# 20 years of fun with periodic orbits and trace formulae

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Talk presented at the Workshop “MAGUTZ15”
**Martin Gutzwiller’s scientific Universe:**
**From Wavefunctions over periodic Orbits to Sun, Moon and Earth**
*(MPI-PKS Dresden, 28-31 October 2015)*

# Semiclassical description of gross-shell structures in finite fermion systems

- Nuclei: Systematics of ground-state deformations
- Nuclei: Onset of asymmetric fission ⇐
- Metal clusters: "Supershells" – beat of two shortest orbits
- Mesoscopic physics: Magnetization in external B field
- Trapped dilute Fermi gases: "Supershells"
- Spatial density oscillations (in terms of *non-periodic* closed orbits) ⇐

We had a lot of fun also using POT for the Hénon-Heiles potential (with R.K.Bhaduri, M.V.N.Murthy, J.Law, K.Tanaka *et al.*)

For many examples and illustrations, see M.Brack and R.K.Bhaduri: *"Semiclassical Physics"* (Westview Press, Boulder, USA 2003)

# Trace formulae for finite fermion systems

For $N$ interacting fermions in a (self-consistent) mean field approximation (HF or DFT):

$$\left\{\hat{T} + V[\{\phi_i\}]\right\}\phi_n = E_n\phi_n .$$

Total energy ('Strutinsky theorem'): $E \simeq \widetilde{E} + \delta E$ (with $N = \widetilde{N} + \delta N$), $\widetilde{E}(\widetilde{N})$ from selfconsistent ETF model, $\delta E$ = 'shell-correction energy' defined in terms of the $E_n$ (Strutinsky, 1968).

**Trace formulae** using the periodic orbits ($po$) in the classical hamiltonian $H(\mathbf{r},\mathbf{p}) = \mathbf{p}^2/2m + V(\mathbf{r})$; here $V(\mathbf{r})$ is a model potential for $V[\{\phi_i\}]$.

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

$$\delta N \simeq -\sum_{po}\left(\frac{\hbar}{T_{po}(\lambda_N)}\right)A_{po}(\lambda_N)\sin\left[\frac{1}{\hbar}S_{po}(\lambda_N) - \frac{\pi}{2}\sigma_{po}\right]$$

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

(Strutinsky, 1975) $\lambda_N$ = Fermi energy

# Gross-shell structure given by shortest *pos*

Because of the factor $(\hbar/T_{po})^2$, the shell-correction energy $\delta E$ converges fast with increasing orbit length.

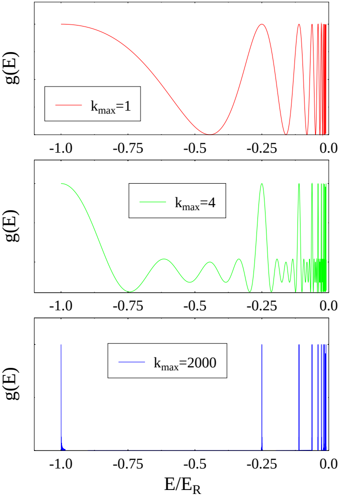
$\Rightarrow$ Often the gross-shell structure of a system is already well described by the shortest (few) orbits!

This holds also for the level density $\delta g(E)$ in integrable systems.

# Exact trace formula for the hydrogen spectrum

The exact level density is given by ($E_R$ = Rydberg energy)

$$g(E) = \sum_n d_n\, \delta(E - E_n) = \frac{1}{2}\frac{E_R^{3/2}}{(-E)^{5/2}} \left\{1 + 2\sum_{k=1}^{\infty} \cos\left(2\pi k \sqrt{-E_R/E}\right)\right\}$$




The lowest Fourier component ($k = 1$), i.e., the shortest periodic orbit family, already yields maxima at the positions of the quantum energies.

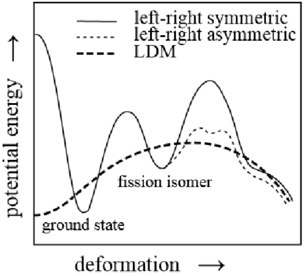
⇒ "gross-shell structure"!

$k_{max} = 2000$ gives practically the exact quantum spectrum: $E_n = -E_R/n^2$.

# Asymmetric fission of an actinide nucleus

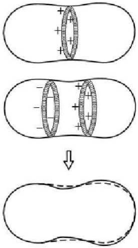
Schematic deformation energy of a typical actinide nucleus:

[after "Funny Hills": M.Brack, J.Damgård, A.S.Jensen, H.C.Pauli, V.M.Strutinsky, C.Y.Wong, Rev. Mod. Phys. **44**, 320 (1972)]




The instability against asymmetry is due to pairs of 'diabatic' single-particle states localized on parallel planes perpendicular to the symmetry axis at and near the waist-line of the nucleus. Their energies repel each other.

[C.Gustafsson, P.Møller, and S.G.Nilsson, Phys.Lett. **34B**, 349 (1971)]



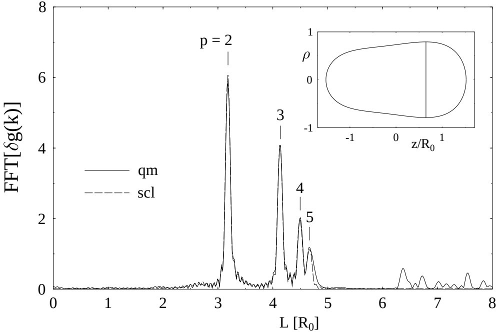
⇒ The (experimentally known) fragment mass asymmetry in fission was understood as a **quantum shell effect** which could not be explained in the (semi-)classical liquid drop model!

# Semiclassical fission model

[M.Brack, S.M.Reimann, M.Sieber, Phys.Rev.Lett. **79**, 1817 (1997)]

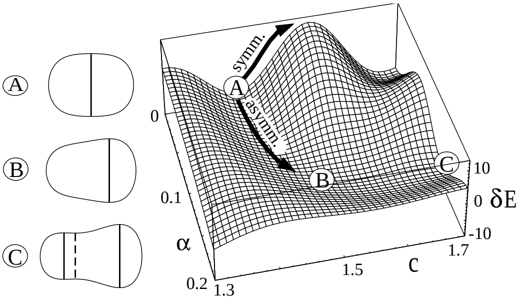
- cavity model with "Funny Hills" $(c, h, \alpha)$ shapes
- simple: only one kind of particles; no Couloumb, no spin-orbit
- only one adjusted parameter: Fermi energy $\lambda_N$
- 4 shortest *po* families in each equator plane are sufficient!

Fourier transform of level density: quantum-mechanical vs. semiclassical (at asymmetric saddle, see point B below):



# Semiclassical fission barrier of $^{240}$Pu

Semiclassical $\delta E$ versus elongation c ($h = 0$) and asymmetry $\alpha$:

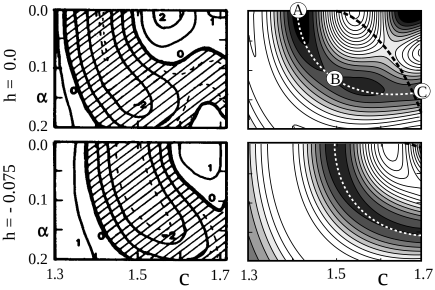



(Includes uniform approximation for bifurcation of orbit planes!)

[M.Brack, S.M.Reimann, M.Sieber, Phys.Rev.Lett. **79**, 1817 (1997)]

# Comparison with realistic old quantum result

Contour plots $\delta E(\alpha, c)$ ($h$ fixed) around second barrier:



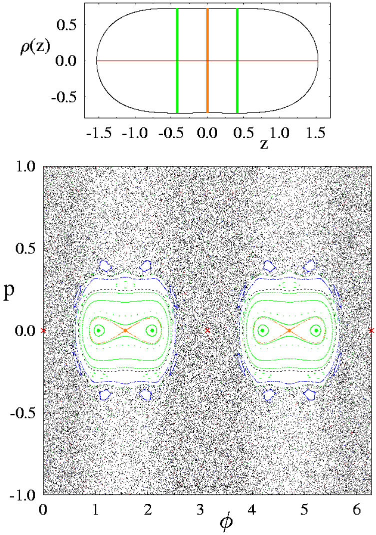

Left: quantum-mechanical $\delta E$ (realistic) ["Funny Hills", RMP 1972]
Right: semiclassical $\delta E$ (cavity model) [M.B. *et al.*, PRL 1997]

Valleys of minimal $\delta E$ (white dashed lines): actions of *pos* are constant

$$\boxed{\delta S_{po} = 0}$$

$\Rightarrow$ Classical least-action principle determines adiabatic fission path!

# Poincaré Surface of Section at the symmetric outer barrier ($\alpha = 0$):



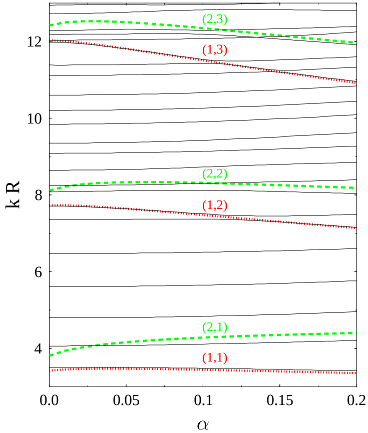

The shortest periodic orbits lie in the same planes (orthogonal to symmetry axis) as the wavefunction extrema of the 'diabatic' single-particle states!

In the Poincaré SS they lie in a small regular island embedded in a chaotic sea.

[M.Brack, M.Sieber and S.M.Reimann, Phys. Scr. T90, 146 (2001)]

# Quantization of the small regular island

Approximate EBK quantization of the linearized motion near the shortest periodic orbits in a “quasimode approximation” (as if in an ellipsoid with the same curvatures at the turning points).




Exact quantum-mechanical levels (black) of the cavity model versus $\alpha$ ($c = 1.53$).

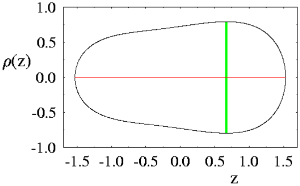
The 'EBK-quantized' levels ($n_\rho, n_\phi$) (dashed, coloured) approximate the 'diabatic' quantum levels that decrease in energy with increasing asymmetry $\alpha$ and lie just underneath the Fermi energy.

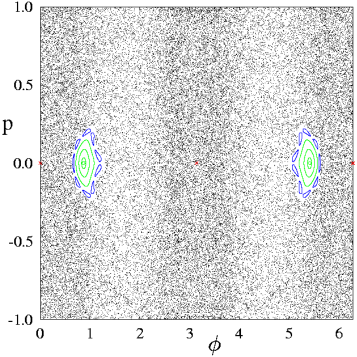
$\Rightarrow$ The total energy of the system is decreased by 'going asymmetric'!

[M.Brack, M.Sieber and S.M.Reimann,

Phys. Scr. T90, 146 (2001)]

# Poincaré Surface of Section at the asymmetric saddle ($\alpha = 0.13$):




The only (stable) periodic orbits lie in the same plane as the wavefunction extrema of the downgoing 'diabatic' single-particle state.

The tiny regular island containing these orbits has shrunk dramatically. Nevertheless: Its regular orbits drive the onset of the fission mass asymmetry – an experimenally observed phenomenon in a many body system!

[M.Brack, M.Sieber and S.M.Reimann,

Phys. Scr. T90, 146 (2001)]

# Semiclassical theory for spatial density oscillations

We study the spatial densities

$$\rho(\mathbf{r}) = \sum_{E_n \leq \lambda_N} \psi_n^\star(\mathbf{r})\psi_n(\mathbf{r})\,, \quad \tau(\mathbf{r}) = -\frac{\hbar^2}{2m} \sum_{E_n \leq \lambda_N} \psi_n^\star(\mathbf{r})\nabla^2\psi_n(\mathbf{r})\,.$$

Their oscillations can be described by **trace formulae** in terms of **closed non-periodic orbits** (*npo*) starting and ending at **r**.

[J. Roccia and M. Brack, Phys. Rev. Lett. **100**, 200408 (2008)]

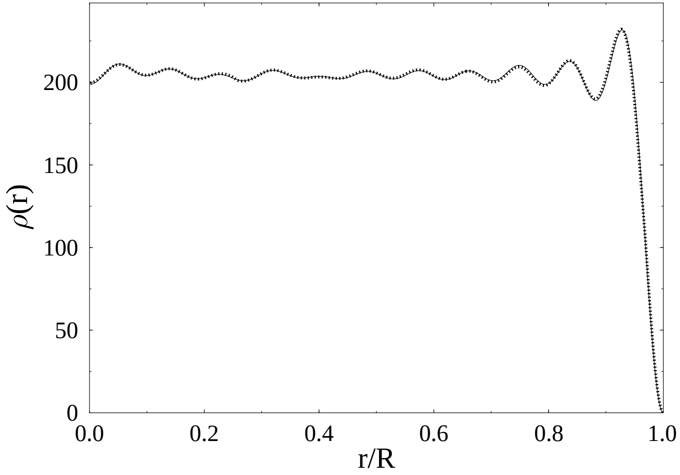
For systems with **spherical symmetry**, as a function of the parameter $r$:

- at $r = 0$: symmetry breaking occurs (here only diametrical orbits)
- at specific radii $r_i$: bifurcations occur, where new orbits are born
- near surface: Friedel oscillations come from the shortest *npo*
- all must be treated in uniform approximations

[M. Brack and J. Roccia, J. Phys. A **42** (2009)]

# Example: 2-dimensional circular billiard

Spatial density $\rho(r)$ for $N = 606$ particles: (solid: qm, dotted: scl)




[from M. Brack and J. Roccia, J. Phys. A **42** (2009)]

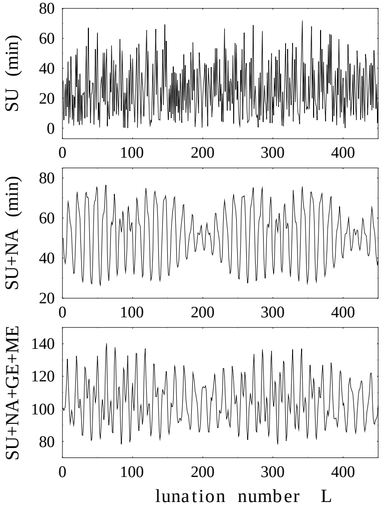
# The Babylonian connection

Martin marvelled at the accuracy to which the old Babylonians had determined the period of the anomalistic Month: $P_☾ = 27.55453$ days. This agrees to within 6 digits with its presently known value of 27.55455 days (calculated for Babylonian times)!
Even on IBM's largest computers in the 1970ies, it took a huge effort to compute $P_☾$ as accurately from the secular perturbation theory of the Moon.

See Martin's accounts in Chap. 4 of his book:
*"Chaos in Classical and Quantum Mechanics"* (Springer Verlag, New York, 1990), and in his review article:
*"Moon-Earth-Sun: The oldest three-body problem"*, Rev. Mod. Phys. **70**, 589 (1998).

But how could the Babylonians more than 2500 years ago find the period of the Moon, without having any dynamical model of our solar system?

# Lunar data from Babylon (since ca. 650 B.C.)




The Babylonians recorded time intervals SU, NA, GE, ME between risings and settings of Sun and Moon at successive oppositions (labeled by the lunation number L) observed along the horizon.

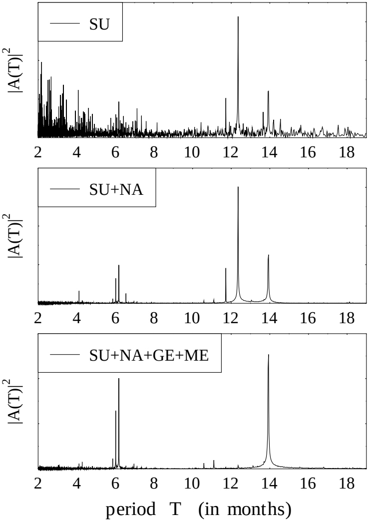
They regularly recorded also the partial sums (SU+NA) and (ME+GE).

The sum (SU+NA)+(GE+ME) was most likely used to determine column Φ having the correct lunar period $T_☾$.

[Lis Brack-Bernsen, Centaurus **33**, 39 (1990)]

Continuous observations over ∼ 600 years allowed for the high accuracy of $T_☾$!

# Fourier analysis of the lunar data




The data SU, NA, GE, ME, (SU+NA), and (GE+ME) are all dominated by the periods $T_\odot \simeq 12.3$ months (Sun) and $T_☾ \simeq 14$ months (Moon).

In the **sum** (SU+NA)+(GE+ME) the influence of $T_\odot$ is eliminated, and $T_☾$ determines the period of the oscillations.
$\Rightarrow$ The Babylonians performed (without knowing it!) a Fourier decomposition of their observed Lunar data to find $T_☾$.

[L.Brack-Bernsen and M.Brack, Int.J.Mod.Phys. E **13**, 247 (2004)]

# Our last encounter in September 2009

Workshop in Regensburg, September 18-19, 2009

Attentive and interested, as ever!

Martin gave a nice talk on Tycho Brahe, Johannes Kepler, and Hill's theory of the moon.

**Thanks, Martin, for your beautiful scientific ideas and for the stimulation you have given to all of us!**