SEMICLASSICAL DESCRIPTION OF SHELL EFFECTS IN FINITE FERMION SYSTEMS

M. Brack, University of Regensburg

(“Nilsson model 50 years”, Lund, 14. June 2005)

1. Semiclassics and POT: basics
   – semiclassical quantization (WKB, EBK)
   – Gutzwiller's trace formula
   – Periodic Orbit Theory (POT) for shell effects

2. Applications to finite fermion systems
   – nuclei (deformations, asymmetry of fission barrier)
   – metal clusters (supershells, deformations)
   – semiconductor nanostructures (conductance fluctuations)
   – trapped dilute fermionic gases (supershells)[1)]

[1)] omitted due to lack of time; see the talk of Magnus Ögren!

For a general introduction to POT, see:
M. Brack and R. K. Bhaduri: *Semiclassical Physics*
(Westview Press, Boulder CO, USA 2003)

Semiclassical quantization

Bohr-Sommerfeld quantization + WKB: (1-dim.)

Quantization of action integral along periodic orbit:

$$S(E) = \oint p(x) \cdot dx = 2\pi \hbar \, (n + \alpha) \qquad n = 0, 1, 2, \ldots$$

$\Rightarrow$ quantized eneriges E_n, become exact in limit $n \gg 1$ (Bohr's correspondence principle!), i.e., for

$$\boxed{S \gg \hbar}$$

(but works often well already for n = 0, 1, 2, . . . !)

In $(N>1)$ dimensions: **torus (EBK) quantization,** works only for **integrable systems!**

Gutzwiller's trace formula:

derived (1971) from the Feynman path-integral formulation of quantum mechanics in the limit $S \gg \hbar$: works also for **non-integrable and chaotic systems**!

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 Weyl expansion)

Oscillating part $\delta g(E)$: semiclassical trace formula (to leading order in $\hbar$)

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

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)

$\sigma_{po} =$ Maslov index

[M. Gutzwiller, J. Math. Phys. **12**, 343 (1971)]

Trace formulae for finite fermion systems

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

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

Total energy (using Strutinsky theorem): $E = \widetilde{E} + \delta E$ with $N = \widetilde{N} + \delta N$.[1)]

Trace formulae from classical $H(\mathbf{p}, \mathbf{q}) = T + V$: [practically: using model potential $V[\phi] \rightarrow V(\mathbf{q})$]

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

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

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

$E_F(N) =$ Fermi energy

[1)] Average $\widetilde{E}(N)$: from selfconsistent ETF (or liquid drop) model

Coarse graining and finite temperatures

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:

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

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

Similarly at finite temperatures T (for grand canonical ensemble):

$$\delta g_T(E) \sim \sum_{po} A_{po}(E)\, \frac{\tau_{po}}{\mathrm{Sinh}(\tau_{\mathrm{po}})}\, \cos\left[\frac{1}{\hbar} S_{po}(E) - \frac{\pi}{2}\,\sigma_{po}\right]$$

with $\tau_{po} = k_B T \pi T_{po}/\hbar$ $\Rightarrow$ trace formula for free energy:

$$\delta F = \sum_{po} \left(\frac{\hbar}{T_{po}}\right)^2 \frac{A_{po}(E_F)\, \tau_{po}}{\mathrm{Sinh}(\tau_{\mathrm{po}})}\, \cos\left[\frac{1}{\hbar} S_{po}(E_F) - \frac{\pi}{2}\,\sigma_{po}\right]$$

Bifurcations

At a bifurcation (e.g., $E = E_{bif}$) of a periodic orbit, the amplitude $A_{po}(E_{bif})$ diverges!

Remedy: go beyond the second-order stationary phase approximation in the integral(s) used for the derivation of $A_{po}(E)$. This leads to

Uniform approximations:

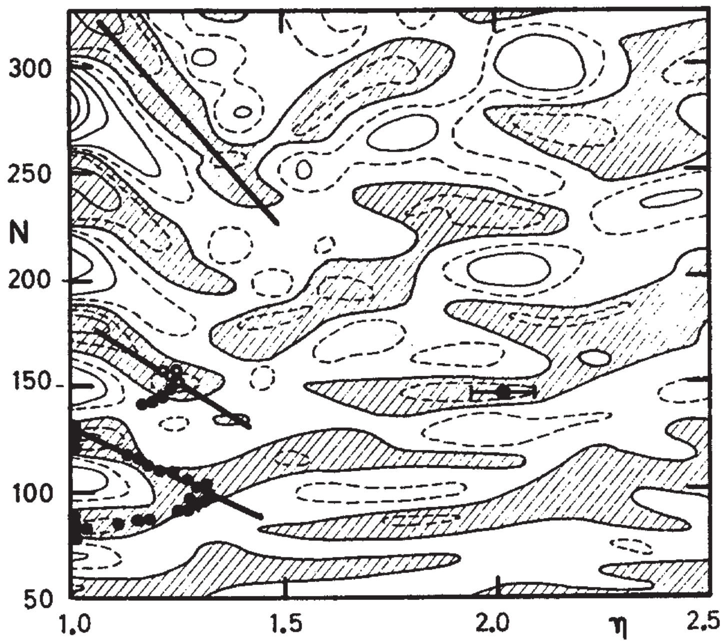
- local, near a bifurcation: see Ozorio de Almeida and Hannay, J. Phys. **A 20**, 5873 (1987)

- global, to recover also the asymptotic Gutzwiller amplitudes far from the bifurcation: see Sieber and H. Schomerus, J. Phys. **A 31**, 165 (1998)
(and earlier work quoted therein)

Attention: No physical meaning should be attached to the diverging amplitudes A_{po} near bifurcations without doing appropriate uniform approximations!

Nuclear deformations

Neutron shell-correction energy $\delta E_n(\eta, N)$ versus deformation (axis ratio) η and neutron number N:



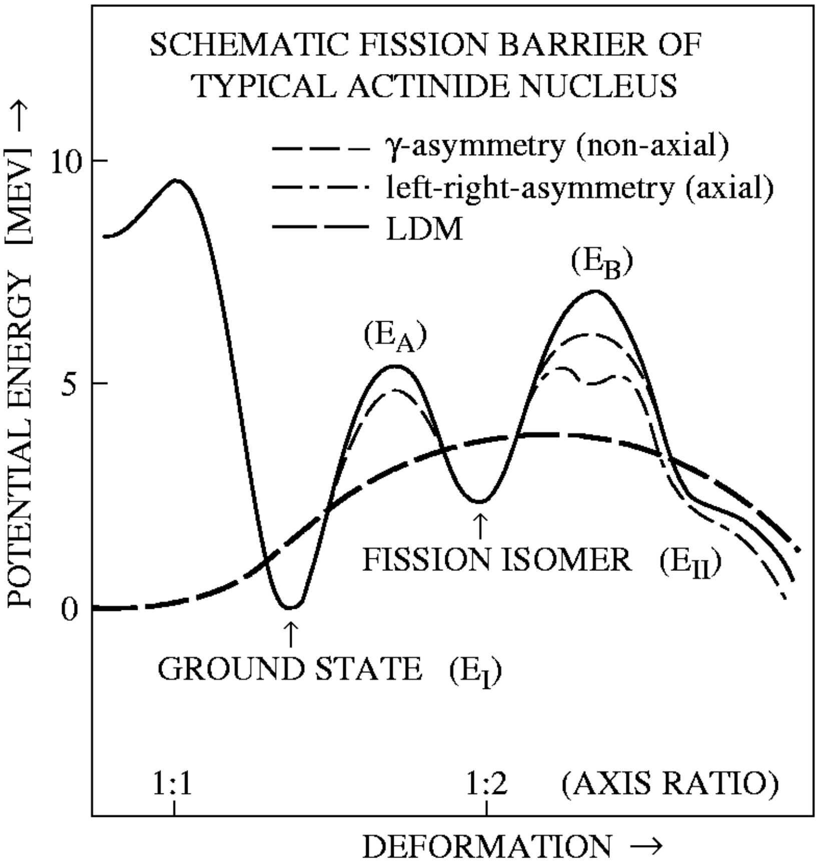
Contours: quantum-mechanics with spheroidal Woods-Saxon potential (including spin-orbit interaction)

Bars: semiclassical valleys of minima: $\delta S_{po} = 0$ for actions of shortest periodic orbits in ellipsoidal cavity (no spin-orbit; Fermi energy adjusted to reproduce correct magic numbers!)

[V. M. Strutinsky, A. G. Magner, S. R. Ofengenden and T. Døssing, Z. Phys. **A 283**, 269 (1977)]

The “double-humped” fission barrier

Deformation energy of a typical actinide nucleus (schematic, projected onto one-dimensional deformation variable):



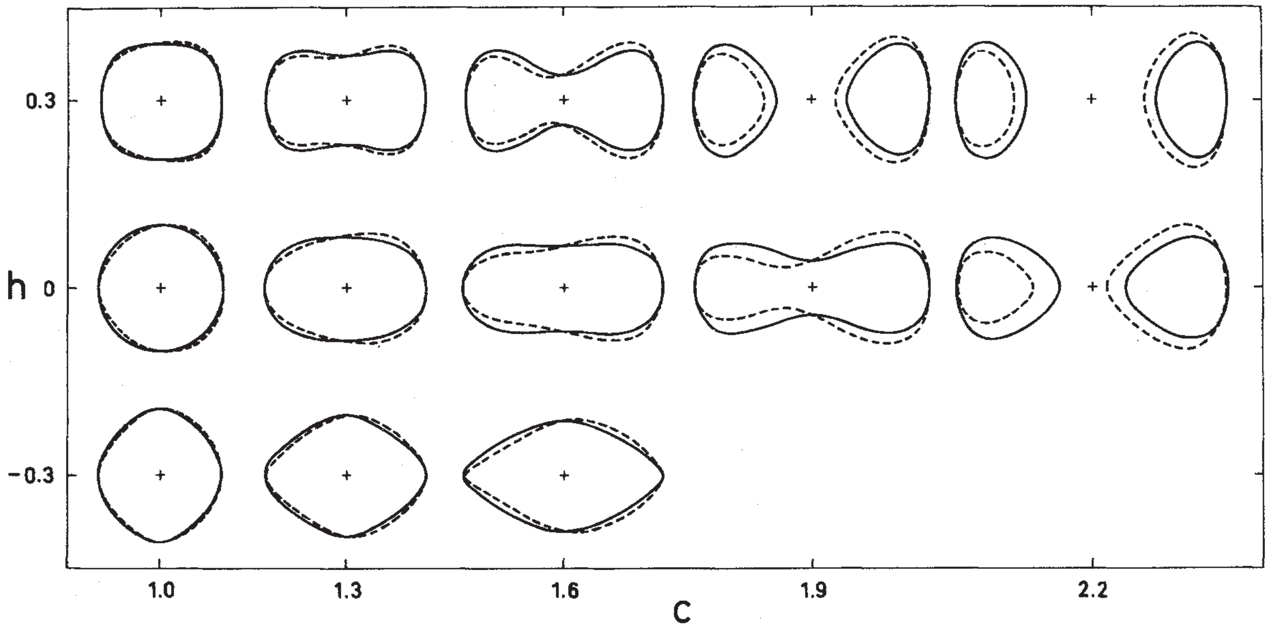
- Difference from smooth (classical) liquid drop model (LDM) behaviour: *quantum shell effects* ('shell-correction' energy)
- Lowest outer barrier for *left-right asymmetric shapes*
- Leads to *mass asymmetry* of the fragment distribution (Classical LDM would give symmetric distribution)

A short 'Lund history' of the fission asymmetry:

- 1962: *S. A. E. Johansson* [Nucl. Phys. **22**, 529 (1962)] studies octopole deformations in the single-particle model, finds instability at LDM fission barrier of heavy nuclei.
- 1970: *P. Möller and S. G. Nilsson* [Phys. Lett. **31 B**, 283 (1970)] obtain instability of outer fission barrier with respect to suitable combinations of ϵ_3 and ϵ_5 deformations in the Nilsson model using Strutinsky's shell-correction method.
- 1971: *C. Gustafsson, P. Möller and S. G. Nilsson* [Phys. Lett. **34 B**, 349 (1971)] explained the quantum-mechanical mechanism of this instability by certain pairs of 'diabatic' single-particle states whose energy levels are particularly sensitive to the ϵ_3-ϵ_5 deformations.
- 2001: *S. M. Reimann* contributes to a semiclassical interpretation of this instability as due to periodic orbits, along which the wavefunctions of the same type of single-particle states have their maxima, and whose local EBK quantization gives the correct single-particle energies of the 'diabatic' states.
  [M. Brack, M. Sieber and S. M. Reimann, Physica Scripta **T90**, 146 (2001)].

A simple semiclassical model for fission:

Axially symmetric shapes from LDM model:



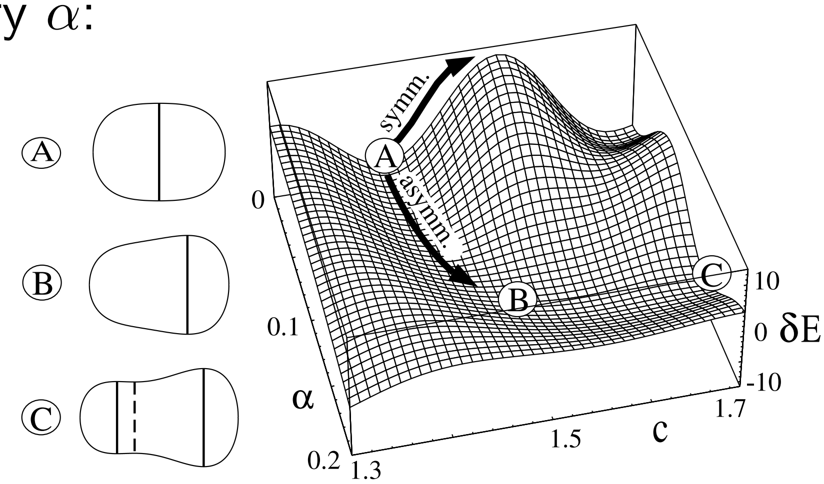
c: elongation parameter
h: neck parameter
$\alpha \neq 0$: left-right asymmetry parameter

- Replace nuclear mean field by 3d cavity with the same shapes (c, h, α)

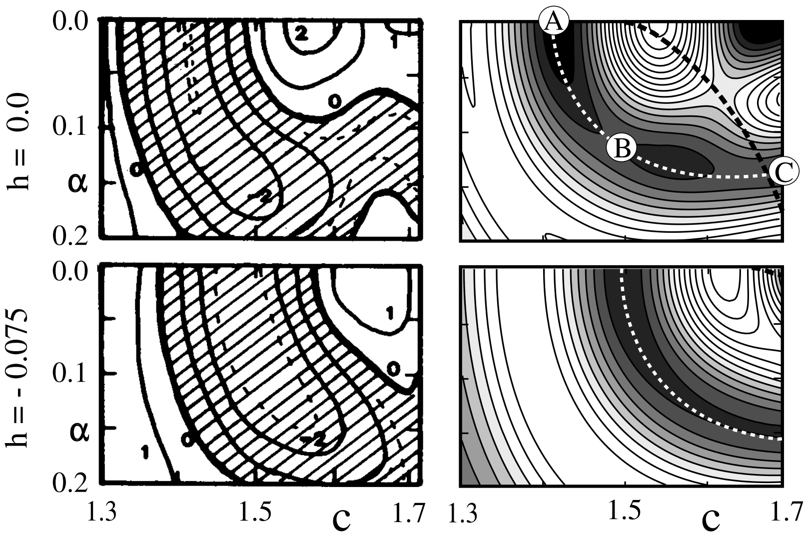
- Find the shortest periodic orbits and calculate shell-correction energy $\delta E(c, h, \alpha)$ using the semiclassical trace formula!

Semiclassical fission barrier

Fission barrier of ^{240}Pu nucleus versus elongation c and asymmetry α:



Comparison with quantum-mechanical results:



Valley of minimal energy (A-B-C): classical action of dominant orbits is constant!

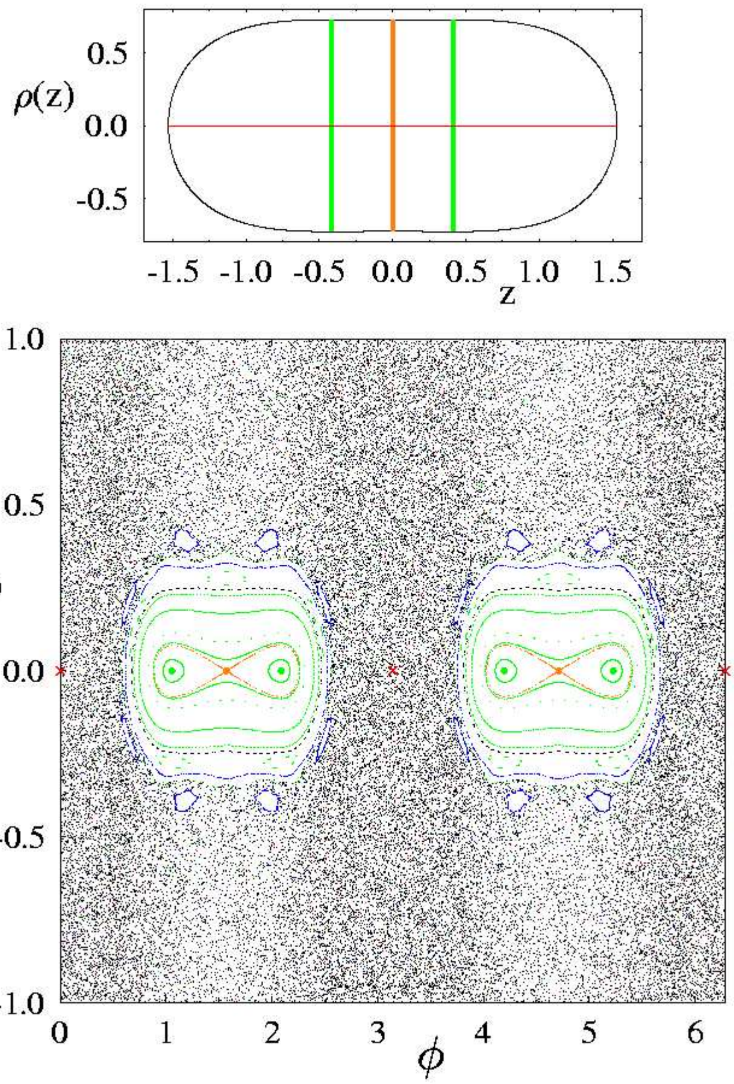
$\boxed{\delta S_{po} = 0}$

Left: quantum-mechanical δE (Strutinsky) (1971)

Right: semiclassical δE with only 2 orbits in equator plane(s)

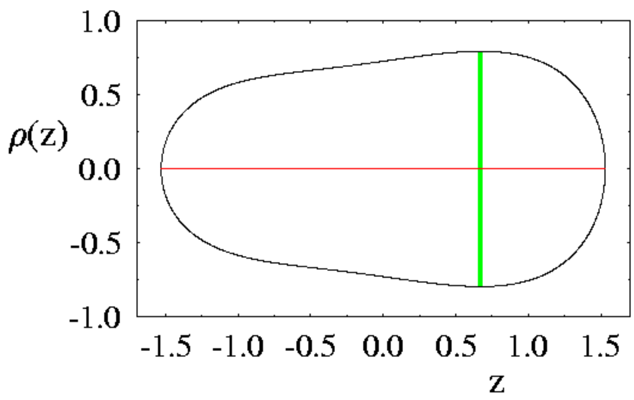
[M. Brack, S. Reimann, M. Sieber, PRL **79**, 1817 (1997)]

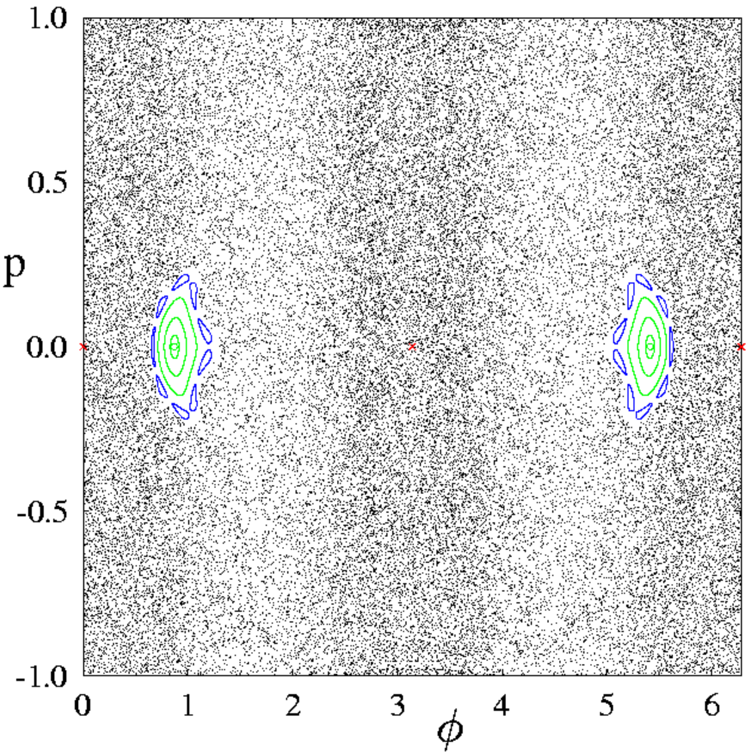
Poincaré surface of section (not area conserving!)
at symmetric barrier (c=1.53, h=0, α=0):



Shortest periodic orbits lie in same planes as the wavefunction extrema of the 'diabatic' single-particle states! [M. Brack, M. Sieber and S. M. Reimann, Physica Scripta T90, 146 (2001)]

Poincaré surface of section (not area conserving!)
at asymmetric saddle (point B: c=1.53, h=0, α=0.13):

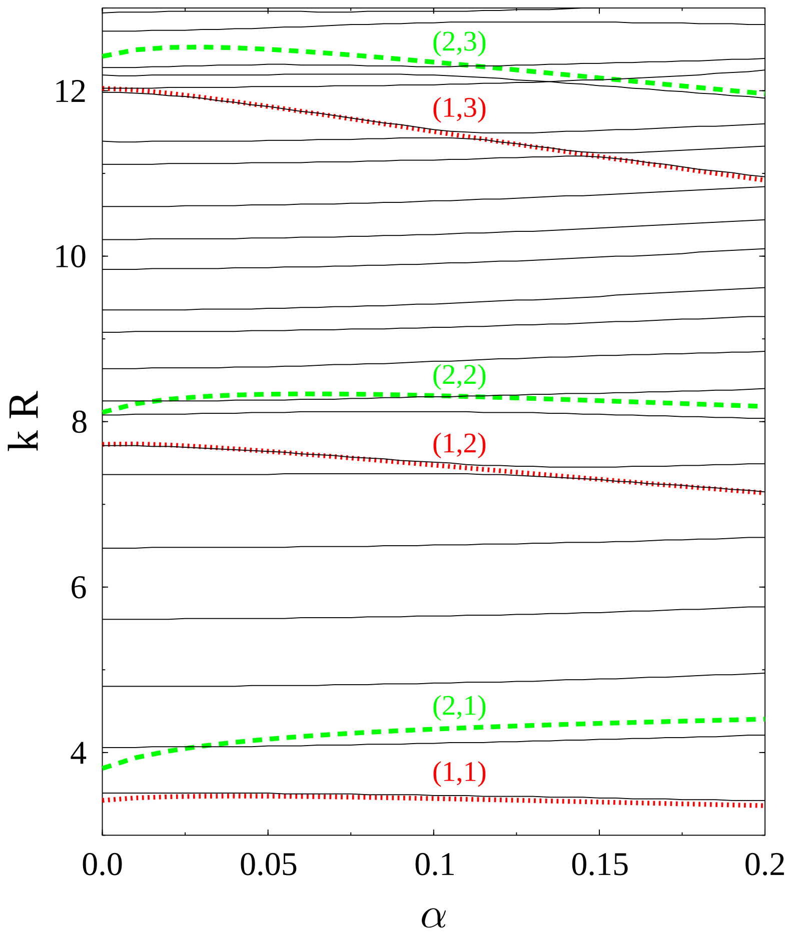




A tiny regular island in the middle of a sea of chaos causes the onset of the mass asymmetry!

Quantization of small regular island

Approximate EBK quantization of the linearized motion near the shortest periodic orbits[1]:



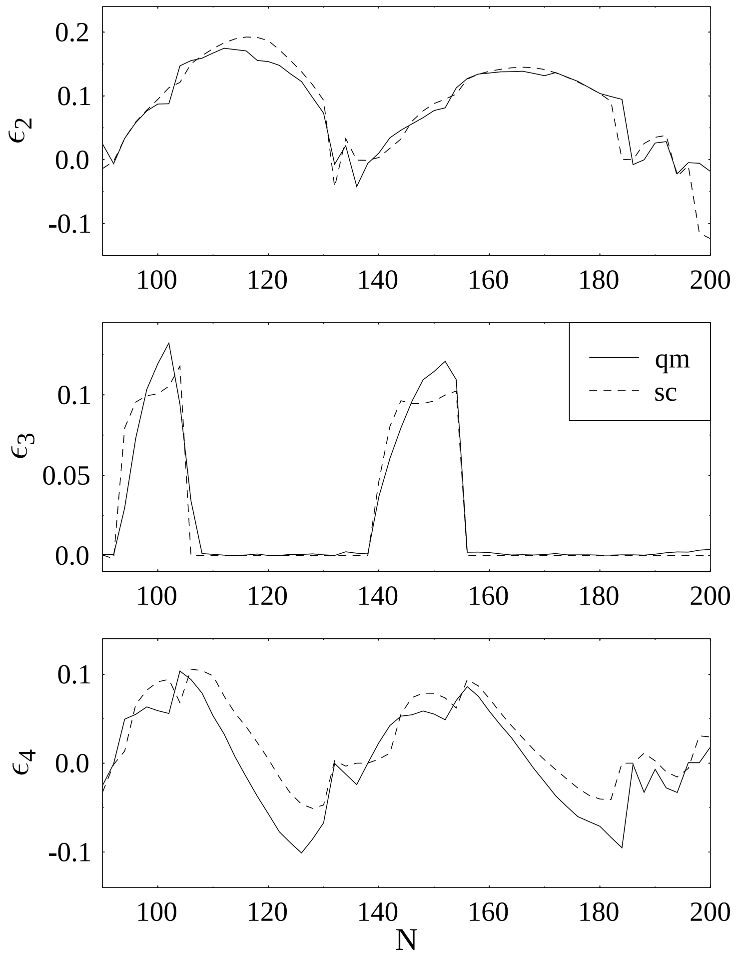
Coloured dashed lines: 'EBK' levels (n_z, n_ρ), approximate the 'diabatic' quantum states!

Black lines: exact quantum-mechanical levels

[1] as if in ellipsoid with same curvatures at turning points

Multipole deformations of metal clusters

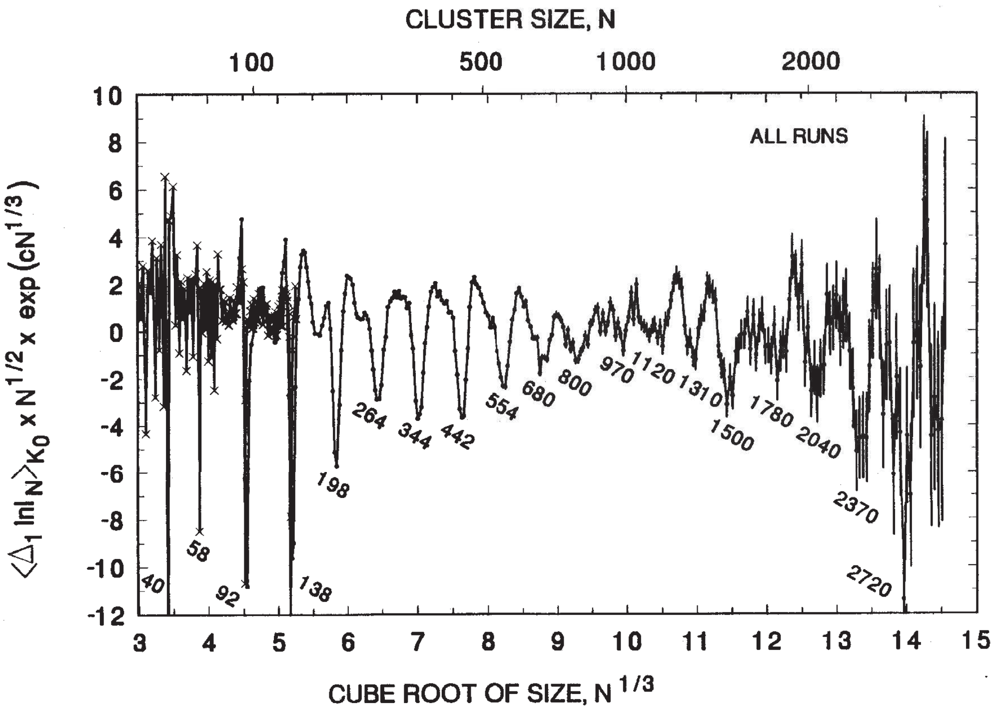
Deformations ϵ_2, ϵ_3, ϵ_4 of axial 3d cavities with N particles (minimizing $E_{tot} = E_{LDM} + \delta E$):



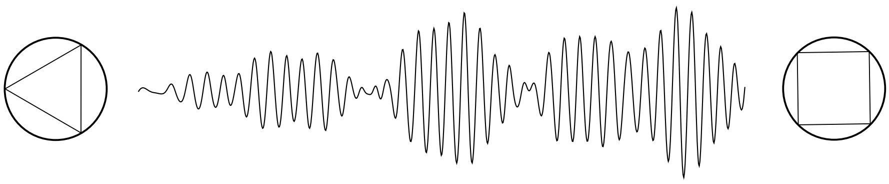
Solid lines: quantum-mechanical δE with Strutinsky method
Dashed lines: semiclassical δE with perturbative trace formula

[V. V. Pashkevich, P. Meier, M. Brack and A. V. Unzhakova, Phys. Lett. **A 294**, 314 (2002)]

Supershells in metal clusters



Abundance of Na clusters with N atoms (most stable for "magic numbers" N_i) [J. Pedersen *et al.*, Nature **353**, 733 (1991)].

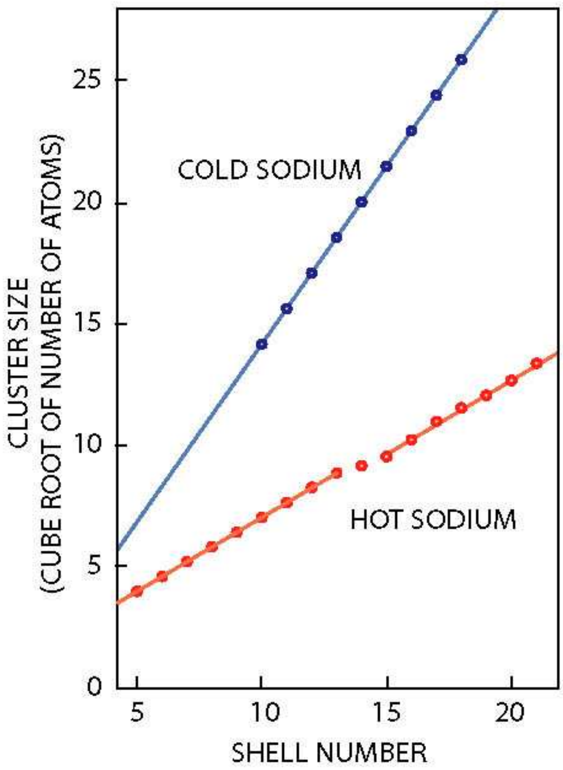


Semiclassically: interference of triangle and square orbits in spherical cavity [R. Balian and C. Bloch, Ann. Phys. **69**, 76 (1972)] or Woods-Saxon potential [H. Nishioka, K. Hansen and B. R. Mottelson, Phys. Rev. B **42**, 9377 (1990)].

Quantum-mechanically: DFT (Kohn-Sham eqs.) in jellium model [H. Genzken and M. Brack, Phys. Rev. Lett. **67**, 3286 (1991)].

Experimental “magic radii” of Na clusters:

plot of $R_i = r_0 N_i^{1/3}$ (dots) against shell number i:



← ignore this

← look here!

Experiment: Slope of red line (also for other metals: Li, Ga):

$$s_{exp} = 0.61 \pm 0.01$$

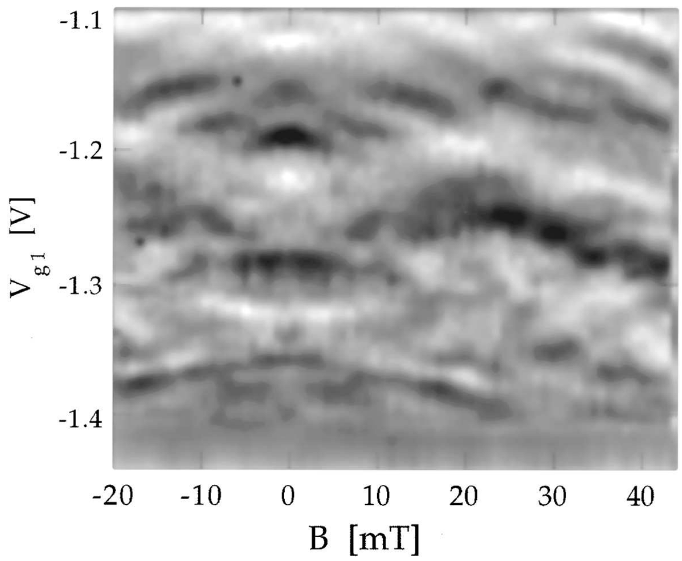
Semiclassics: From the mean length of triangular (3,1) and square (4,1) orbits in the Balian-Bloch sphere one gets:

$$s_{POT} = 0.603$$

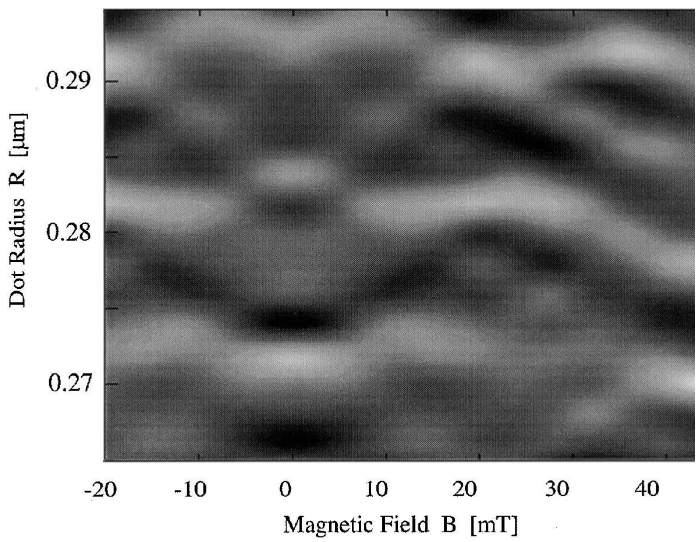
Quantum-mechanics: (Jellium + LDA-Kohn-Sham): $s = 0.61$

Magnetoconductance in a quantum dot

Experimental conductance of a circular quantum dot with ~ 1500 electrons (NBI/Chalmers, 1995); gray-scale plot of δG:



Semicl. trace formula (circular billard); gray-scale plot of $\delta g(E_F)$:



period ($\uparrow$) $\Delta R \sim$ average **length** of shortest orbit(s)!

period ($\longrightarrow$) $\Delta B \sim$ average **area** of shortest orbit(s)!

Effect of a (homogeneous) magnetic field B:

Canonical momentum: $\mathbf{p} \to \mathbf{p} - \frac{e}{c}\mathbf{A}$

Action: $S_{po} \to S_{po} - \frac{e}{c}\oint_{po} \mathbf{A} \cdot d\mathbf{q}$

$$= S_{po} - \frac{e}{c} B F_{po} = S_{po} - \frac{e}{c}\Phi_{po}$$

$\Rightarrow$ shift of phase by magnetic flux Φ_{po} of periodic orbit; analogous to Aharonov-Bohm (AB) effect!

In weak homogeneous magnetic field B (perturbation theory!):

$$\delta g(E_F, B) \simeq \sum_{po} A_{po} \cos\left(\frac{1}{\hbar} S_{po} - \frac{\pi}{2}\sigma_{po}\right) \cos\left(\frac{e}{\hbar c} B F_{po}\right)$$

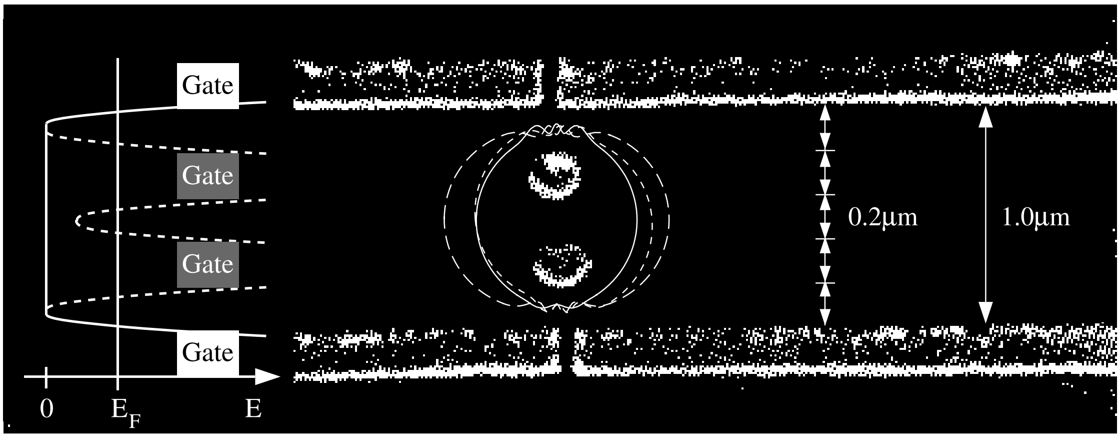
First factor: $B = 0$ case $\Rightarrow$ "shell oscillations" versus energy E or radius R

Last factor: $\Rightarrow$ "AB oscillations" versus B

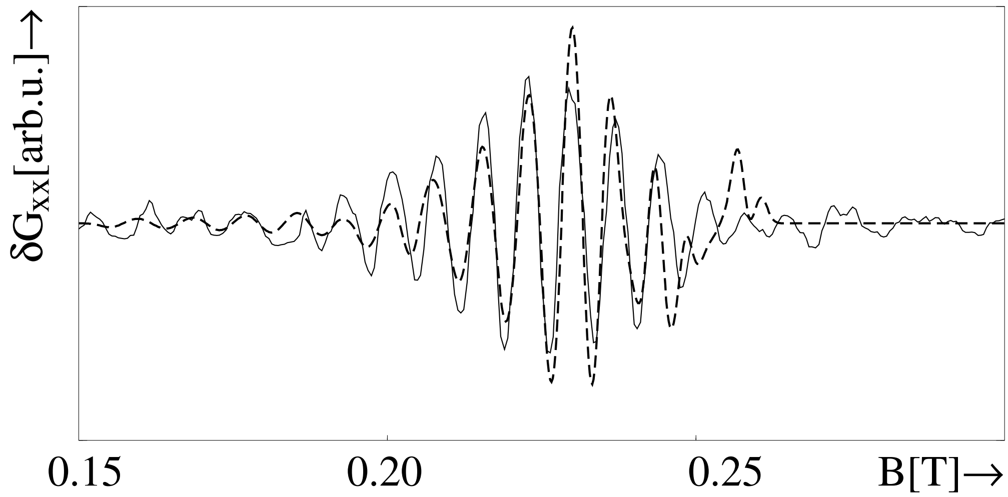
[S. M. Reimann, M. Persson, P. E. Lindelof, M. Brack, Z. Phys. B **101**, 377 (1996)]

Magnetoconductance oscillations in a mesoscopic channel with antidots

The device (A. Sachraida *et al.*, Ottawa):



Conductance (Aharonov-Bohm) oscillations δG_{xx}:



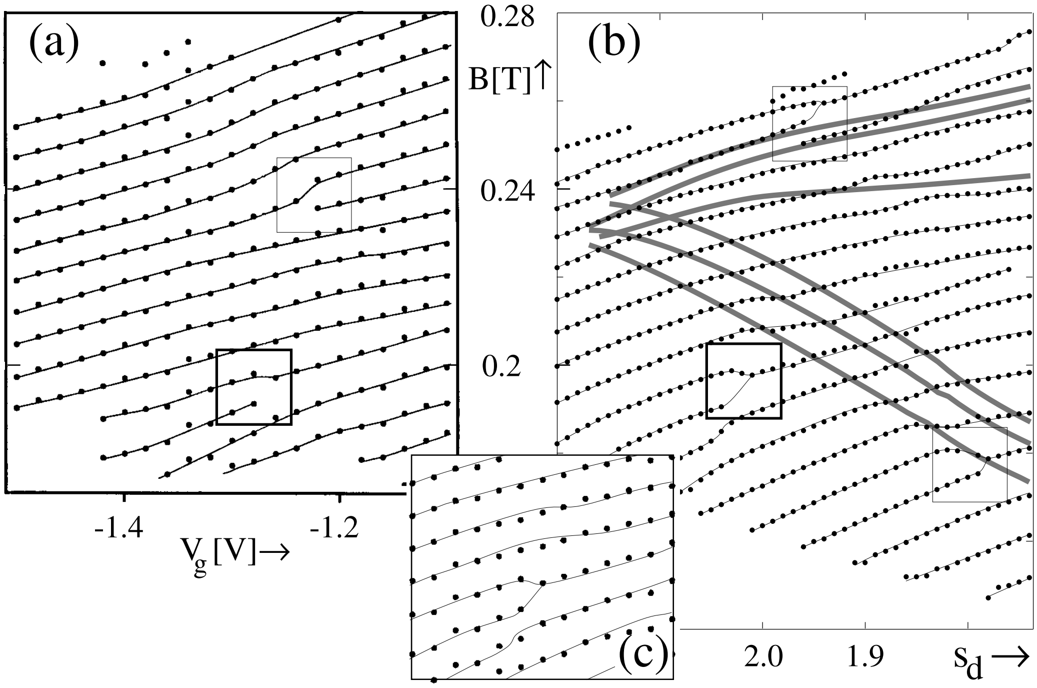
solid line: experimental, dashed line: semiclassical results.

[J. Blaschke, PhD Thesis (Regensburg, 1999);

J. Blaschke and M. Brack, Europhys. Lett. **50**, 294 (2000)]

Observable footprints of periodic orbit bifurcations

Plots of oscillation maxima of δG_{xx} versus magnetic field B (vertical) and gate voltage V_g or antidot radius s_d (horizontal):



(a) experimental results

(b) semiclassical theory: shaded lines mark bifurcation loci of leading periodic orbits

(c) local comparison experiment ↔ semiclassical theory

⇒ dislocations are signatures of orbit bifurcations!

Thanks

1. To my postdocs and students at Regensburg:
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