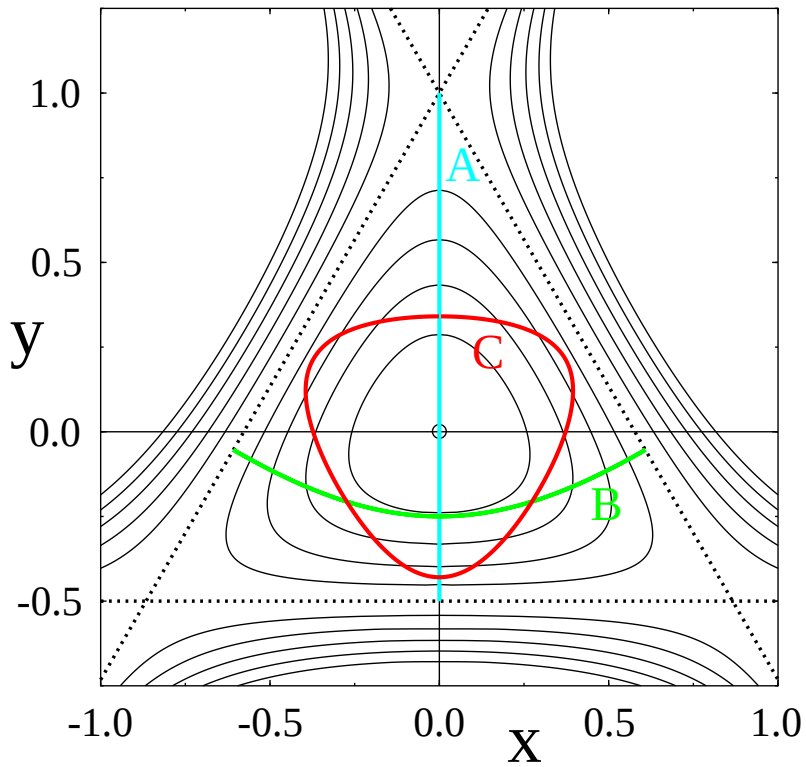
- Model for an electron in a triangular quantum dot with 3 external leads

- Formally: 3-particle cyclic Toda chain (integrable, bound!), Taylor expanded around $x{=}y{=}0$ and truncated at 3rd order (becomes open and non-integrable!)

- Has become a textbook example of a non-integrable mixed system with transition from regular ($E \to 0$ or $\alpha \to 0$) to chaotic motion ($E \gg E_{th}$)

The shortest orbits

Equipotential lines and the three shortest periodic orbits A, B and C (at scaled energy $e = 6E\alpha^2 = 1$, i.e. at threshold energy $E = E_{th}$) – note D_3 symmetry!



3 orbits B, always unstable, exist at all energies

2 orbits C, stable up to $e \simeq 0.892$, exist at all energies

3 orbits A, stable up to $e \simeq 0.97$, but then .....

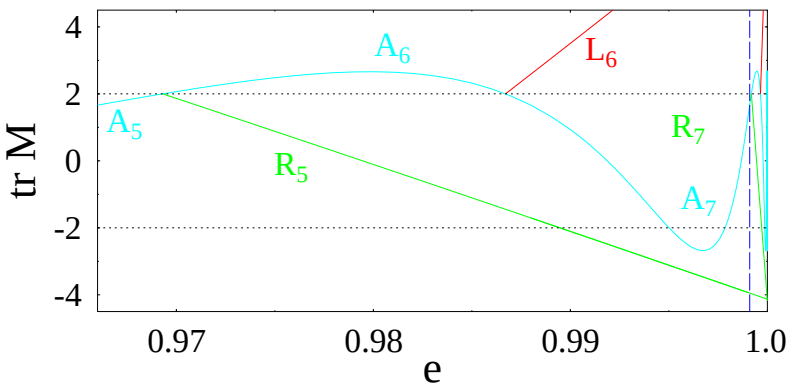
A, B, C correspond to vibrational modes in a triatomic molecule! [N. Fulton *et al.*, J. Chem. Phys. **99**, 906 (1993)]

Bifurcation cascade of the A orbit:

Orbit A undergoes an infinite sequence of pitchfork bifurcations before it reaches the barrier at $e = 1$ with period $T_A = \infty$!

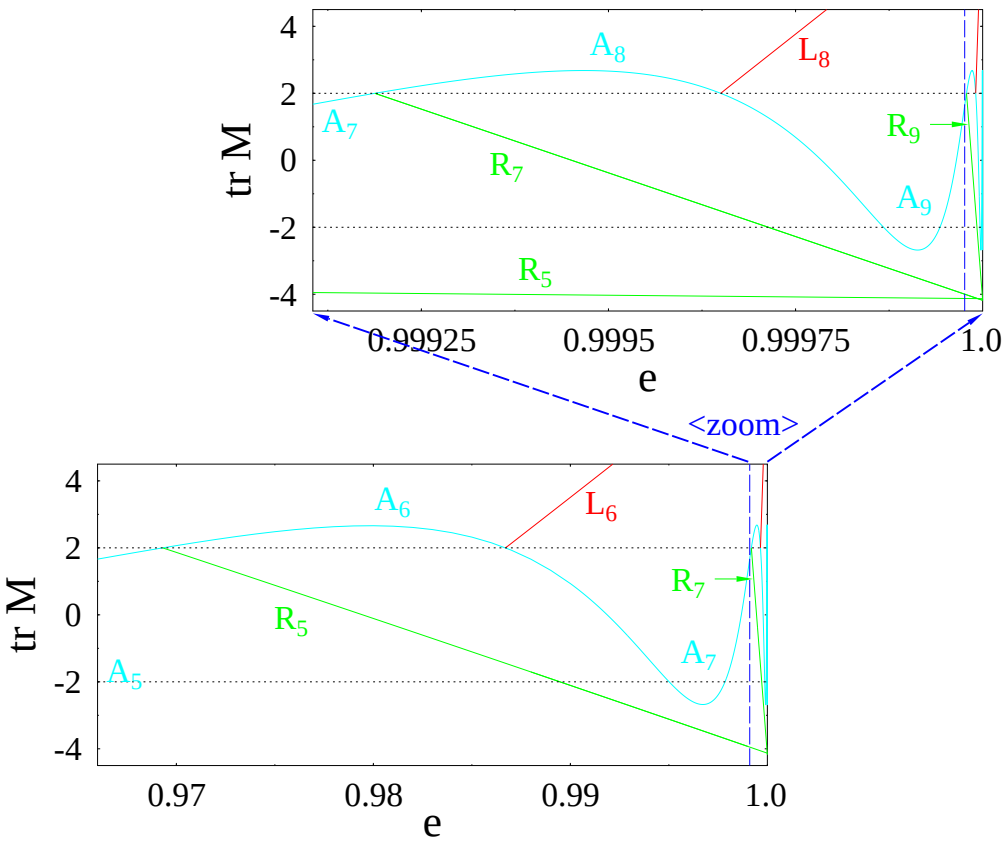
The orbits R_n and L_m born at these bifurcations exist up to infinite energy (all unstable for $e \geq 1$)!

Trace of stability matrix of A orbit versus energy e: bifurcation of orbits R_5 and L_6

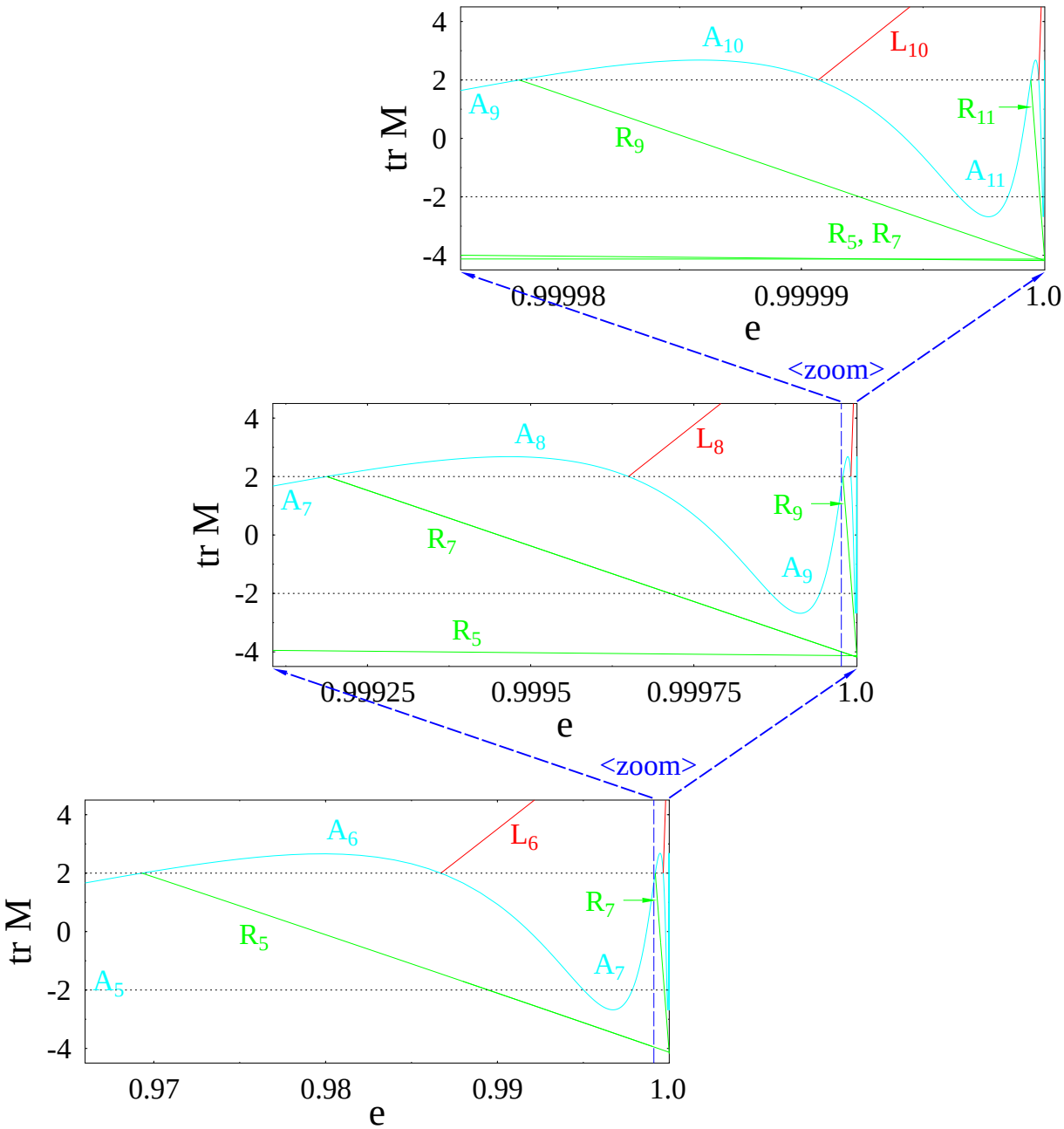


Bifurcation cascade of the A orbit:

Zoom into the last 0.1% of the energy scale:
bifurcation of orbits R_7 and L_8



Zoom again: orbits R_9 and L_{10}, and so on .....

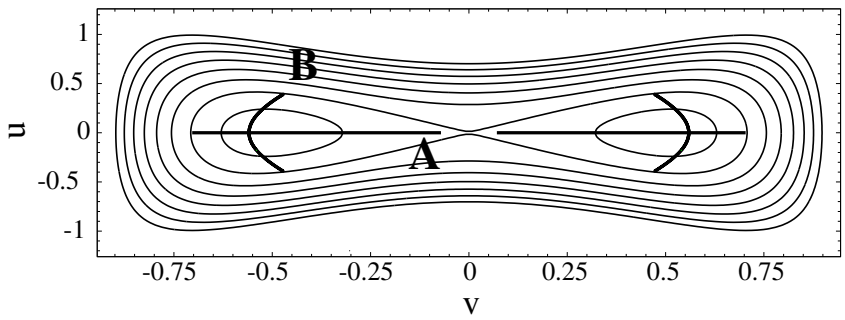


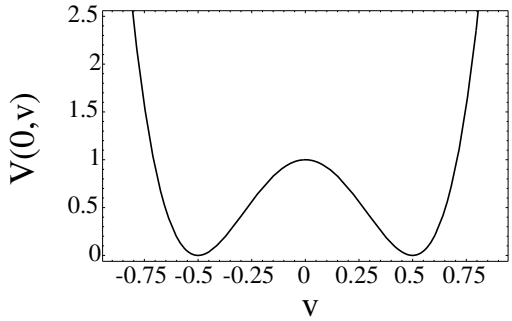
"HH fan": TrM $\simeq -4.183$ for all R orbits; similar for L orbits!

Bifurcation cascades in a double-well potential

$$V(u,v) = \frac{1}{2}\left(u^2 - v^2\right) + \lambda\left(v^4 - \frac{1}{2}u^2v^2\right) + \frac{1}{16\lambda}$$

equipotential lines and projection along $u = 0$:



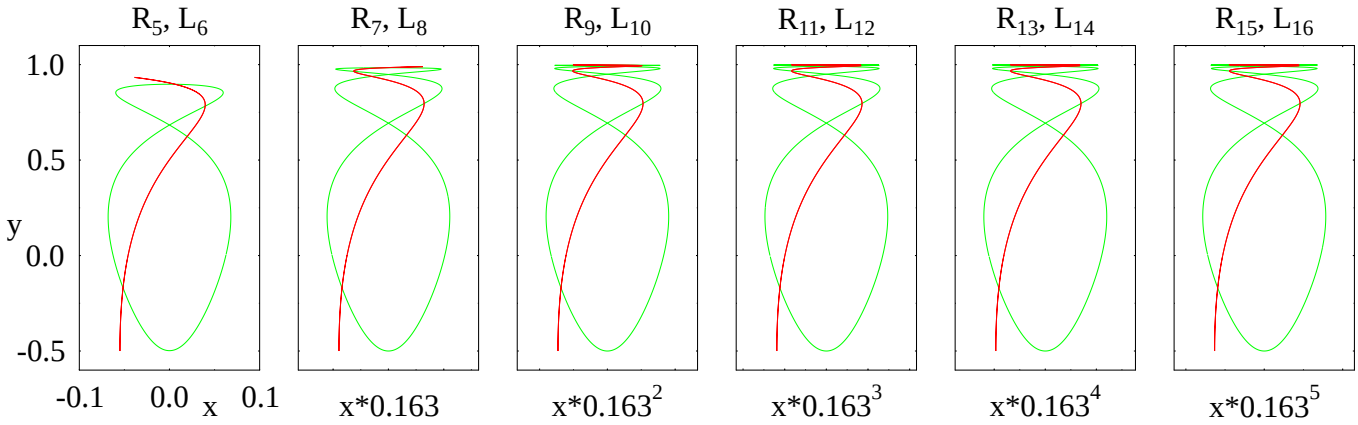


barrier at scaled energy $e = 1$; system is (quasi-)bound up to $e = 9$

A orbit in v direction has bifurcation cascades both below barrier (for $e \uparrow 1$) and above barrier (for $e \downarrow 1$)! ($T_A \to \infty$ in both cases)

Self-similarity of R and L orbits

Shapes or R and L orbits in (x, y) plane at $e = 1$, successively zoomed in the x direction by factor 0.163[1]:

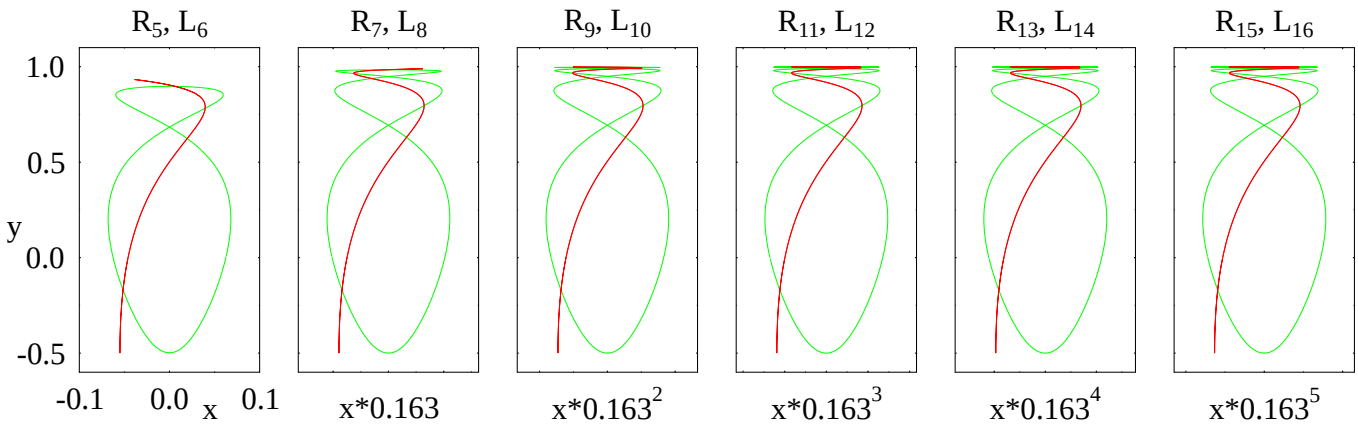


[1]more precisely: $\exp(-\pi/\sqrt{3}) = 0.1630335\ldots$
(an analytical 'Feigenbaum constant'!)

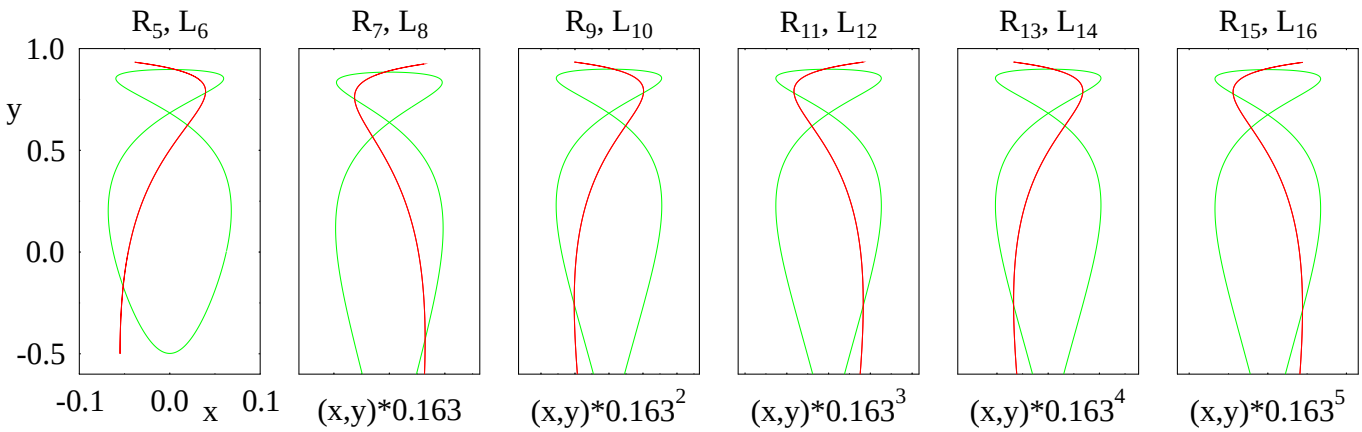
[M. Brack, Foundations of Physics **31**, 209 (2991)]

Self-similarity of R and L orbits

Shapes or R and L orbits in (x, y) plane at $e = 1$, successively zoomed in the x direction by factor 0.163:



Now zoom also in y direction by factor 0.163 (from barrier position at $y = 1$):



Analytical form of these shapes near bifurcations given by Lamé functions

[M. Brack, M. Mehta, K. Tanaka, J. Phys. A **34**, 8199 (2001)]

The "Hénon-Heiles fan"

Numerical finding:
[M. Brack, Foundations of Physics **31**, 209 (2991)]

for $n, m \to \infty$ (i.e., for $e \to 1$), the values of trM of the R_n orbits intersect linearly at $\mathrm{trM}_{R_n} = -4.183$, those of the L_m orbits at $\mathrm{trM}_{L_m} = +8.183$, thus

$$\mathrm{trM}_{R,L}(e) \longrightarrow 2 \mp 6.183 \left(\frac{e - e^*}{1 - e^*} \right)$$

where e^* are their respective bifurcation energies.

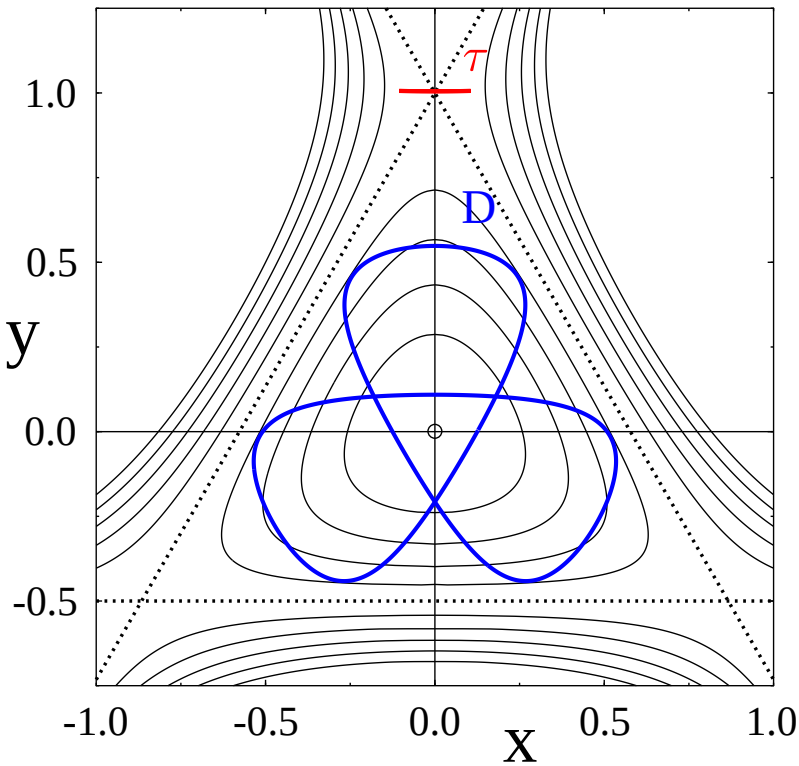
Explanation by first-order perturbation theory, following Creagh [Ann. Phys. **248**, 60 (1996)]:

using the term $x^2 y$ as a perturbation for the rational tori bifurcating in the separable HH potential ($\alpha = 1$) $V(x, y) = \frac{1}{2}(x^2 + y^2) - \frac{1}{3} y^3$ from the A orbit, we get:

$$\mathrm{trM}_{R,L}(e) \longrightarrow 2 \mp 5.069 \left(\frac{e - e^*}{1 - e^*} \right)$$

[S. Fedotkin, and M. Brack, work in progress]

Other orbits above the barrier ($e \geq 1$)

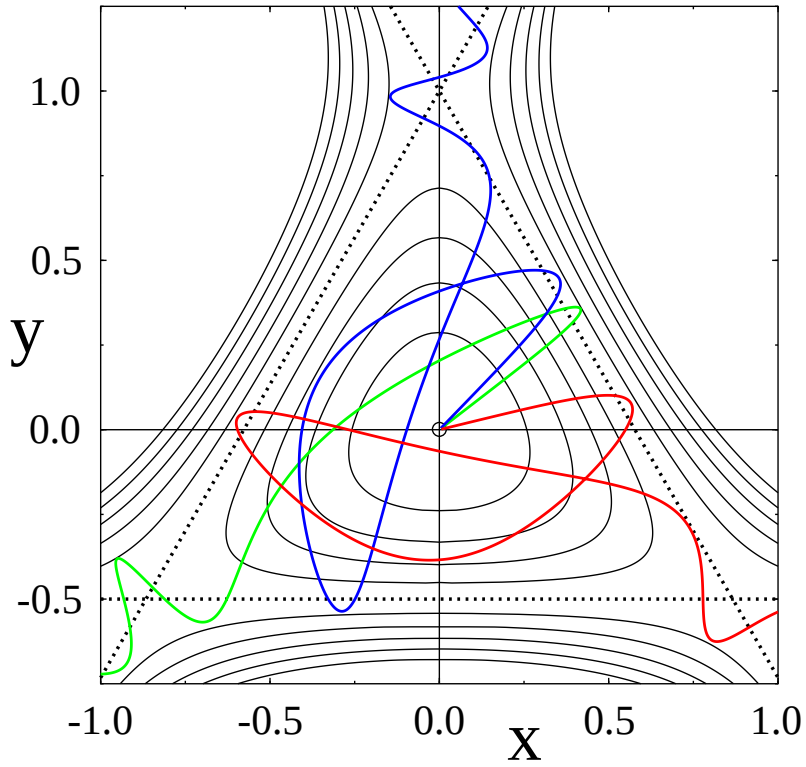


2 orbits D born at a bifurcation from C^2 at $e \simeq 0.892$, stable until $e \simeq 1.238$, then always unstable

3 orbits τ exist for all $e > 1$, always unstable (play the roles of PODS!)

Escape from the Hénon-Heiles potential

Unbound non-periodic orbits starting from $(x, y) = (0, 0)$ at $e = 1.2$:

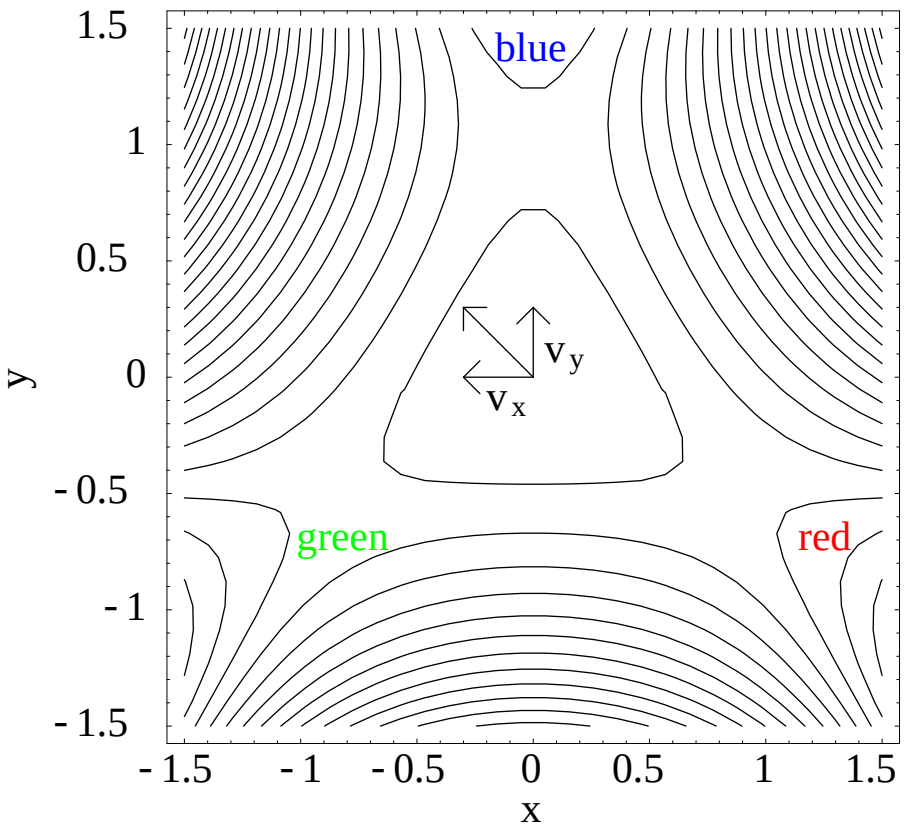


Note the sensitive dependence of the exit barrier on the initial direction!

Escape from the Hénon-Heiles potential

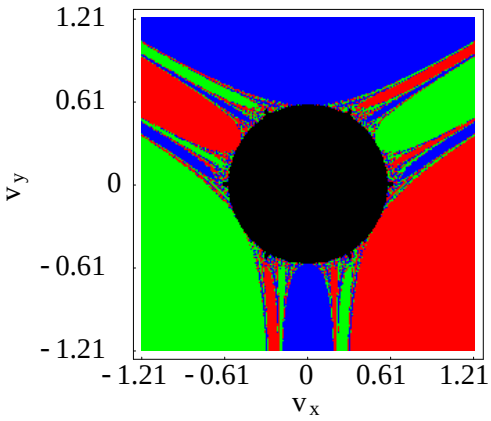
Where does the particle exit, when it starts from the point (x,y) = (0,0) ?

We vary the initial velocity (components v_x,v_y)



and insert coloured points corresponding to the exit barrier (blue, green, red) into a diagram (v_x,v_y)

Escape from the Hénon-Heiles potential



Colour gives exit barrier:

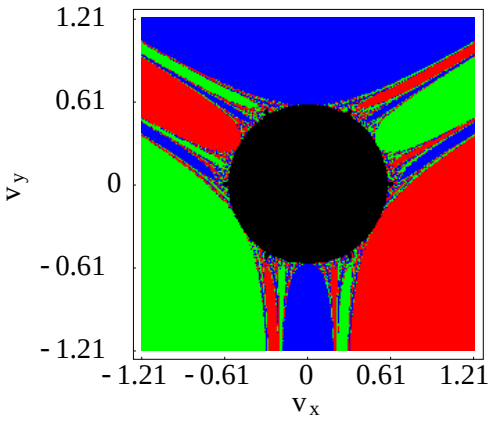
blue: upwards

red: down right

green: down left

black: no escape (circle: $e \leq 1$)

Escape from the Hénon-Heiles potential



Colour gives exit barrier:

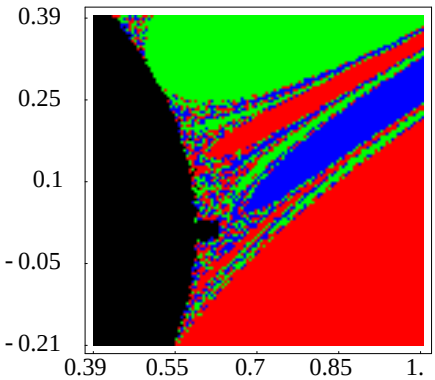
blue: upwards

red: down right

green: down left

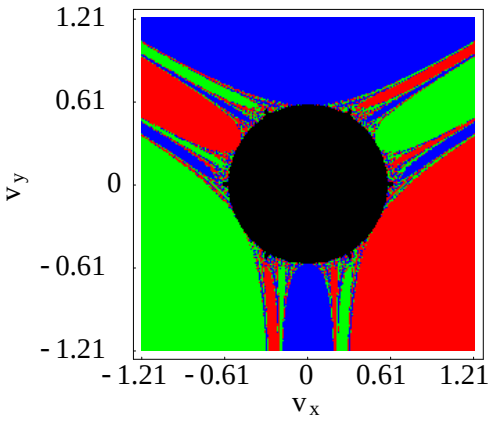
black: no escape (circle: $e \leq 1$)

zoom $\longrightarrow$



Appearance of a fractal structure!

Escape from the Hénon-Heiles potential



Colour gives exit barrier:

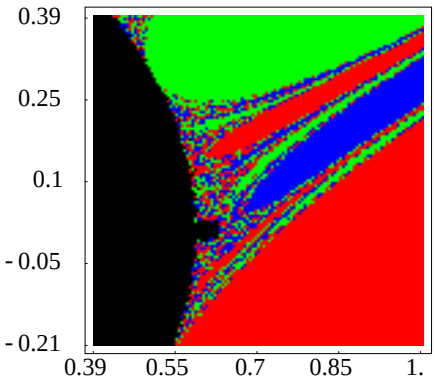
blue: upwards

red: down right

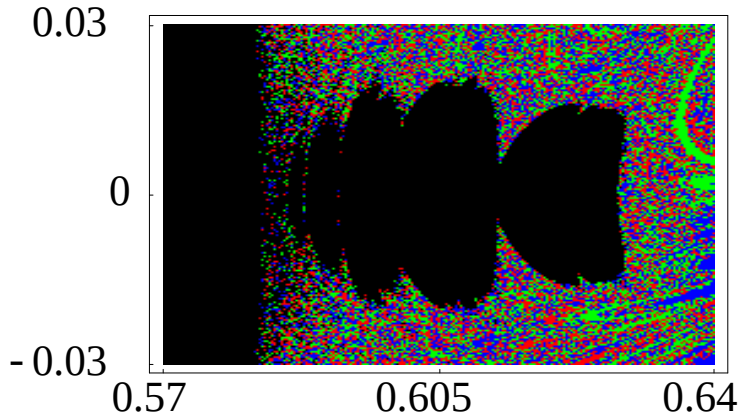
green: down left

black: no escape (circle: $e \leq 1$)

zoom $\longrightarrow$



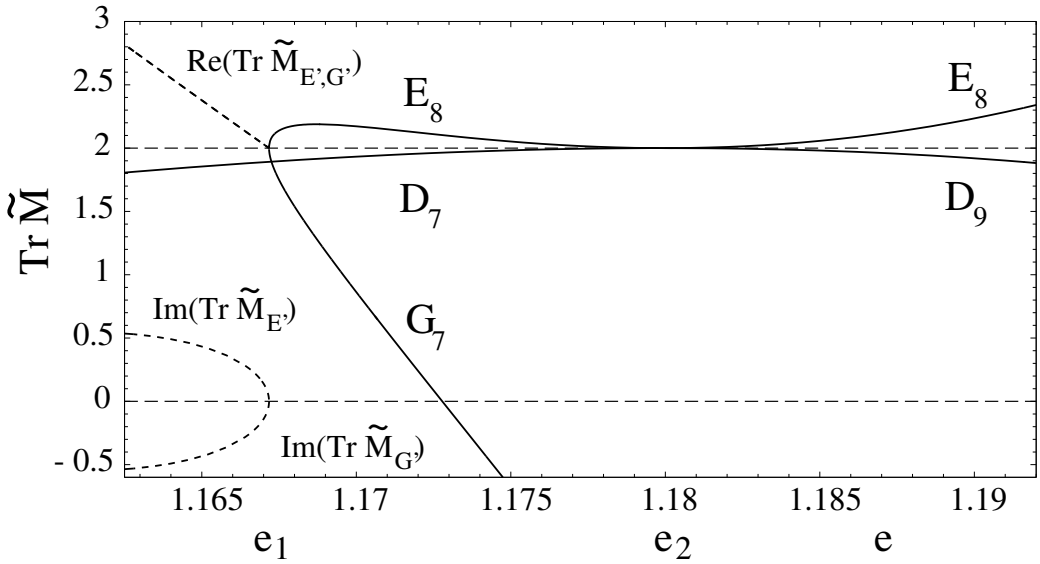
further zoom $\longrightarrow$



black island for $e > 1$: capture by stable orbit D above barrier!

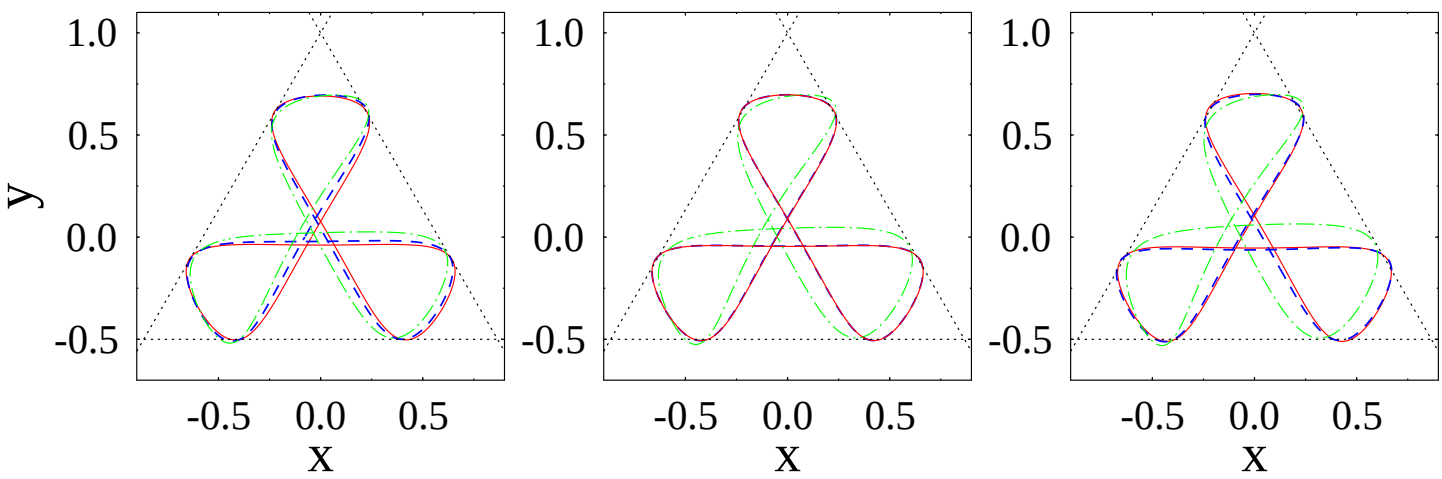
Bifurcation of the D orbit

trace of stability matrix:



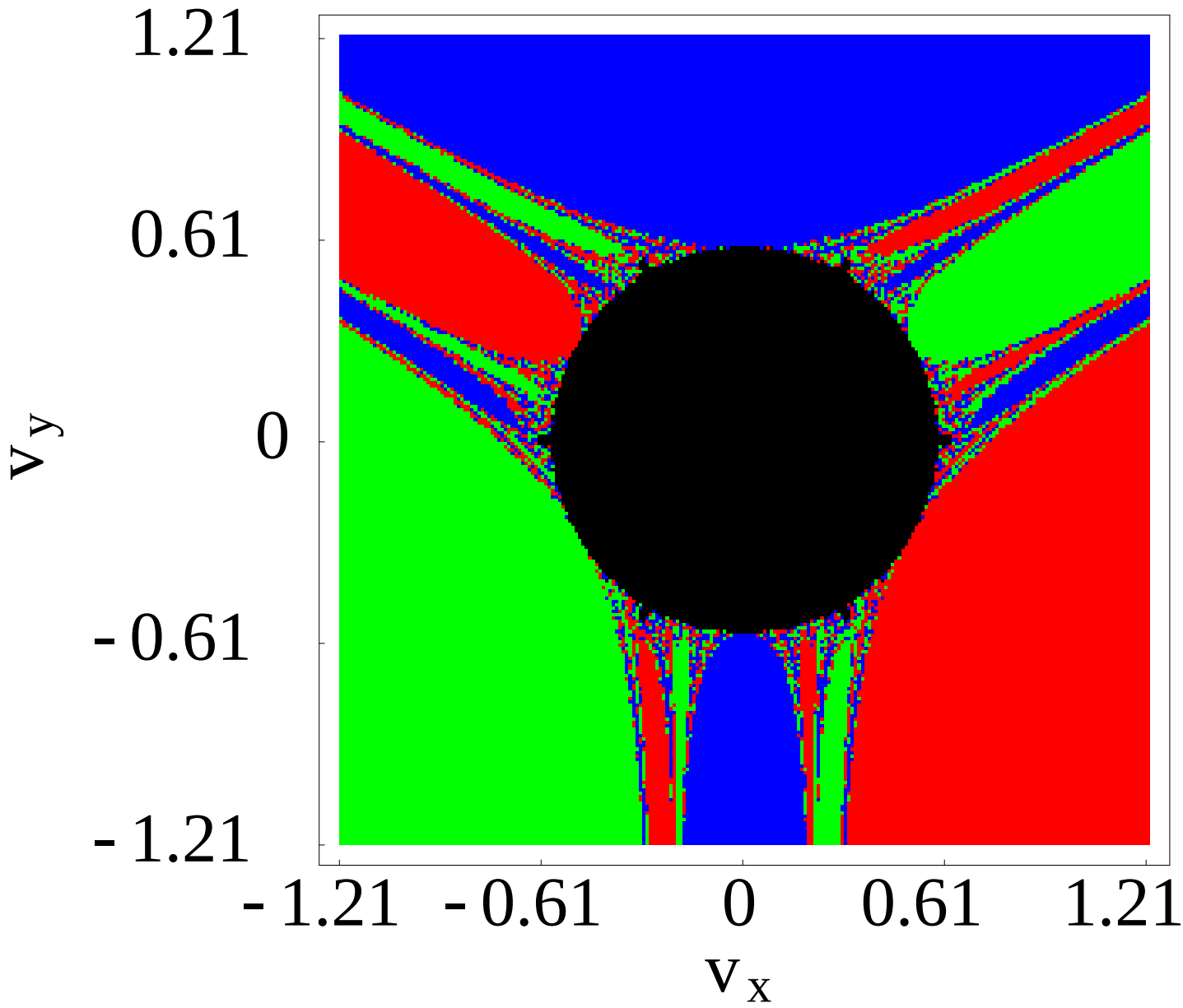
dashed lines show "ghost orbits" (needed for trace formula)

shapes of orbits D, E and G: (at $e = 1.17$, 1.18 and 1.19)



solid: D, dashed: E, dash-dotted: G

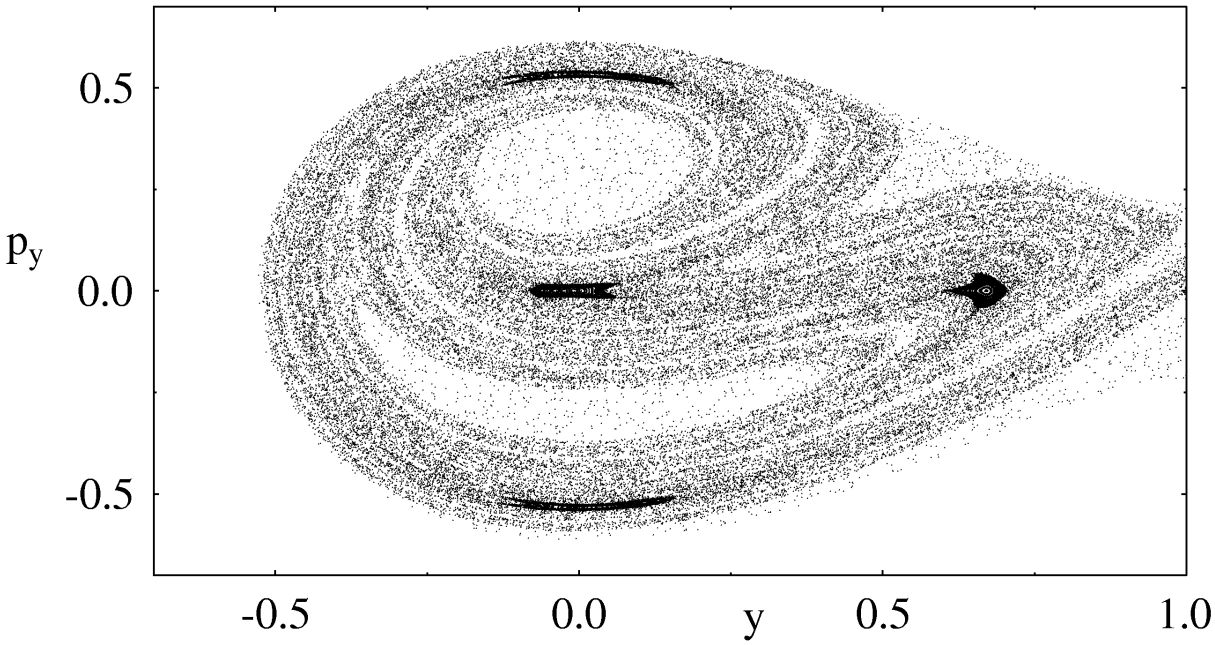
A closer look at the captures by the D orbit:

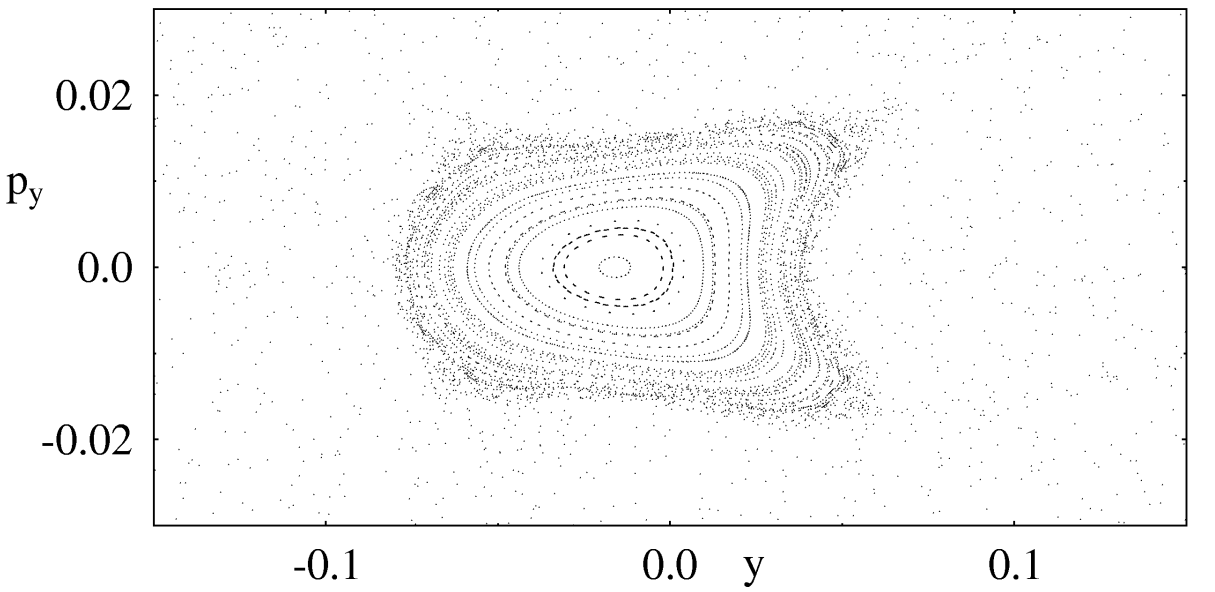


note the "capture islands" at angles $n \cdot 2\pi/6$ $(n = 0, 1, 2, 3, 4, 5)$!

Poincaré surface of section ($x = 0$)

at $e = 1.14$, zoom of central stability island of D orbit





The Gutzwiller trace formula

The quantum-mechanical **density of states**:

$$g(E) = \sum_n \delta(E - E_n) = \widetilde{g}(E) + \delta g(E)$$

Smooth part $\widetilde{g}(E)$: from extended Thomas-Fermi (ETF) model or Strutinsky smoothing of $\{E_n\}$

Oscillating part $\delta g(E)$: semiclassical trace formula
[M. Gutzwiller, J. Math. Phys. **12**, 343 (1971)]

$$\boxed{\delta g(E) \simeq \sum_{po} A_{po}(E) \cos\left[\frac{1}{\hbar} S_{po}(E) - \frac{\pi}{2}\sigma_{po}\right]}$$

Sum over periodic orbits (po) of the *classical system!*

$S_{po} = \oint_{po} \mathbf{p} \cdot d\mathbf{q}$ = action integral along po

A_{po} = amplitude (related to stability and degeneracy)

σ_{po} = Maslov index (= Conley-Zehnder index for symplectic path on a Lagrangian manifold)

In systems with mixed classical dynamics:
no convergence of po sum due to bifurcations!

Influence of periodic orbit bifurcations

Amplitude $A_{po}(E)$ for isolated orbit:

$$A_{po}(E) = \frac{T_{po}(E)}{r_{po}\sqrt{|\det\left(\mathrm{M}_{po}(E) - 1\right)|}}$$

M_{po} = stability matrix, r_{po} = repetition number of primitive periodic orbit

A_{po} diverges at po bifurcations, where $\det \mathrm{M}_{po} = 1$! (Reason: break-down of stationary-phase approximation in doing trace integrals)

Remedy: go beyond saddle-point approximation! This yields so-called uniform approximations

[Ozorio de Almeida & Hannay, Tomsovic *et al.*, Creagh, Sieber, Schomerus & Sieber, Brack *et al.*, ...]

But: this becomes increasingly complicated with increasing orbit lengths. (Number of bifurcations grows exponentially!)

Coarse graining

For *finite resolution* of energy spectrum, convolute level density over energy range γ

$$g_\gamma(E) = \frac{1}{\sqrt{\pi}\gamma} \sum_n e^{-\left(\frac{E-E_n}{\gamma}\right)^2}$$

$\Rightarrow$ get exponential damping factor in trace formula, suppressing orbits with longer periods T_{po}:

$$\delta g_\gamma(E) \sim \sum_{po} A_{po}(E)\, e^{-(\gamma T_{po}/2\hbar)^2} \cos\left[\frac{1}{\hbar} S_{po}(E) - \frac{\pi}{2}\sigma_{po}\right]$$

$\Rightarrow$ Only shortest orbits relevant for gross-shell effects!

Solves problem of convergence of po sum!

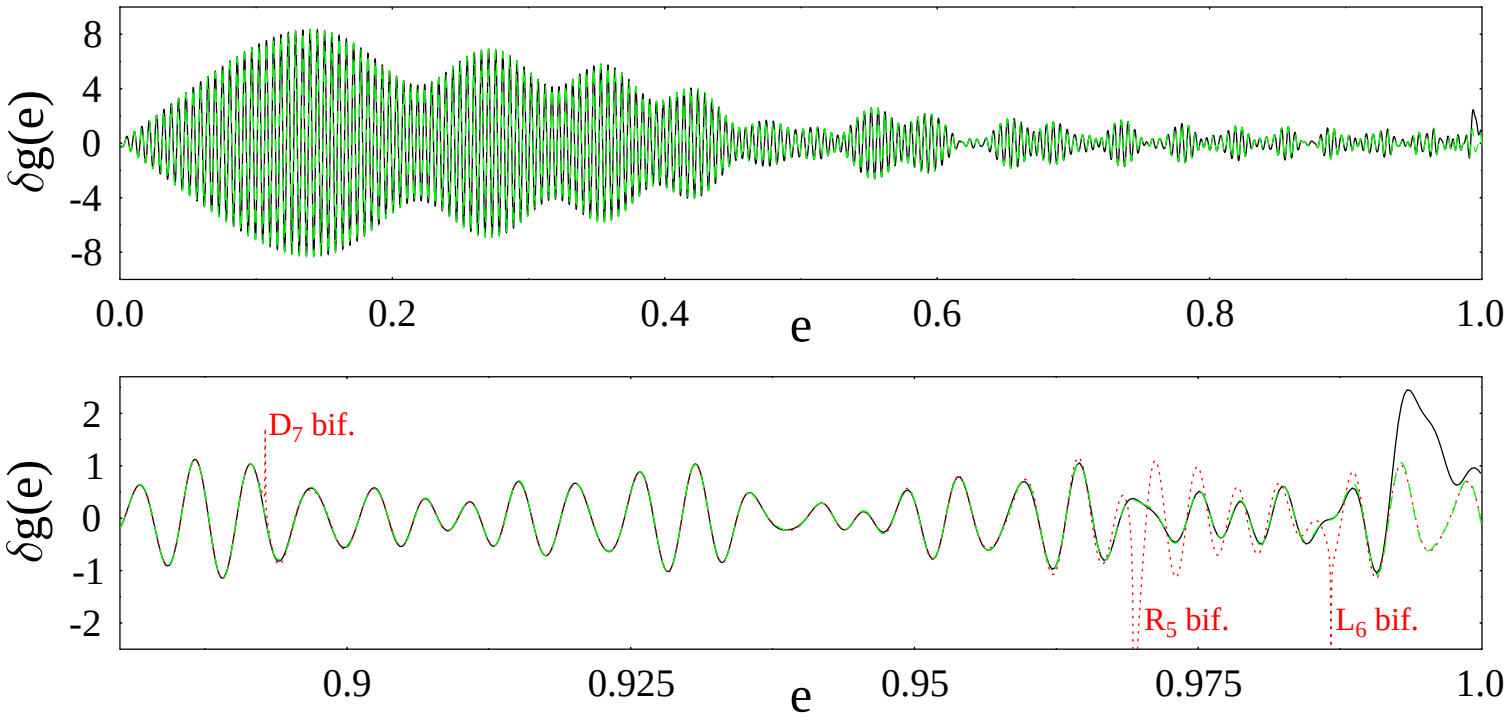
The Hénon-Heiles level density below barrier

with semiclassical trace formula ($\gamma = 0.4\,\hbar\omega$):

solid line: quantum-mechanical (α=0.03)

dotted line: semiclassical, Gutzwiller trace formula[1]

dashed line: semiclassical, Gutzwiller + uniform approximations[2]



only 11 periodic orbits contribute: (up to $e \sim 0.85$ only A,B,C!)

$A_{5/6/7}$, C_3, B_4, R_5 and L_6 ($k = 1, 2$), D_7 ($k = 1$)

[1]including uniform approximation for U(2) symmetry breaking [M. Brack, P. Meier, K. Tanaka, J. Phys. A **32**, 331 (1999)]

[2][J. Kaidel, M. Brack, Phys. Rev. E **70**, 016206 (2004)]

Level density in continuum

The trace formula is mathematically justifiable also in continuum regions. There, it describes the density of resonances:

$$E_n \longrightarrow E_n - i\Gamma_n$$

Γ_n = width of resonance, $\hbar/\Gamma_n \propto$ escape time from potential

Then, the level density $g(E)$ is given by

$$\sum_n \delta(E - E_n) \longrightarrow -\frac{1}{\pi} \mathrm{Im} \sum_n \frac{1}{E - E_n + i\Gamma_n/2}$$

after subtraction of non-resonating continuum density ($\propto \sqrt{E}$ in 3d, constant in 2d)

Role of finite widths Γ_n:

- affect smooth level density $\widetilde{g}(E)$ [cf. H. Schomerus and J. Tworzydlo, Phys. Rev. Lett. **93**, 154102 (2004)]
- give "natural" coarse-graining (selection of shortest orbits) in semiclassical trace formula for $\delta g(E)$

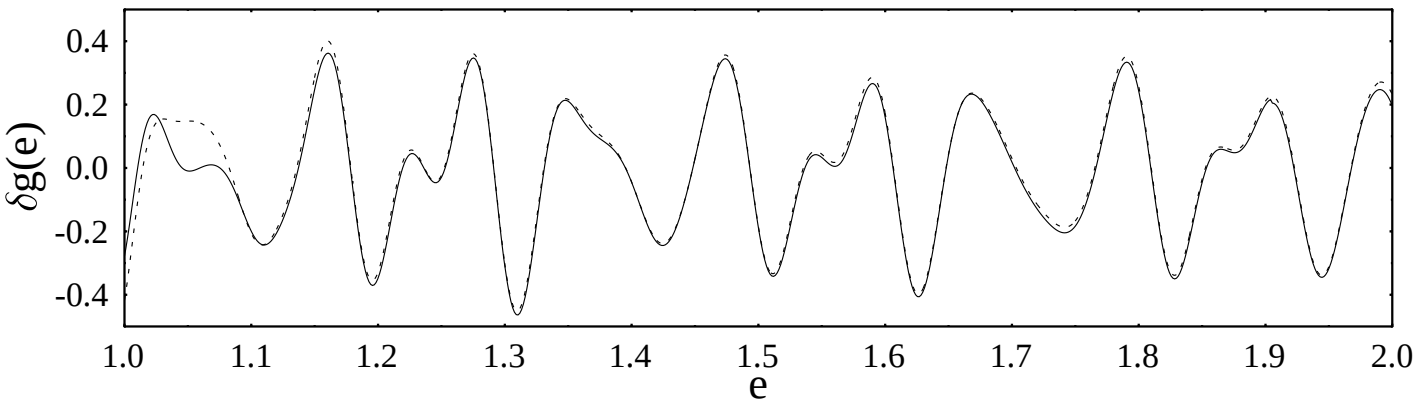
The Hénon-Heiles level density above barrier

using semiclassical trace formula with uniform approximation of orbit D bifurcation (codimension two) (smooth part $\widetilde{g}(E)$ obtained by complex Strutinsky smoothing; has small uncertainties at $e \gtrsim 1$!)

Coarse-graining with $\gamma = 0.5$ (energy unit $\hbar\omega = 1$):

dashed line: semiclassical

solid line: quantum-mechanical (with complex spectrum, α=0.1)



only 7 periodic orbits contribute (all unstable):

C_3, B_4, R_5 and L_6 ($k = 1$), τ ($k = 1, 2, 3$)

Note the pronounced regular shell structure in a 99.9% chaotic system!

[J. Kaidel, P. Winkler, M. Brack, Phys. Rev. E **70**, 066208 (2004)]

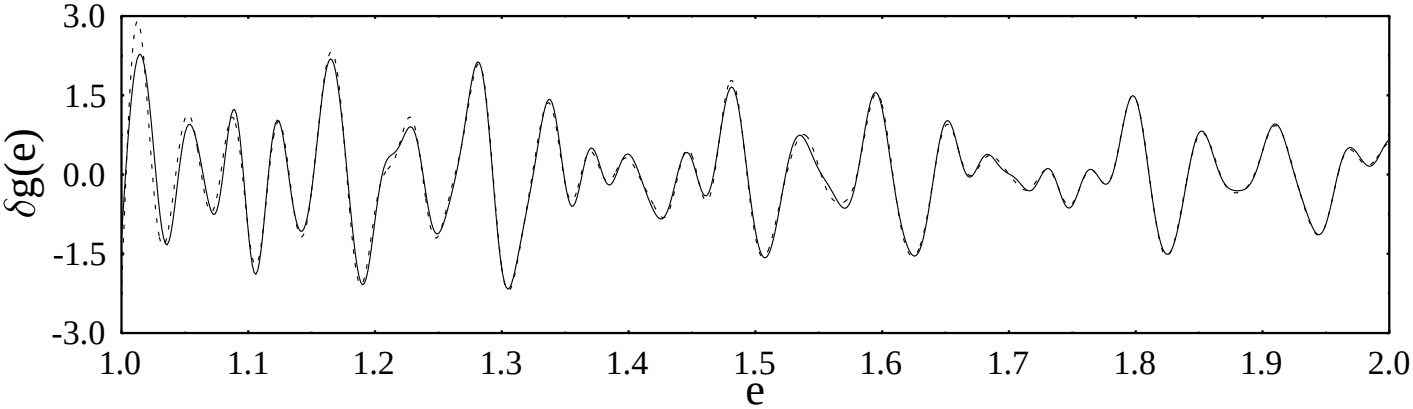
The Hénon-Heiles level density above barrier

using semiclassical trace formula with uniform approximation of orbit D bifurcation (codimension two) (smooth part $\widetilde{g}(E)$ obtained by complex Strutinsky smoothing; has small uncertainties at $e \gtrsim 1$!)

Coarse-graining with $\gamma = 0.25$ (energy unit $\hbar\omega = 1$):

dashed line: semiclassical

solid line: quantum-mechanical (with complex spectrum, α=0.1)



18 periodic orbits contribute:

C_3, B_4 ($k = 1, 2$); R_5, L_6, R_7 and L_8 ($k = 1$) (all unstable)

$D_{7/9}$, G_7 ($k = 1$, stable); E_8 ($k = 1$, unstable) + 2 "ghosts"

τ ($k = 1, 2, 3, 4, 5$, all unstable)

[J. Kaidel, P. Winkler, M. Brack, Phys. Rev. E **70**, 066208 (2004)]

Summary and Conclusions

1. Semiclassical trace formula (with uniform approximations for bifurcating orbits) reproduces detailed shell structure in the quantum-mechanical density of states in the continuum region

2. Only real orbits needed[1] for reproducing density of complex resonances

3. Pronounced shell structure in an (almost) chaotic system

4. Good prospectives for semiclassical calculations of molecular (or other few-body) reactions including quantum effects

[1] apart from "ghosts" required for uniform approximations near bifurcations

Thanks

1. To my collaborators and former students:
   - R. K. Bhaduri (McMaster, Canada)
   - M. V. N. Murthy (I.M.Sc. Madras, India)
   - S. Creagh (Nottingham, UK)
   - K. Tanaka (Saskatoon, Canada)
   - P. Winkler (Reno, USA)
   - S. Fedotkin, A. Magner (I.N.R. Kiev, Ukraine)
   - P. Meier, Ch. Amann, J. Kaidel (Regensburg)

2. To my sponsors:
   - Deutsche Forschungsgemeinschaft
   - NSERC (Canada)

3. To a patient audience!