

# Closed-orbit theory for spatial density oscillations in finite fermion systems

Matthias Brack and Jérôme Roccia

*Institute for Theoretical Physics, University of Regensburg, Germany*

(Kazimierz Dolny, 26.09.09)

Introduction:

Reminder of semiclassical periodic orbit theory

## Semiclassical quantization

**Bohr-Sommerfeld quantization** (+WKB, in one dimension)

Quantization of action integral along periodic orbit:

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

$\Rightarrow$  quantized energies  $E_n$ , become exact in limit  $n \gg 1$

(Bohr's correspondence principle!), i.e., for  $S \gg \hbar$

(but works often well already for  $n = 0, 1, 2, \dots$ !)

In  $D > 1$  dimensions: **torus (EBK) quantization** (Einstein 1916)

but works only for **integrable systems!**

**Gutzwiller's trace formula:** (derived 1971 from the Feynman path-integral formulation of quantum mechanics in limit  $S \gg \hbar$ ):

works also for **non-integrable and chaotic systems!**

# The Gutzwiller trace formula

The **quantum-mechanical density of states** for spectrum  $\{E_n\}$ :

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

*Smooth part*  $\tilde{g}(E)$ : from extended Thomas-Fermi (ETF) model (or Weyl expansion)

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

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

Sum over periodic orbits (*POs*) 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 of *PO*)

$\alpha_{PO}$  = Maslov index (a kind of winding number)

## Trace formula for finite fermion systems

$N$  (non-)interacting fermions in a (self-consistent) *local mean field* (Skyrme-HF or DFT, or model potential):

$$\left\{ \hat{T} + V(\mathbf{r}) \right\} \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r})$$

Total energy (using Strutinsky theorem):  $E(N) = \tilde{E}(N) + \delta E(N)$   
using  $\tilde{E}(N)$  from selfconsistent ETF (or liquid drop) model

Semiclassical trace formula for shell-correction energy  $\delta E$ :

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

using  $PO$ s from classical system  $H(\mathbf{p}, \mathbf{r}) = \mathbf{p}^2/2m + V(\mathbf{r})$

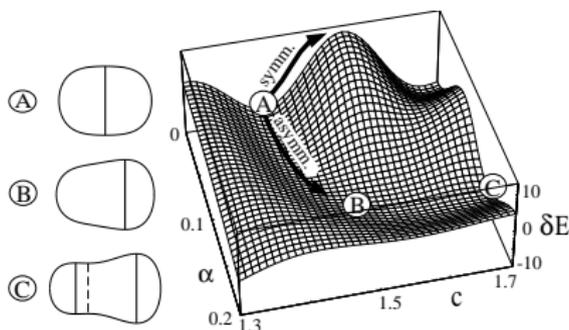
$T_{PO} = dS_{PO}(E)/dE|_{E=\lambda_N} = \text{period}$

$\lambda_N = \lambda(N) = \text{Fermi energy: } \int^{\lambda_N} g(E) dE = N$

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

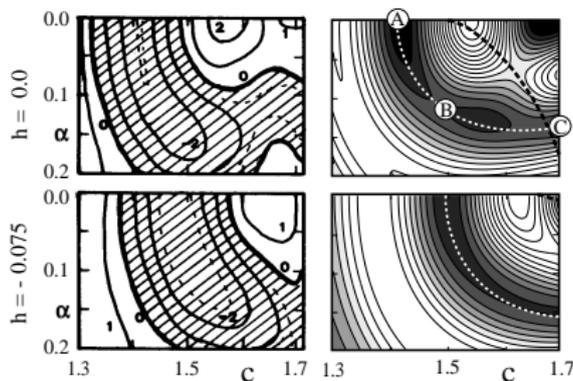
- Cavity model with “Funny Hills” ( $c, h, \alpha$ ) shapes
- **simple**: one kind of particles; no Coulomb, no spin-orbit!
- only adjusted parameter: Fermi energy  $\lambda_N$
- two shortest orbits in each equator plane are sufficient!

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



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

## Comparison of scl with quantum result:



Left: quantum-mechanical  $\delta E$  ("Funny Hills", 1972)

Right: semiclassical  $\delta E$

Valley of minimal energy: action of dominant orbits is constant

$$\delta S_{PO} = 0$$

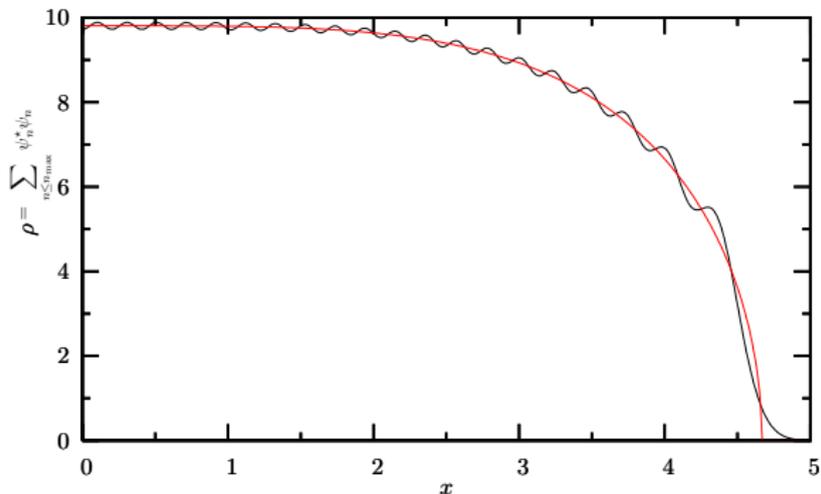
Classical least-action principle determines adiabatic fission path!

First part:

## Semiclassical theory for spatial density oscillations

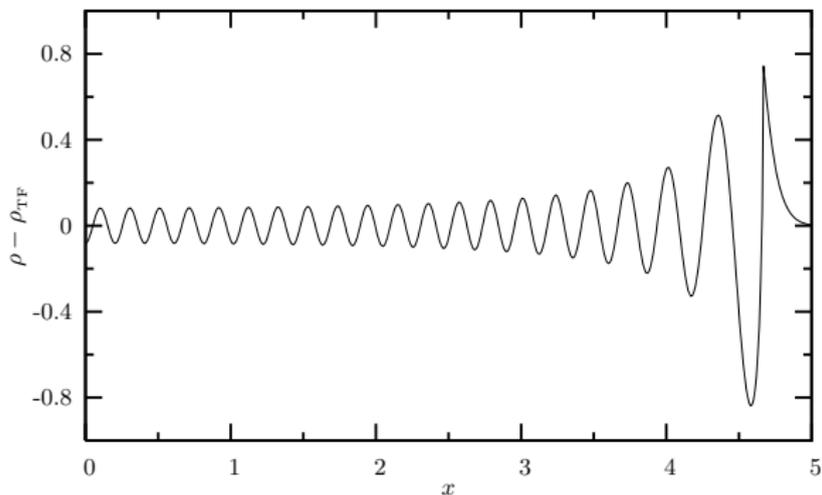
- Question: Can we also describe quantum oscillations in **spatial densities** in terms of classical orbits?
- Answer: Yes!
  - J.R.+M.B., Phys. Rev. Lett. **100**, 200408 (2008)
  - M.B.+J.R., J. Phys. A **42** (2009)
  - J.R.+M.B.+A.Koch+M.V.N.Murthy, arXiv:math-ph/0903.2172

A typical density distribution  $\rho(x)$  (here: HO in one dimension)



exhibits quantum oscillations around a smooth part, given here by the Thomas-Fermi density  $\rho_{TF}(x)$

Looking at the oscillating part  $\delta\rho(x) = \rho(x) - \rho_{TF}(x)$ :



Note the **Friedel oscillations** with increasing amplitude near the surface!

## Spatial densities:

$N$  fermions are bound in a local (mean-field) potential  $V(\mathbf{r})$   
in  $D$  dimensions

We define the spatial densities as

$$\rho(\mathbf{r}) = \sum_{E_n \leq \lambda_N} \psi_n^*(\mathbf{r}) \psi_n(\mathbf{r}) \quad \text{particle density}$$

$$\tau(\mathbf{r}) = -\frac{\hbar^2}{2m} \sum_{E_n \leq \lambda_N} \psi_n^*(\mathbf{r}) \nabla^2 \psi_n(\mathbf{r}) \quad \text{kinetic-energy density}$$

$$\tau_1(\mathbf{r}) = \frac{\hbar^2}{2m} \sum_{E_n \leq \lambda_N} |\nabla \psi_n(\mathbf{r})|^2 \quad \text{also kinetic-energy density!}$$

Consider also the following kinetic-energy density:

$$\xi(\mathbf{r}) = \frac{1}{2} [\tau(\mathbf{r}) + \tau_1(\mathbf{r})]$$

## Green function formulation

$$[\hat{H}_r - E]G(E, \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$

$G(E, \mathbf{r}, \mathbf{r}')$  in terms of eigenfunctions and -energies:

$$G(E, \mathbf{r}, \mathbf{r}') = \sum_n \frac{\psi_n^*(\mathbf{r})\psi_n(\mathbf{r}')}{E + i\epsilon - E_n} \quad (\epsilon > 0)$$

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Using  $1/(E + i\epsilon - E_n) = \mathcal{P}[1/(E - E_n)] - i\pi\delta(E - E_n)$ , we get

the level density:

$$g(E) = -\frac{1}{\pi} \text{Im} \int d^D r G(E, \mathbf{r}, \mathbf{r}' = \mathbf{r})$$

(trace integral over space)

and the spatial densities:

$$\rho(N, \mathbf{r}) = -\frac{1}{\pi} \operatorname{Im} \int_0^{\lambda_N} dE G(E, \mathbf{r}, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}$$

$$\tau(N, \mathbf{r}) = \frac{\hbar^2}{2\pi m} \operatorname{Im} \int_0^{\lambda_N} dE \nabla_{\mathbf{r}'}^2 G(E, \mathbf{r}, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}$$

$$\tau_1(N, \mathbf{r}) = -\frac{\hbar^2}{2\pi m} \operatorname{Im} \int_0^{\lambda_N} dE \nabla_{\mathbf{r}} \nabla_{\mathbf{r}'} G(E, \mathbf{r}, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}}$$

(energy integral up to Fermi energy)

## Semiclassical approximation (1)

- Replace  $G(E, \mathbf{r}, \mathbf{r}')$  by Gutzwiller's semiclassical Green function  $G_{\text{Scl}}(E, \mathbf{r}, \mathbf{r}')$  derived from Feynman path integral (Gutzwiller 1967)

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Semiclassical Green function in  $D$  dimensions:

$$G_{\text{scl}}(E, \mathbf{r}, \mathbf{r}') = \alpha_D \sum_{\gamma} |\mathcal{D}_{\gamma}(E, \mathbf{r}, \mathbf{r}')|^{1/2} e^{\frac{i}{\hbar} S_{\gamma}(E, \mathbf{r}, \mathbf{r}') - i\mu_{\gamma} \frac{\pi}{2}},$$

- sum over **classical trajectories**  $\gamma$  from  $\mathbf{r}$  to  $\mathbf{r}'$
- $\mathcal{D}_{\gamma}(E, \mathbf{r}, \mathbf{r}')$ : Van Vleck determinant (related to stability of orbit)
- $S_{\gamma}(E, \mathbf{r}, \mathbf{r}') = \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{p} \cdot d\mathbf{q}$ : action integral along  $\gamma$
- $\mu_{\gamma}$ : Morse index (number of conjugate points)
- $\alpha_D = 2\pi(2i\pi\hbar)^{-(D+1)/2}$

## Semiclassical approximation (2)

Now we use leading-order terms in  $1/\hbar$ :

- $\nabla_{\mathbf{r}} G_{\text{scl}}(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') \approx \frac{i}{\hbar} \nabla_{\mathbf{r}} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}')$
- $\lambda_N = \tilde{\lambda} + \delta\lambda$ , with  $\int^{\tilde{\lambda}} \tilde{g}(E) dE = N$   
 $\tilde{g}(E) = \text{smooth (ETF or Weyl) part of level density}$

Furthermore, use classical canonical relations:

- $\nabla_{\mathbf{r}} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') = -\mathbf{p}(\tilde{\lambda}, \mathbf{r}) =: -\mathbf{p}_{\lambda}$  (initial momentum)
- $\nabla_{\mathbf{r}'} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') = \mathbf{p}(\tilde{\lambda}, \mathbf{r}') =: \mathbf{p}'_{\lambda}$  (final momentum)
- $p(\tilde{\lambda}, \mathbf{r}) = |\mathbf{p}(\tilde{\lambda}, \mathbf{r})| = \{2m[\tilde{\lambda} - V(\mathbf{r})]\}^{1/2}$
- **Note:** modulus  $p(\tilde{\lambda}, \mathbf{r})$  does **not** depend of the particular orbit; only on  $\mathbf{r}$ !

## Semiclassical approximation (3)

Spatial densities to leading order in  $\hbar$ :  $\gamma = \text{closed orbits!}$  ( $\mathbf{r} = \mathbf{r}'$ )

$$\rho(\mathbf{r}) = \frac{m\hbar}{\pi} \text{Re} \alpha_D \sum_{\gamma} \frac{\sqrt{|\mathcal{D}_{\perp}|_{\mathbf{r}'=\mathbf{r}}}}{\rho(\tilde{\lambda}, \mathbf{r}) T_{\gamma}(\tilde{\lambda}, \mathbf{r})} e^{i\Phi_{\gamma}(\tilde{\lambda}, \mathbf{r})}$$

$$\tau(\mathbf{r}) = \frac{\hbar}{2\pi} \text{Re} \alpha_D \sum_{\gamma} \frac{\rho(\tilde{\lambda}, \mathbf{r}) \sqrt{|\mathcal{D}_{\perp}|_{\mathbf{r}'=\mathbf{r}}}}{T_{\gamma}(\tilde{\lambda}, \mathbf{r})} e^{i\Phi_{\gamma}(\tilde{\lambda}, \mathbf{r})}$$

$$\tau_1(\mathbf{r}) = \frac{\hbar}{2\pi} \text{Re} \alpha_D \sum_{\gamma} \frac{\{(\mathbf{p}_{\lambda} \cdot \mathbf{p}'_{\lambda}) \sqrt{|\mathcal{D}_{\perp}|}\}_{\mathbf{r}'=\mathbf{r}}}{\rho(\tilde{\lambda}, \mathbf{r}) T_{\gamma}(\tilde{\lambda}, \mathbf{r})} e^{i\Phi_{\gamma}(\tilde{\lambda}, \mathbf{r})}$$

- $\Phi_{\gamma}(\tilde{\lambda}, \mathbf{r}) = \frac{1}{\hbar} S_{\gamma}(\tilde{\lambda}, \mathbf{r}, \mathbf{r}) - \mu_{\gamma} \frac{\pi}{2}$
- $T_{\gamma}(\tilde{\lambda}, \mathbf{r}) = \frac{d}{dE} S_{\gamma}(E, \mathbf{r}, \mathbf{r})|_{E=\tilde{\lambda}}$ : running time

## Semiclassical approximation (4)

- Under the sum over closed orbits  $\gamma$ :
  - non-periodic orbits (NPOs) give oscillating parts of  $\rho, \tau, \tau_1$  because of  $\mathbf{r}$  dependence of  $S_{\text{NPO}}(\tilde{\lambda}, \mathbf{r}, \mathbf{r})$  in phase
  - periodic orbits (POs) give smooth (ETF) parts of  $\rho, \tau, \tau_1$  because actions  $S_{\text{PO}}(\tilde{\lambda})$  are independent of  $\mathbf{r}$
- $\Rightarrow$  write:  $\rho(\mathbf{r}) = \tilde{\rho}(\mathbf{r}) + \delta\rho(\mathbf{r}), \quad \tilde{\rho}(\mathbf{r}) = \rho_{\text{ETF}}(\mathbf{r})$  etc.  
(ETF for extended Thomas-Fermi model)
- Oscillating parts  $\delta\rho(\mathbf{r}), \delta\tau(\mathbf{r}), \delta\tau_1(\mathbf{r})$  are governed by the NPOs!
- (different from trace formulae for oscillations in **energy**, which are governed by the POs!)

# 'Local Virial Theorem' and Thomas-Fermi functional

Without knowledge of the orbits  $\gamma$ , we find directly the

Local Virial Theorem:

$$\delta\tau(\mathbf{r}) = [\tilde{\lambda} - V(\mathbf{r})] \delta\rho(\mathbf{r})$$

valid for any **integrable** or **chaotic** potential  
(except near turning points)

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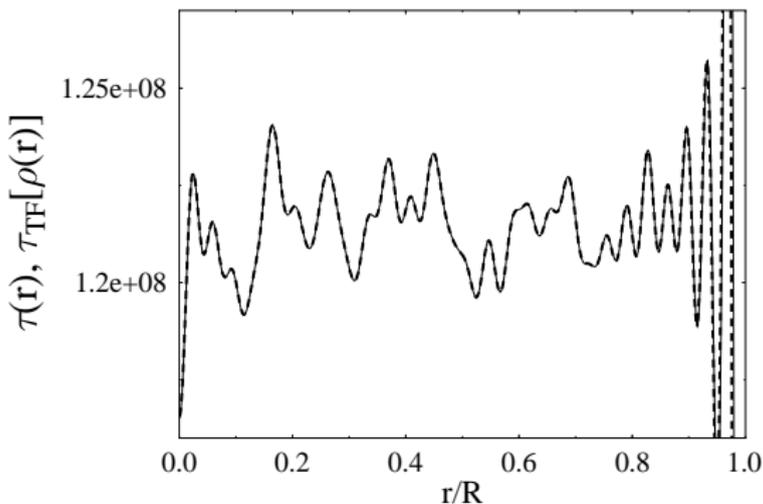
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- $\Rightarrow$  The TF functional reproduces the shell effects to first order in  $\delta\rho$  and  $\delta\tau$  (known numerically for a long time, but not understood until now!)
- No such relations for  $\delta\tau_1(\mathbf{r})$  in general!

## Example: 3D spherical billiard (integrable) with $N = 100068$

solid:  $\tau(r)$ , dashed:  $\tau_{TF}[\rho(r)]$ , with exact q.m.  $\tau(r)$  and  $\rho(r)$

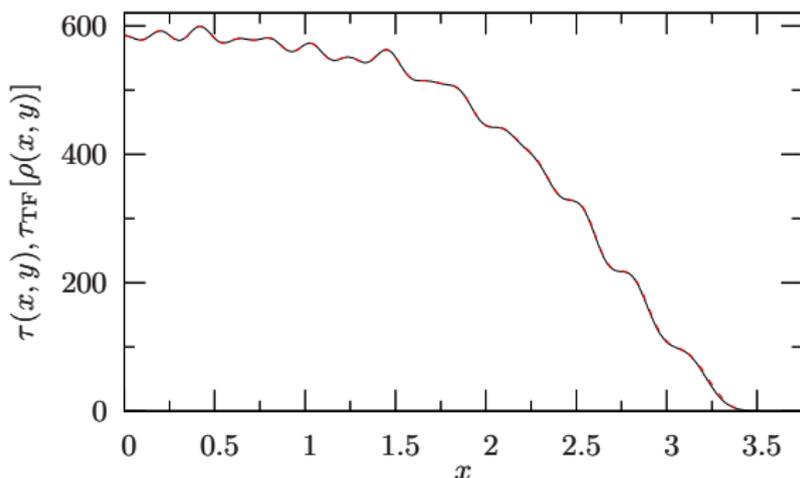


**Note superposition of fast regular and slow irregular oscillations!**  
(characteristic of spherical systems in  $D > 1$ )

Example: 2D potential  $V(x, y) = (x^4 + y^4)/4 - \kappa x^2 y^2$

with  $\kappa = 0.6$  (chaotic dynamics!),  $N = 632$

black:  $\tau(x, y)$ , red:  $\tau_{TF}[\rho(x, y)]$ , with exact q.m.  $\tau(x, y)$  and  $\rho(x, y)$



(all taken along  $x = y$ )

## $D$ -dimensional systems with radial symmetry:

- radial NPOs with  $\mathbf{p} = -\mathbf{p}'$  give fast regular oscillations
- nonradial NPOs with  $\mathbf{p} \neq \mathbf{p}'$ :  
give slow, irregular oscillations

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The fast regular oscillations (from radial NPOs) satisfy

- $\delta_{\text{reg}}\tau_1(r) = -\delta_{\text{reg}}\tau(r)$

Near  $r = 0$ , where  $V(r) \ll \lambda_N$ , find universal relation:

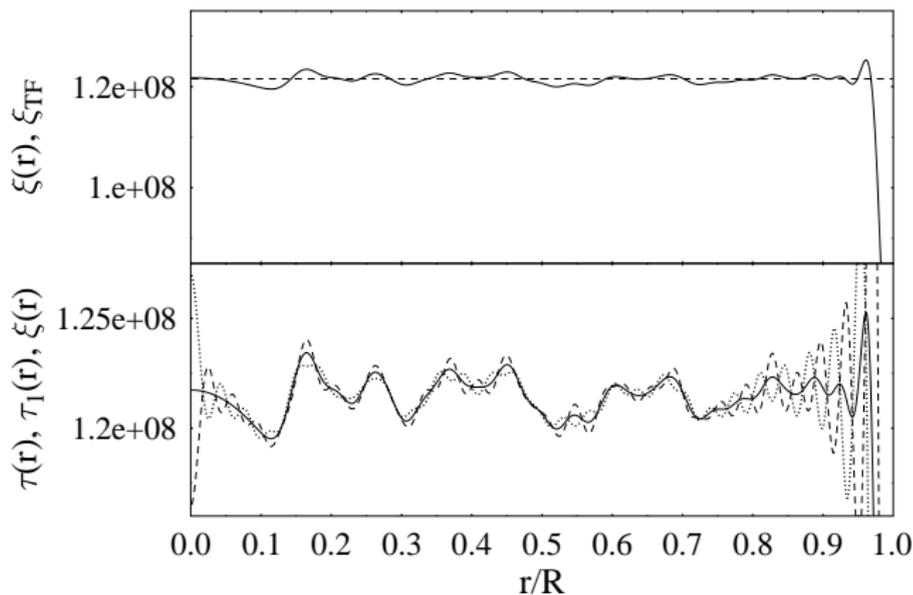
- $-\frac{\hbar^2}{8m}\nabla^2\delta_{\text{reg}}\rho(r) = \tilde{\lambda}\delta_{\text{reg}}\rho(r)$ , with solution:

- $\delta_{\text{reg}}\rho(r) = (-1)^{M-1}\frac{m}{2\hbar T_{r1}(\tilde{\lambda})}\left(\frac{p_\lambda}{4\pi\hbar r}\right)^\nu J_\nu(2rp_\lambda/\hbar)$

$M$ : number of occupied main shells,  $p_\lambda = \sqrt{2m\tilde{\lambda}}$ ,

$T_{r1}$ : period of shortest periodic orbit (diameter orbit)

## Example: 3D spherical billiard, $N = 100068$



- $\xi(r)$  (solid line) has only slow and irregular oscillations
- rapid oscillations of  $\tau(r)$  (dashed) and  $\tau_1(r)$  (dotted): same amplitude but opposite phase

## $D$ -dimensional systems with radial symmetry:

Consequences:

- Fast regular oscillations cancel in quantity  $\xi(r)$
- Note:  $\xi(r)$  is smooth ( $\simeq \xi_{ETF}$ ) in:
  - isotropic harmonic oscillators
  - all 1-dimensional potentials
  - linear potentials  $V(\mathbf{r}) = \mathbf{a} \cdot \mathbf{r}$because these systems have no nonradial NPOs  
(known since long, but not understood until now!)

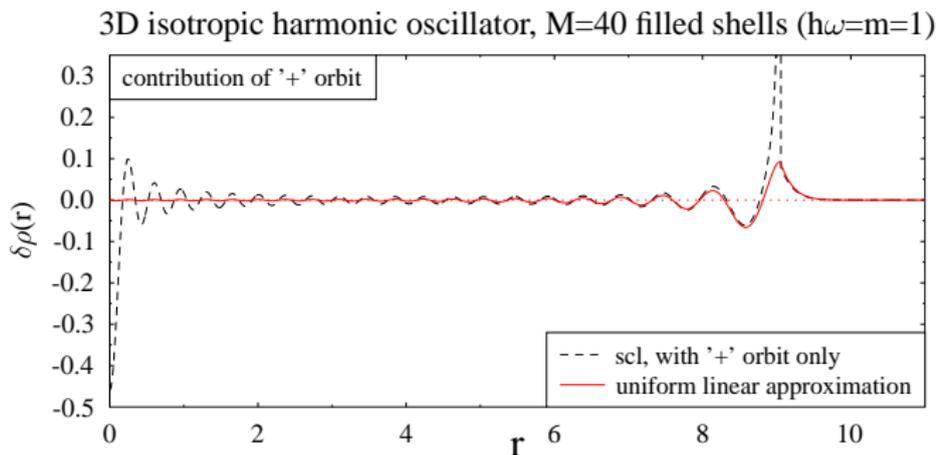
## Approaching the classical turning points

- semiclassical approximation breaks down:
  - in denominator:  $T_\gamma(\tilde{\lambda}, \mathbf{r}) \rightarrow 0$  for shortest orbit (going from  $\mathbf{r}$  to closest turning point and back) goes to zero
  - for smooth potentials:  $\rho_{ETF}(\mathbf{r})$  etc. diverge
- $\Rightarrow$  construct uniform approximations
- for smooth potentials:
  - linearize potential around turning point
  - use exact solution for linearized potential (in terms of Airy functions) near turning point
- for billiards:
  - use regularized uniform propagator for short times

## Friedel oscillations

- Friedel oscillation near surface comes from shortest linear NPO (one single reflection; '+' orbit) orthogonal to plane touching the turning point
- uniform approximation required

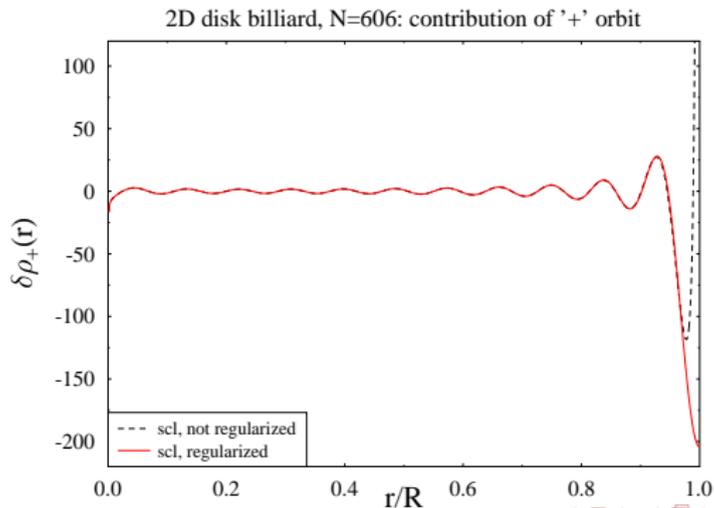
Smooth potentials: use Airy solution for linearized potential



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Billiards: use regularized short-time propagator



Second part:

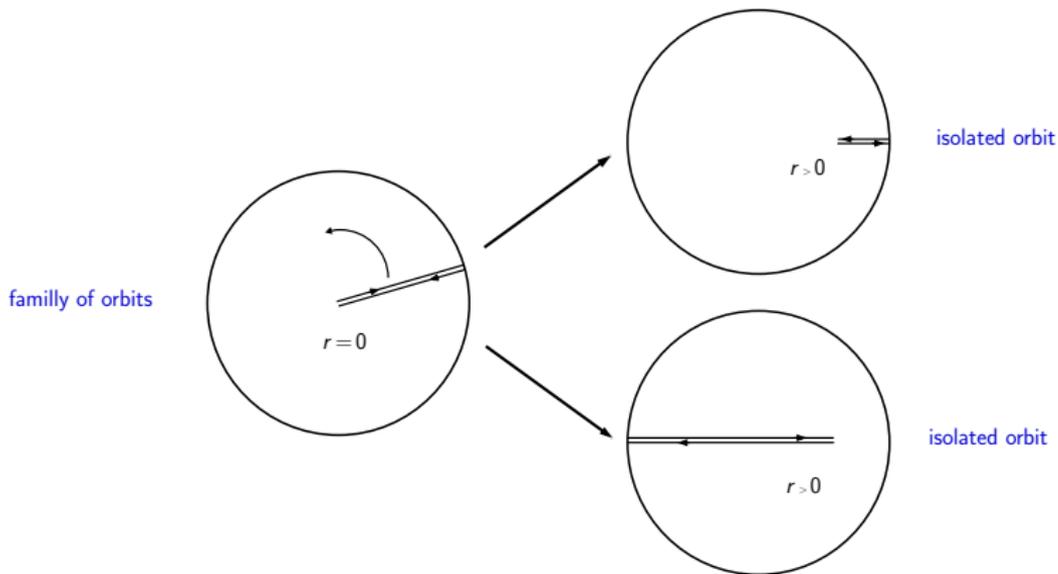
## Case study: 2-dimensional circular billiard

- All closed orbits (NPOs and POs) are classified
- All their properties calculated analytically
- At  $r = 0$ , **U(1) symmetry breaking**: **families** of orbits (invariant under rotation inside the circle) are broken into **isolated orbits** for  $r > 0$
- **Bifurcations** (as a function of **parameter  $r$** ) take place at specific distances  $r_i$  where new orbits (NPOs or POs) are born

[MB + JR, J. Phys. A **42** (2009)]

## 2-dimensional circular billiard

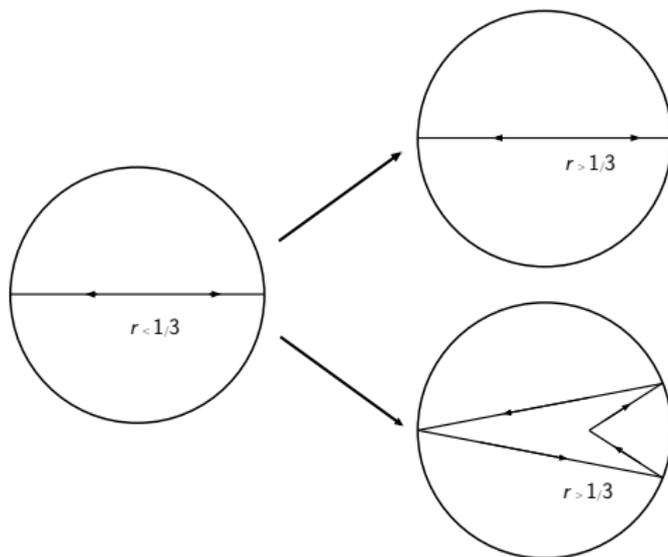
$r = 0$ :  $U(1)$  symmetry breaking



(happens in all radially symmetric potentials!)

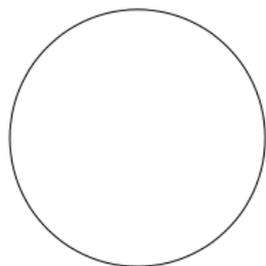
## 2-dimensional circular billiard

(pitchfork) bifurcation at  $r = R/3$ :

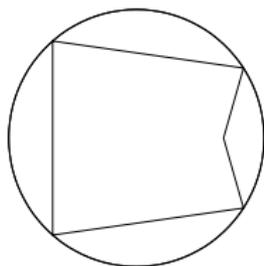


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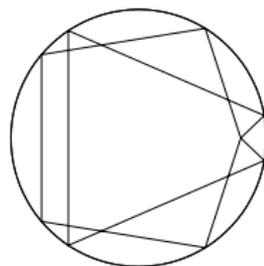
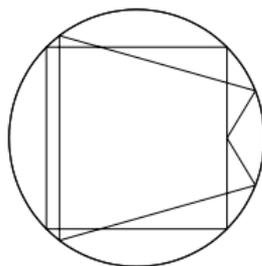
(tangent) bifurcation at  $r_0 = 0.6824... R$ :



$$r < r_0$$



$$r \geq r_0$$



## 2-dimensional circular billiard

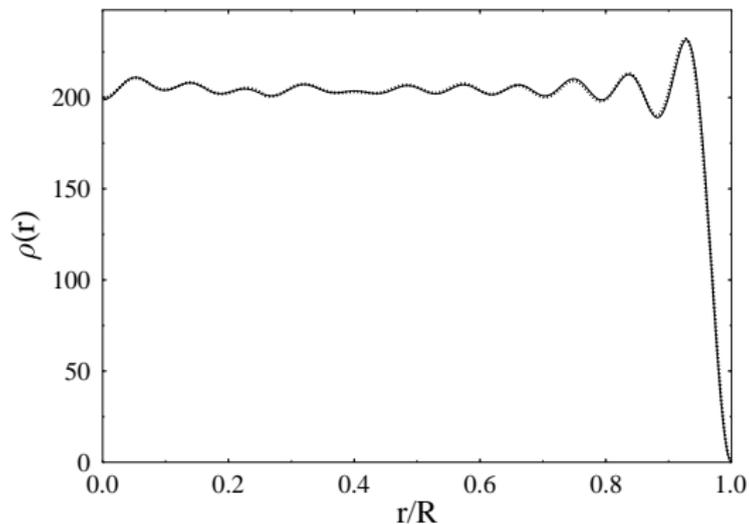
At all critical points ( $r = 0$  and bifurcations  $r_i > 0$ ),  $\mathcal{D}_\gamma$  in semiclassical amplitudes **diverges!**

**remedy:** use global **uniform approximations** via normal forms known (from periodic orbits)

- for symmetry breaking (Tomsovic *et al.*, 1995) and
- for bifurcations (Sieber and Schomerus, 1998)

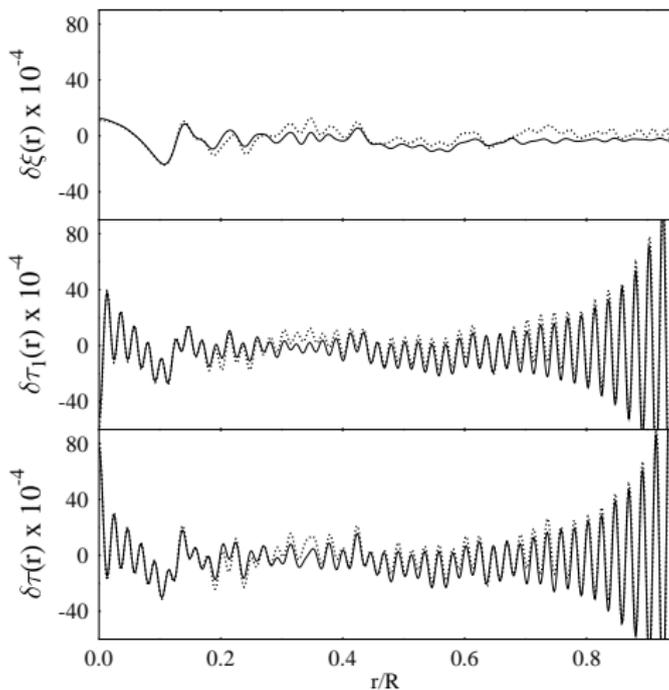
## 2-dimensional circular billiard

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



## 2-dimensional circular billiard

$\delta\tau(r)$ ,  $\delta\tau_1(r)$  and  $\delta\xi(r)$  for  $N = 606$ : (solid: qm, dotted: scl)



## Summary:

- Semiclassical closed-orbit theory for spatial density oscillations
- 'Local Virial Theorem'
- In spherical systems:
  - radial orbits with  $\mathbf{p} = -\mathbf{p}'$  cause regular rapid oscillations
  - nonradial orbits cause slow irregular oscillations
- $\mathbf{r}$  as bifurcation parameter (studied so far in circular billiard)
- good reproduction of quantum densities in circular billiard (and other integrable systems, see preprint)

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## Outlook:

- Look at density matrix  $\rho(\mathbf{r}, \mathbf{r}')$ : **open orbits!**
- Extend theory to finite temperatures
- Include pairing correlations (e.g. for nuclei)
- Cold trapped atoms at unitarity (using fractional statistics)