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

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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

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Motivation

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

\[ V(x, y) = \frac{1}{2} (x^2 + y^2) + \alpha (x^2y - \frac{1}{3} y^3) \]

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

- Model for the deformation (vibrational) energy of triatomic molecules such as \( \text{H}_3^+ \), 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 \( (E \gg E_{\text{th}}) \)
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 .....  

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": $\text{Tr} M \simeq -4.183$ for all $R$ orbits; similar for $L$ orbits!
Bifurcation cascades in a double-well potential

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

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\(^1\):

\[ \exp(-\pi/\sqrt{3}) = 0.1630335 \ldots \]

(an analytical 'Feigenbaum constant'!)

\[ \text{[M. Brack, Foundations of Physics 31, 209 (2991)]} \]
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:

![Graphs of R and L orbits zoomed in x direction](image)

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

![Graphs of R and L orbits zoomed in y direction](image)

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 $\text{trM}$ of the $R_n$ orbits intersect linearly at $\text{trM}_{R_n} = -4.183$, those of the $L_m$ orbits at $\text{trM}_{L_m} = +8.183$, thus

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

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:

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

[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 \(\tau\) 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
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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: \( e \leq 1 \))

black island for \( e > 1 \): capture by stable orbit D above barrier!
Bifurcation of the D orbit

trace of stability matrix:

![Trace of stability matrix diagram]

- Dashed lines show "ghost orbits" (needed for trace formula)
- Shapes of orbits D, E and G: (at $e = 1.17, 1.18$ and $1.19$)

![Orbit shapes diagram]
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:

\[ g(E) = \sum_n \delta(E - E_n) = \tilde{g}(E) + \delta g(E) \]

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

Oscillating part \( \delta g(E) \): semiclassical trace formula


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

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

\( S_{po} = \oint_{po} p \cdot dq = \) action integral along \(po\)

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

\( \sigma_{po} = \) 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:

$$A_{po}(E) = \frac{T_{po}(E)}{r_{po} \sqrt{|\det (M_{po}(E) - 1)|}}$$

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

$A_{po}$ diverges at $po$ bifurcations, where $\det M_{po} = 1$!
(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 $\gamma$

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

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

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

⇒ 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 ($\alpha=0.03$)
- dotted line: semiclassical, Gutzwiller trace formula
- dashed line: semiclassical, Gutzwiller + uniform approximations

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
$^2$[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:

\[
E_n \rightarrow E_n - i \Gamma_n
\]

\( \Gamma_n = \) width of resonance, \( \hbar/\Gamma_n \propto \) escape time from potential

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

\[
\sum_n \delta(E - E_n) \rightarrow -\frac{1}{\pi} \text{Im} \sum_n \frac{1}{E - E_n + i\Gamma_n/2}
\]

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

Role of finite widths \( \Gamma_n \):

- affect smooth level density \( \tilde{g}(E) \) [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 $\tilde{g}(E)$ obtained by complex Strutinsky smoothing; has small uncertainties at $\epsilon \gtrsim 1$!)

Coarse-graining with $\gamma = 0.5$ (energy unit $\hbar \omega = 1$):
dashed line: semiclassical
solid line: quantum-mechanical (with complex spectrum, $\alpha = 0.1$)

only 7 periodic orbits contribute (all unstable):
$C_3$, $B_4$, $R_5$ and $L_6$ ($k = 1$), $\tau$ ($k = 1, 2, 3$)

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 $\tilde{g}(E)$ 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, $\alpha=0.1$)

18 periodic orbits contribute:
$C_3, B_4 \ (k = 1, 2); R_5, L_6, R_7 \text{ and } L_8 \ (k = 1) \ (\text{all unstable})$
$D_{7/9}, G_7 \ (k = 1, \text{stable}); E_8 \ (k = 1, \text{unstable}) + 2 \text{ “ghosts”}$
$\tau \ (k = 1, 2, 3, 4, 5, \text{all unstable})$

[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!