Semiclassical approaches to the kinetic-energy functionals $T_s[\rho]$ and $\tau[\rho]$

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Detailed references to Sects. 1 - 3 see in the text book *"Semiclassical Physics"* by M. Brack and R. K. Bhaduri (Westview Press, Bolder, USA, 2003)

1.a) Our object: the kinetic energy functional $T_s[\rho]$

From DFT we know that the total energy of an interacting fermion system is a functional of the local density $\rho(\mathbf{r})$:

$$E_{tot}[\rho] = T_s[\rho] + \int V_{ext}(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}\mathbf{r} + E_H[\rho] + E_{xc}[\rho]$$

$T_s[\rho]$ = kinetic energy of non-interacting fermions
$V_{ext}(\mathbf{r})$ = external potential
$E_H[\rho]$ = Hartree (direct, classical) potential energy
$E_{xc}[\rho]$ = exchange-correlation energy (per definition!)

Because we don't know $T_s[\rho]$ explicitly, we have to write

$$\rho(\mathbf{r}) = \sum_{E_n \leq \lambda} |\psi_n(\mathbf{r})|^2 \qquad (\lambda = \text{Fermi energy})$$

and solve the Kohn-Sham equations for the $\psi_n(\mathbf{r})$ and E_n.

The **Kohn-Sham (KS) equations**:

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r}) + V_{KS}[\rho(\mathbf{r})]\right\}\psi_n(\mathbf{r}) = E_n\,\psi_n(\mathbf{r})\,,$$

where $V_{KS}[\rho(\mathbf{r})]$ is given by the variational derivative
$V_{KS}[\rho(\mathbf{r})] = \delta(E_H[\rho] + E_{xc}[\rho])/\delta\rho(\mathbf{r}) = V_H(\mathbf{r}) + V_{xc}(\mathbf{r})\,.$

We define a **kinetic-energy density** $\tau(\mathbf{r})$ by

$$\tau(\mathbf{r}) = -\frac{\hbar^2}{2m}\sum_{E_n\leq\lambda}\psi_n^*(\mathbf{r})\nabla^2\psi_n(\mathbf{r})\,.$$

Then, $T_s[\rho]$ is given exactly by the integral $T_s[\rho] = \int\tau(\mathbf{r})\,\mathrm{d}\mathbf{r}\,.$
(The crux: $E_{xc}[\rho]$ and hence $V_{xc}[\rho(\mathbf{r})]$ are not exactly known!)

In this talk, we shall discuss semiclassical approximations to $T_s[\rho]$ and $\tau(\mathbf{r})$ as explicit functionals of $\rho(\mathbf{r})$.

1.b) Smooth and oscillating components

In the mean-field approximation, many quantities (e.g., energy E_{tot}, level density $g(E)$, spatial densities) can be decomposed into a smooth and an oscillating component. Examples:

- $E_{tot} = \tilde{E}_{tot} + \delta E$ (cf. Strutinsky; δE ="shell correction")
- $g(E) = \tilde{g}(E) + \delta g(E)$ (cf. Gutzwiller, Berry & Tabor, Balian & Bloch)
- $\rho(\mathbf{r}) = \tilde{\rho}(\mathbf{r}) + \delta\rho(\mathbf{r})$ etc. (see below)

Caveat: This decomposition is not unique. It makes sense only when (truncated) **semiclassical** (or asymptotic) expansions are used separately for both components!

1.c) Two kinds of semiclassical expansions

The smooth and oscillating components are accessible to different types of semiclassical (asymptotic) expansions in powers of $\hbar$

For the smooth components:

- Leading terms are given by the Thomas-Fermi (TF) model (equivalent to the local density approximation, LDA) (cf. Thomas, Fermi, Bethe & Weizsäcker, Simon, Lieb)
- Semiclassical corrections are obtained in terms of an $\hbar$ expansion (Wigner & Kirkwood), or equivalently for smooth potentials $V(\mathbf{r})$, an expansion in gradients of $V(\mathbf{r})$ (Kirzhnits), leading to the so-called extended Thomas-Fermi (ETF) model
- ETF expansion of $\tilde{g}(E)$ or $\tilde{E}_{tot}$ is equivalent to Strutinsky averaging

- For billiard systems (cavities with ideally reflecting walls), the ETF model is equivalent to the Weyl expansion (cf. Weyl, Baltes & Hilf, Berry & Howles)
- Alternatively, a $1/N$ (large N) expansion may be used (cf. liquid drop model, LDM)
- Caveat: large-N and $\hbar$ expansions generally agree only in leading terms!

For the oscillating components of level density and energy:

- To leading order in $\hbar$, so-called **trace formulae** can be used to express the quantum oscillations in terms of **classical periodic orbits** and their properties (Gutzwiller, Berry & Tabor, Balian & Bloch, ...)
- (Higher-order corrections in $\hbar$ are tedious, but usually not important)

2. Extended Thomas-Fermi (ETF) expansion of the smooth kinetic energy

TF expressions for $\rho(\mathbf{r})$ and $\tau(\mathbf{r})$ for non-interacting fermions in a potential $V(\mathbf{r})$ in D dimensions:

$$\rho_{TF}(\mathbf{r},\lambda) = \frac{1}{(2\pi)^{D/2}} \frac{4}{D} \frac{1}{\Gamma(\frac{D}{2})} [\lambda - V(\mathbf{r})]^{D/2} \Theta[\lambda - V(\mathbf{r})]$$

$$\tau_{TF}(\mathbf{r},\lambda) = \frac{1}{(2\pi)^{D/2}} \frac{4}{(D+2)} \frac{1}{\Gamma(\frac{D}{2})} [\lambda - V(\mathbf{r})]^{D/2+1} \Theta[\lambda - V(\mathbf{r})]$$

Semiclassical $\hbar$ corrections in terms of gradients of $V(\mathbf{r})$ (Wigner & Kirkwood, Kirzhnits) yield ETF expressions which

- are *a priori* only good for **smooth, non-divergent** densities
- diverge at classical turning points, where $[\lambda = V(\mathbf{r})]$, and are not defined outside the classically allowed region
- but, after elimination of $[\lambda - V(\mathbf{r})]$ and its gradients, lead to a functional $\tau_{ETF}[\rho]$ that can be used over all space for physically acceptable densities $\rho(\mathbf{r})$ (see below)

TF functional for the kinetic energy density in D dimensions:

$$\tau_{TF}[\rho(\mathbf{r})] = \frac{\hbar^2}{2m}\,\frac{4\pi D}{(D+2)}\left[\frac{D}{4}\,\Gamma\left(\frac{D}{2}\right)\right]^{2/D}\rho^{1+2/D}(\mathbf{r})$$

Historically, Weizsäcker (1935) derived an "inhomogeneity correction":

$$\tau_{W}[\rho(\mathbf{r})] = \frac{\hbar^2}{8m}\frac{(\nabla\rho)^2}{\rho} \qquad \text{(for } D = 3\text{)}$$

The ETF model leads yields a unique series of corrections to $\tau_{TF}[\rho(\mathbf{r})]$ in terms of gradients $\nabla\rho$, $\nabla^2\rho$, ... of $\rho(\mathbf{r})$.

Under the integral $\int \mathrm{d}^3r\,\tau_{ETF}[\rho(\mathbf{r})] = T_{ETF}[\rho]$ many terms vanish.

ETF kinetic energy functional in $D = 3$ dimensions:

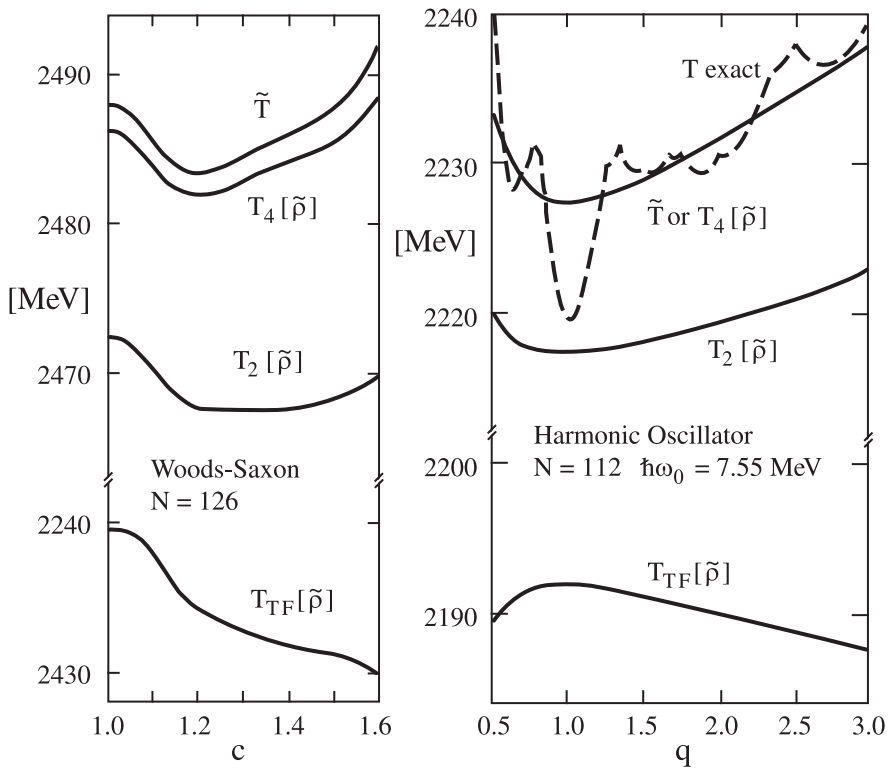
$$T_{ETF}[\rho] = T_{TF}[\rho] + T_2[\rho] + T_4[\rho] =$$

$$\frac{\hbar^2}{2m}\int \mathrm{d}^3 r \left\{ \kappa_0 \rho^{5/3} + \kappa_2 \frac{(\nabla\rho)^2}{\rho} + \kappa_4 \left[8\left(\frac{\nabla\rho}{\rho}\right)^4 - 27\left(\frac{\nabla\rho}{\rho}\right)^2 \frac{\nabla^2\rho}{\rho} + 24\left(\frac{\nabla^2\rho}{\rho}\right)^2 \right] \right\}$$

with $\kappa_0 = \frac{3(3\pi^2)^{2/3}}{5}$, $\kappa_2 = \frac{1}{36}$ (9 times smaller than Weizsäcker!),
and $\kappa_4 = \frac{1}{6480\,(3\pi^2)^{2/3}}$

In order to test $T_{ETF}[\rho]$, we compute it as a functional of selfconsistently averaged (variational) densities $\tilde{\rho}(\mathbf{r})$
and compare the results to the selfonsistently averaged quantum-mechanical kinetic energies $\widetilde{T}_s$ in terms of the eigenfunctions $\psi(\mathbf{r})$ of the selfconsistently averaged potential $\tilde{V}(\mathbf{r})$

Tests of $T_{ETF}[\tilde{\rho}]$ for average kinetic deformation energy:



Left: Woods-Saxon potential with $N = 126$ nucleons at typical deformations for nuclear fission.

Right: Axially symmetric harmonic-oscillator potential with frequency ratio q and $N = 112$ particles.

$\Rightarrow$ Good convergence of $T_{ETF}[\tilde{\rho}]$ up to 4th order towards $\widetilde{T}_s$!

3. Periodic Orbit Theory (POT)

For a quantum system given by

$$\hat{H}\,\psi_n = [\hat{T} + V]\,\psi_n = E_n\,\psi_n$$

the quantum-mechanical level density (density of states) is given by

$$g(E) = \sum_n \delta(E - E_n) \; = \tilde{g}(E) \; + \; \delta g(E) \qquad [\,\tilde{g}(E) \to g_{ETF}(E)\,]$$

Gutzwiller derived (1967-1972) a **semiclassical trace formula** relating $\delta g(E)$ to the periodic orbits of the corresponding **classical Hamiltonian** $H(\mathbf{p},\mathbf{r}) = \mathbf{p}^2/2m + V(\mathbf{r})$.

Alternative trace formulae were also proposed by Berry & Tabor, Balian & Bloch and many others, leading to the so-called **periodic orbit theory** (POT).

Trace formula for the level density

For the oscillating part of the level density, the following asymptotic identity holds to leading order in $\hbar$:

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

The sum is over the **periodic orbits** (POs) of the **classical** system $H(\mathbf{p},\mathbf{r}) = \mathbf{p}^2/2m + V(\mathbf{r})$

Ingredients:
$S_{PO} = \oint_{PO} \mathbf{p}\cdot \mathrm{d}\mathbf{q}$ = action integral along PO
A_{PO} = amplitude (related to stability and degeneracy)
σ_{PO} = Maslov index (for isolated orbits: a winding number)

It's actually a **Fourier decomposition** of $g(E)$!

Also studied a lot in mathematics (e.g., Selberg trace formula)

Trace formulae for finite fermion systems

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

$$\hat{H}\psi_n = \left\{ \hat{T} + V[\psi] \right\} \psi_n = E_n \psi_n$$

Total interacting energy can be split (by "Strutinsky theorem"):
$E_{tot} = \tilde{E}_{tot} + \delta E \qquad$ (and $N = \tilde{N} + \delta N$)
[Average $\tilde{E}_{tot}(\tilde{N})$ e.g. from selfconsistent ETF model]

Trace formulae for δE and δN (Strutinsky *et al.*, 1975):

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

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

$T_{PO}(\lambda) = \frac{\mathrm{d}}{\mathrm{d}E} S_{PO}(E)|_{E=\lambda}$ = period; λ = Fermi energy

Merits of POT:

- Very successful for quantum oscillations in many-body systems in different fields (nuclear physics, metal clusters, mesoscopic and nano-systems)
- Applicable also for other integrated observables (e.g., magnetization, conductivity, other transport phenomena)
- Fostered the field of "quantum chaos (chaology)"

Problems with POT:

- POT sum converges only for integrable systems; in chaotic and mixed-dynamic systems, special tricks required to obtain (partial) convergence
- At orbit bifurcations, uniform approximations needed

For many examples and technical details, see the textbook Brack and Bhaduri: *"Semiclassical Physics"*

4. Oscillations in spatial densities

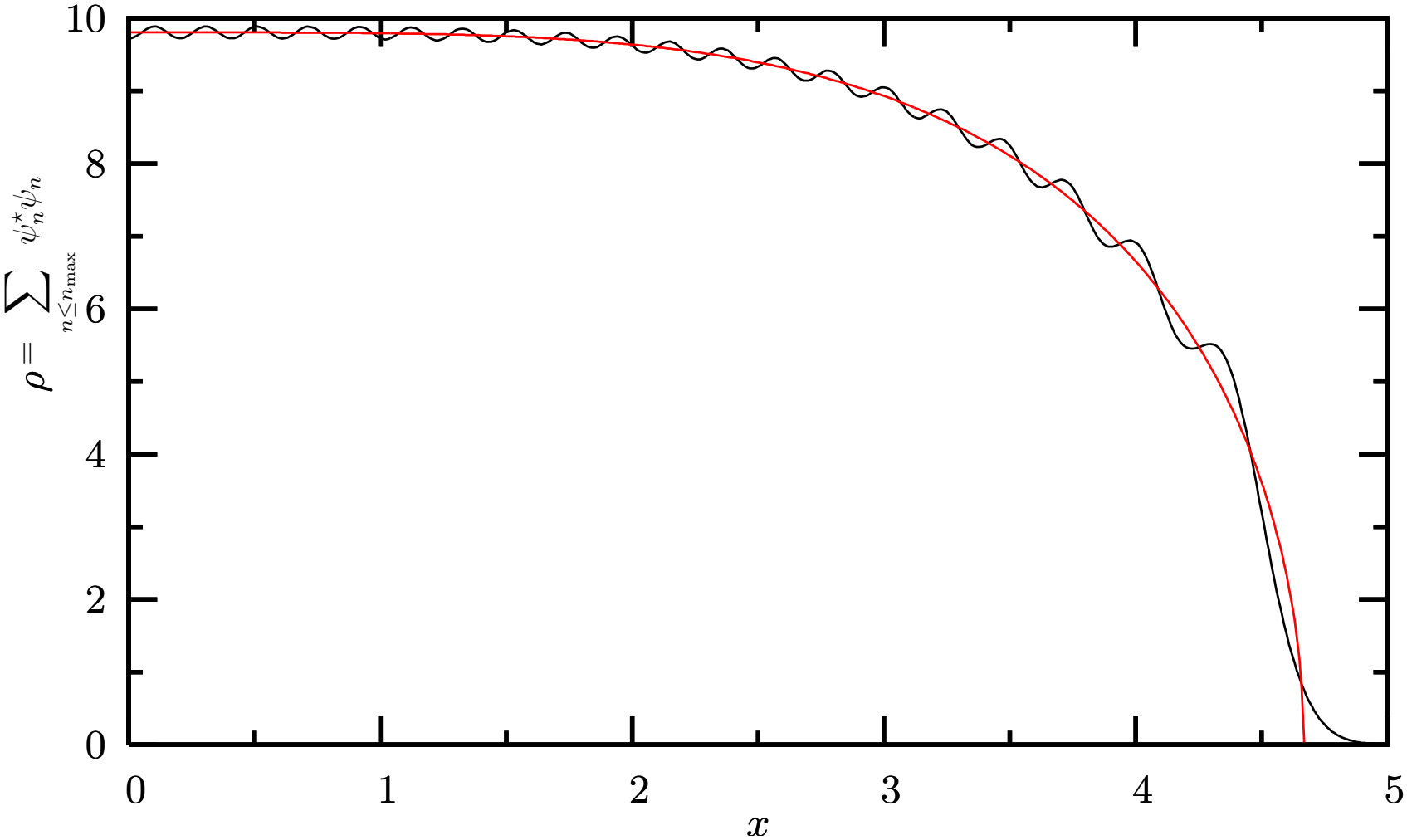
Question: Can such a semiclassical theory also be used to describe quantum oscillations in **spatial densities**?

Answer: Yes! (but it's a Closed Orbit Theory - COT!)

Collaboration with J. Roccia, A. Koch and M.V.N. Murthy:

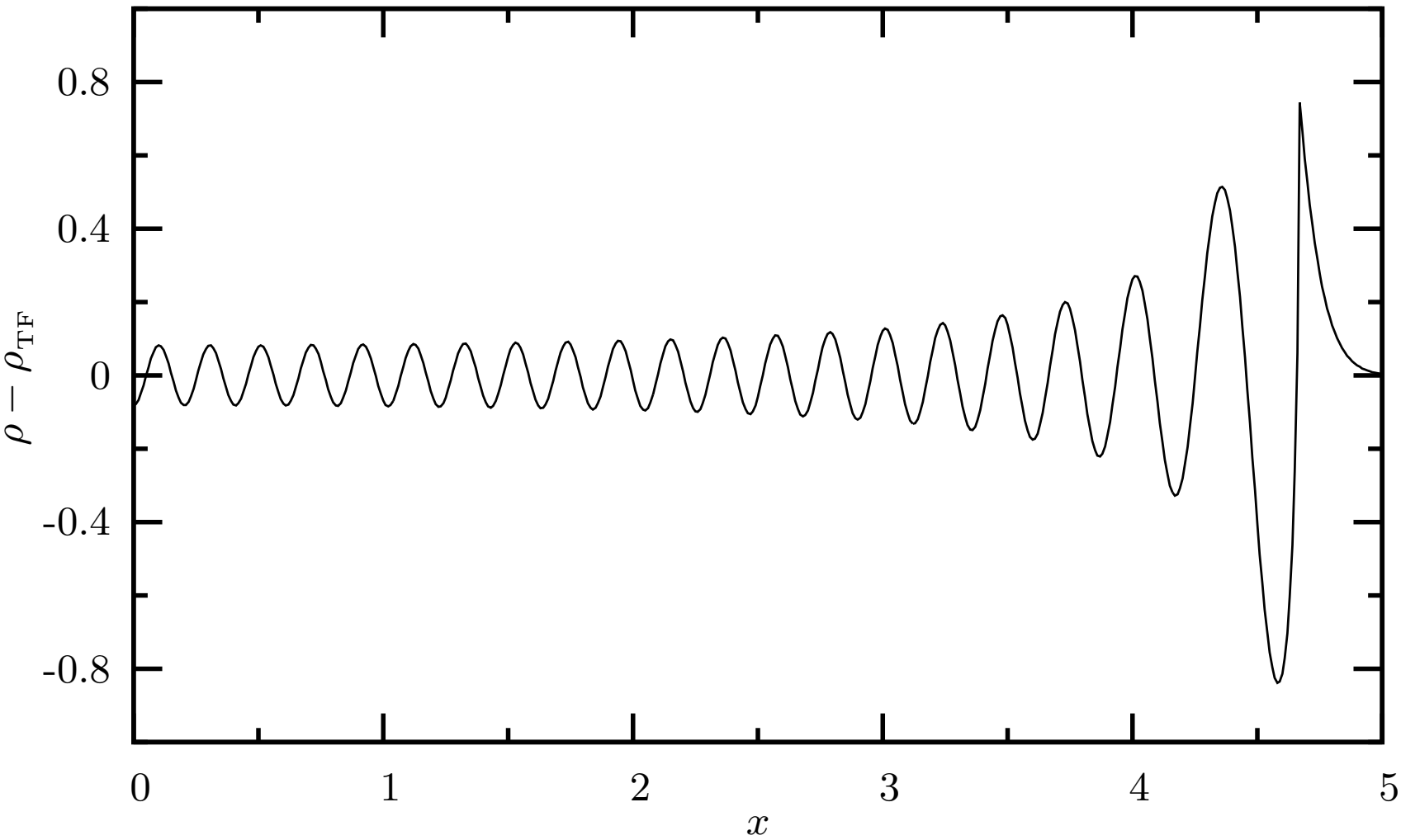
J.R.+M.B., Phys. Rev. Lett. **100**, 200408 (2008)
M.B.+J.R., J. Phys. A **42**, 355210 (2009)
J.R.+M.B.+A.K., Phys. Rev. E **81**, 011118 (2010)
M.B.+A.K.+M.V.N.M.+J.R., J. Phys. A **43**, 255204 (2010)

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



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

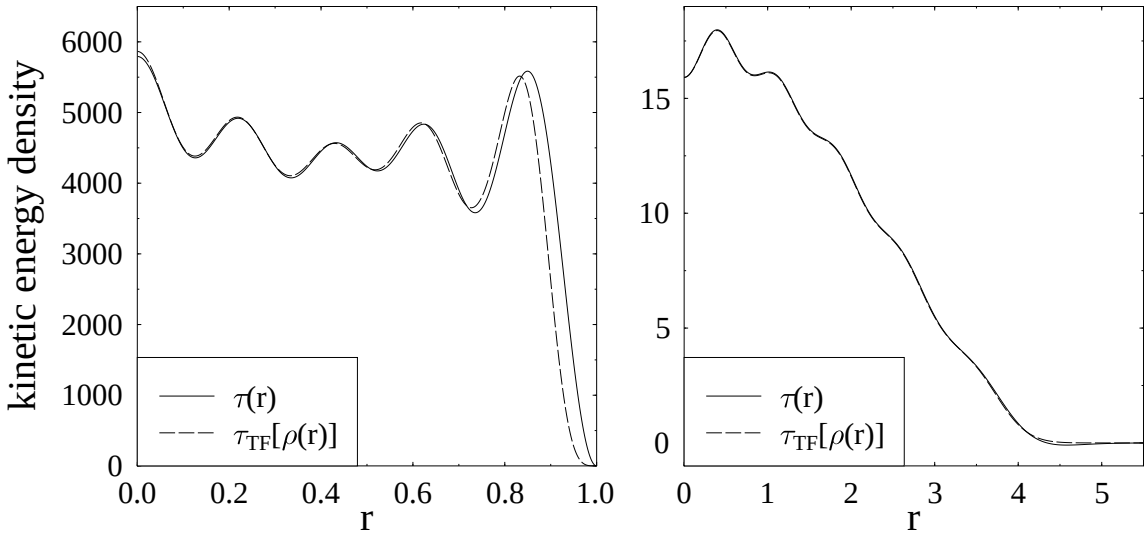
Looking at the oscillating part $\delta\rho(x) = \rho(x) - \rho_{TF}(x)$:



Note the Friedel oscillations with increasing amplitude near the surface!

4.a) A surprise:

What happens if we use the TF functional $\tau_{TF}[\rho(\mathbf{r})]$ with the exact quantum-mechanical $\rho(\mathbf{r})$? does this make sense? ... let's try!



Solid lines: exact kinetic energy density $\tau(r)$
Dashed lines: $\tau_{TF}[\rho(r)]$ using exact spatial density $\rho(r)$
Left: $N = 102$ particles in a circular billiard (with unit radius)
Right: $N = 110$ particles in a 2D isotropic harmonic oscillator

Yields exact $\tau(\mathbf{r})$ amazingly well (except near surface)
but *not* with $\tau_{ETF}[\rho(r)]$! **Why does it work?** semiclassical proof below

4.b) Closed orbit theory for oscillations in spatial densities

We consider a system of N fermions bound in a local potential $V(\mathbf{r})$ in D dimensions: $\hat{H}_{\mathbf{r}}\,\psi_n(\mathbf{r}) = [\hat{T} + V(\mathbf{r})]\,\psi_n(\mathbf{r}) = E_n\,\psi_n(\mathbf{r})$

We define the following spatial densities

$$\rho(\mathbf{r}) = \sum_{E_n \le \lambda} \psi_n^\star(\mathbf{r})\psi_n(\mathbf{r}) \qquad \text{particle density}$$

$$\tau(\mathbf{r}) = -\frac{\hbar^2}{2m} \sum_{E_n \le \lambda} \psi_n^\star(\mathbf{r})\nabla^2\psi_n(\mathbf{r}) \qquad \text{kinetic-energy density}$$

$$\tau_1(\mathbf{r}) = \frac{\hbar^2}{2m} \sum_{E_n \le \lambda} |\nabla\psi_n(\mathbf{r})|^2 \qquad \text{another kinetic-energy density}$$

$$\xi(\mathbf{r}) = \frac{1}{2}\left[\tau(\mathbf{r}) + \tau_1(\mathbf{r})\right] \qquad \text{still another kinetic-energy density}$$

The Fermi energy is a function of the particle number N:

$$N = \int \mathrm{d}\mathbf{r}\, \rho(\mathbf{r}) = \int^{\lambda} g(E)\, \mathrm{d}E \quad \Longrightarrow \quad \lambda = \lambda(N)$$

where $g(E)$ is the level density (density of states):

$$g(E) = \sum_n \delta(E - E_n)$$

Note that all kinetic-energy densities integrate to the exact $T_s[\rho]$:

$$\int \mathrm{d}\mathbf{r}\, \tau(\mathbf{r}) = \int \mathrm{d}\mathbf{r}\, \tau_1(\mathbf{r}) = \int \mathrm{d}\mathbf{r}\, \xi(\mathbf{r}) = T_s[\rho]$$

For time-symmetric systems: $\tau(\mathbf{r}) = \tau_1(\mathbf{r}) - (\hbar^2/4m)\, \nabla^2 \rho(\mathbf{r})$

Use of Green function

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

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

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

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

$$g(E) = -\tfrac{1}{\pi}\,\Im\mathrm{m}\int \mathrm{d}\mathbf{r}\, G(E, \mathbf{r}, \mathbf{r}' = \mathbf{r})$$

(trace integral over space)

and the spatial densities:

$$\begin{aligned}
\rho(N,\mathbf{r}) &= -\frac{1}{\pi}\,\Im\mathrm{m}\int_0^{\lambda(N)} \mathrm{d}E\; G(E,\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}} \\
\tau(N,\mathbf{r}) &= \frac{\hbar^2}{2\pi m}\,\Im\mathrm{m}\int_0^{\lambda(N)} \mathrm{d}E\; \nabla^2_{\mathbf{r}'} G(E,\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}} \\
\tau_1(N,\mathbf{r}) &= -\frac{\hbar^2}{2\pi m}\,\Im\mathrm{m}\int_0^{\lambda(N)} \mathrm{d}E\; \nabla_{\mathbf{r}}\nabla_{\mathbf{r}'} G(E,\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}
\end{aligned}$$

(energy integral up to Fermi energy)

Note: **no** integral over space variables **r**!

Semiclassical approximation

Replace $G(E, \mathbf{r}, \mathbf{r}')$ by Gutzwiller's semiclassical Green function $G_{\mathrm{scl}}(E, \mathbf{r}, \mathbf{r}')$ [derived from Feynman path integral (Gutzwiller 1967)]

$$G_{\mathrm{scl}}(E, \mathbf{r}, \mathbf{r}') = \alpha_D \sum_{\gamma} \sqrt{|\mathcal{D}_\gamma(E, \mathbf{r}, \mathbf{r}')|}\, \exp\left[\frac{i}{\hbar} S_\gamma(E, \mathbf{r}, \mathbf{r}') - i\mu_\gamma \frac{\pi}{2}\right]$$

Ingredients:

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

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

- $\nabla_{\mathbf{r}} G_{\mathrm{scl}}(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') \approx \frac{i}{\hbar} \nabla_{\mathbf{r}} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}')$
- $\nabla_{\mathbf{r}} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') = -\mathbf{p}(\tilde{\lambda}, \mathbf{r}) =: -\mathbf{p}_\lambda$ (initial momentum)
- $\nabla_{\mathbf{r}'} S(\tilde{\lambda}, \mathbf{r}, \mathbf{r}') = \mathbf{p}(\tilde{\lambda}, \mathbf{r}') =: \mathbf{p}'_\lambda$ (final momentum)
- the local Fermi momentum is $p(\tilde{\lambda}, \mathbf{r}) = |\mathbf{p}(\tilde{\lambda}, \mathbf{r})| = \{2m\,[\tilde{\lambda} - V(\mathbf{r})]\}^{1/2}$
- hereby: $\lambda(N) = \tilde{\lambda} + \delta\lambda$, with $\int^{\tilde{\lambda}} \tilde{g}(E)\,\mathrm{d}E = N$
- $\tilde{g}(E) =$ smooth (ETF or Weyl) part of level density

Since we always need $\mathbf{r}' = \mathbf{r}$, only **closed** orbits γ (in coordinate space) contribute to the spatial densities!

For the **level density**, we need the spatial trace integral:
$\int \mathrm{d}\mathbf{r}\, G_{scl}(E, \mathbf{r}, \mathbf{r}' = \mathbf{r})$

Doing it in *stationary-phase approximation* yields $\mathbf{p}_\lambda = \mathbf{p}'_\lambda$
$\Rightarrow$ only **periodic orbits** (*PO*) contribute (to leading order in $\hbar$):
$\sum_\gamma = \sum_{PO}$!

But for the **spatial densities**, no spatial integration is required!
$\Rightarrow$ a priori, **all closed orbits (i.e., also the non-periodic orbits) contribute!**

For the density we get:

$$\rho(\mathbf{r}) = \frac{m\hbar}{\pi}\,\Re\mathrm{e}\;\alpha_D \sum_\gamma \frac{\sqrt{|\mathcal{D}_\perp|}_{\mathbf{r}'=\mathbf{r}}}{p(\tilde\lambda,\mathbf{r})\;T_\gamma(\tilde\lambda,\mathbf{r})}\; e^{i\left[S_\gamma(\tilde\lambda,\mathbf{r},\mathbf{r})/\hbar - \mu_\gamma\frac{\pi}{2}\right]}$$

with $T_\gamma(\tilde\lambda,\mathbf{r}) = \frac{\mathrm{d}}{\mathrm{d}E}S_\gamma(E,\mathbf{r},\mathbf{r})|_{E=\tilde\lambda}$ (running time)

- Under the sum over closed orbits γ:
  - periodic orbits (*PO*s) give smooth (ETF) parts $\tilde\rho, \tilde\tau, \tilde\tau_1$ because actions $S_{PO}(\tilde\lambda)$ are independent of $\mathbf{r}$
  - non-periodic orbits (*NPO*s) give oscillating parts $\delta\rho, \delta\tau, \delta\tau_1$ because of $\mathbf{r}$ dependence of $S_{NPO}(\tilde\lambda,\mathbf{r},\mathbf{r})$ in phase
- This gives a natural separation: $\rho(\mathbf{r}) = \tilde\rho(\mathbf{r}) + \delta\rho(\mathbf{r})$, $\tau(\mathbf{r}) = \tilde\tau(\mathbf{r}) + \delta\tau(\mathbf{r})$, etc.

Facit: Oscillating parts $\delta\rho(\mathbf{r})$, $\delta\tau(\mathbf{r})$, $\delta\tau_1(\mathbf{r})$ are governed by the **nonperiodic orbits** (but closed in $\mathbf{r}$ space)!

Trace formulae for oscillating parts of spatial densities

(to leading order in $\hbar$)

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

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

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

- NPO = nonperiodic (closed) orbits
- $\Phi_{NPO}(\tilde{\lambda},\mathbf{r}) = S_{NPO}(\tilde{\lambda},\mathbf{r},\mathbf{r})/\hbar - \mu_{NPO}\frac{\pi}{2}$ (phase function)
- $T_{NPO}(\tilde{\lambda},\mathbf{r}) = \frac{\mathrm{d}}{\mathrm{d}E} S_{NPO}(E,\mathbf{r},\mathbf{r})|_{E=\tilde{\lambda}}$ (running time)

Caveat:

These trace formulae for the spatial densities are **not valid near the classical turning points** since the denominators there go to zero!

Remedy:

Uniform approximations, see J. Phys. A **43**, 255204 (2010) for details

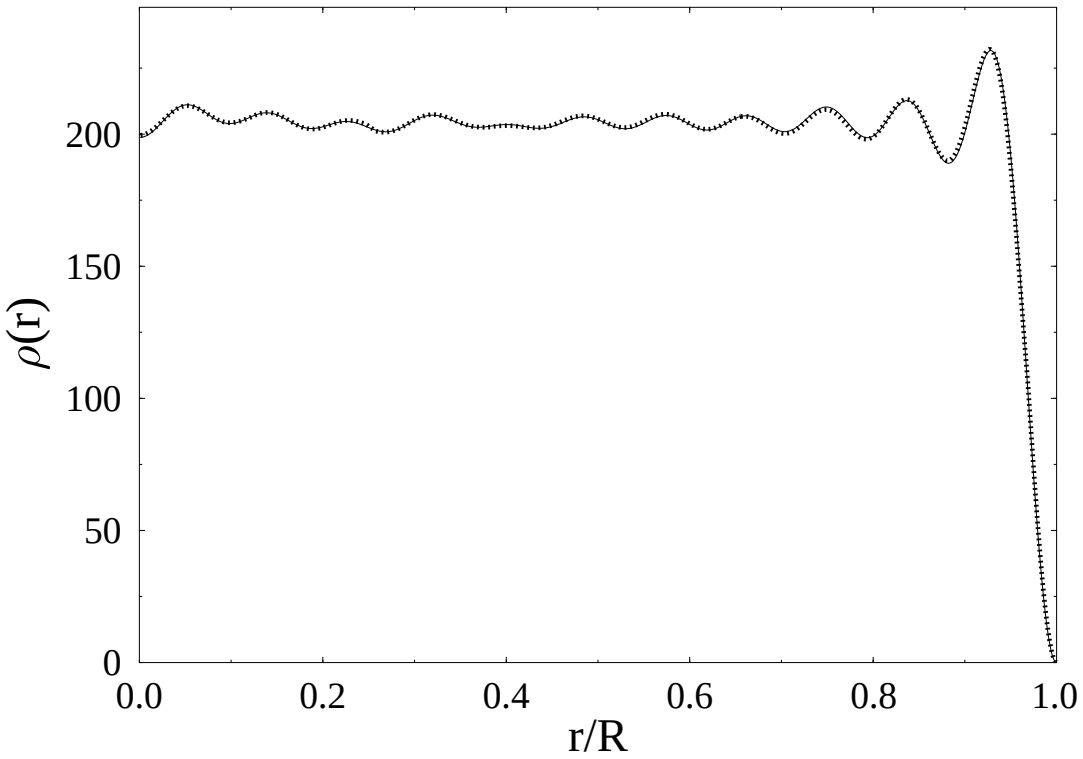
Test case:

Two-dimensional circular billiard (ideally reflecting walls, Dirichlet boundary conditions):

- all POs and NPOs and their properties classified analytically
- uniform approximations for orbit bifurcations (under variation of r)
- see M.B+J.R., J. Phys. A **42** (2009) 355210 for details

The circular billiard ($D = 2$, radius R) for $N = 606$:

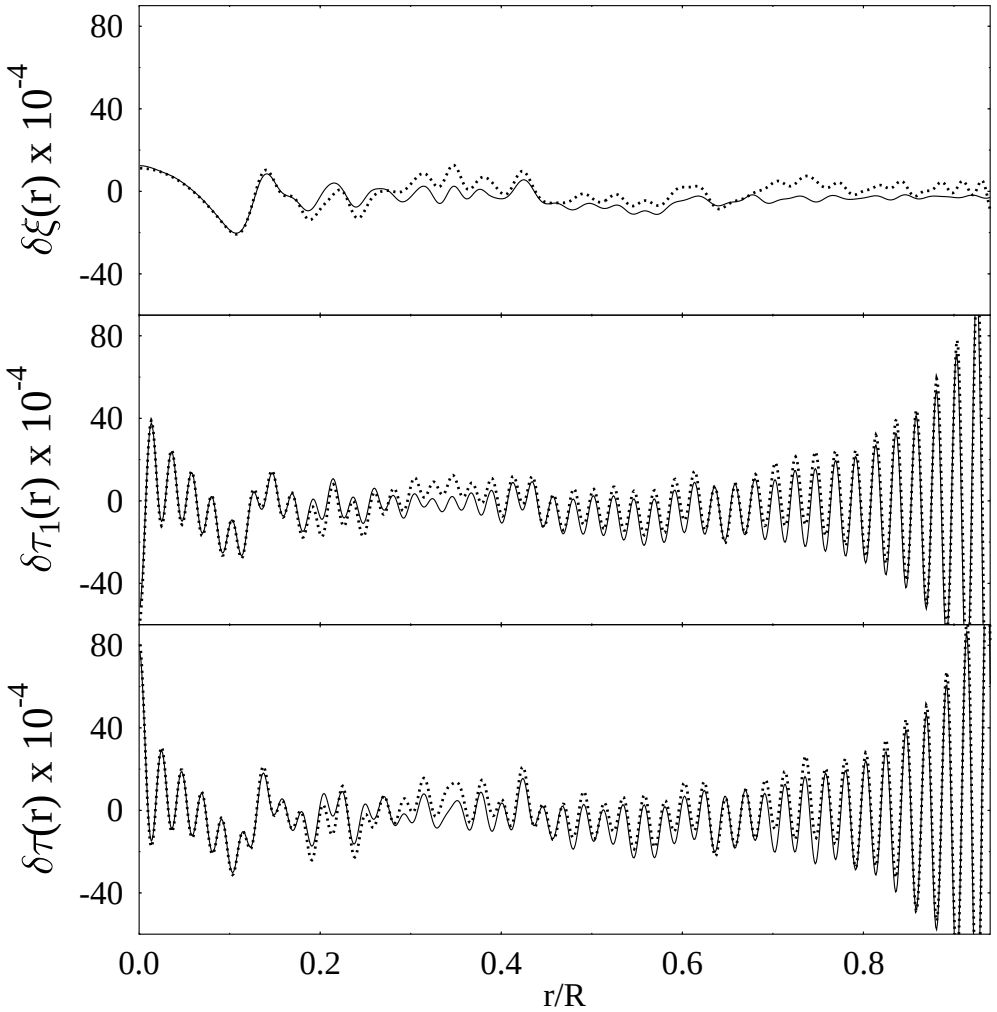
Density $\rho(r)$:



(*solid:* qm, *dotted:* scl) $[\sum_{NPO}$ converged]

The circular billiard ($D = 2$, radius R) for $N = 606$:

Kinetic-energy densities $\delta\tau(r)$, $\delta\tau_1(r)$ and $\delta\xi(r)$:



solid: qm, *dotted:* scl

$\sum_{NPO}$ less well converged (some longer bifurcating orbits were omitted)

Note the opposite phase of the rapid oscillations in $\tau(r)$ and $\tau_1(r)$, and that $\xi(r)$ oscillates less rapidly (all explained by nature of leading NPOs!)

Back to the trace formulae for the spatial densities

(to leading order in $\hbar$)

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

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

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

Note: $(\mathbf{p}_\lambda\cdot\mathbf{p}'_\lambda)$ depends on the nature of the NPO
(namely on the angle between initial and final momentum)

But $p(\tilde{\lambda},\mathbf{r}) = \{2m[\tilde{\lambda} - V(\mathbf{r})]\}^{1/2}$ does not!

4.c) A Local Virial Theorem (LVT)

Since $p(\tilde{\lambda}, \mathbf{r}) = \{2m[\tilde{\lambda} - V(\mathbf{r})]\}^{1/2}$ is independent of the NPOs, we can take it outside of the sums above and find immediately the Local Virial Theorem (LVT):

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

Valid (except near the surface) in the semiclassical limit $\hbar \longrightarrow 0$ for any integrable or chaotic potential $\Rightarrow$ **also for any $V_{KS}(\mathbf{r})$!**

[LVT is exact in the limit $N \longrightarrow \infty$ for the quantum-mechanical densities of harmonic [M.B. and M.V.N.M., J. Phys. A **36**, 1111 (2003)]
and linear potentials [M.B.+A.K.+M.V.N.M.+J.R., J. Phys. A **43**, 255204 (2010)]]

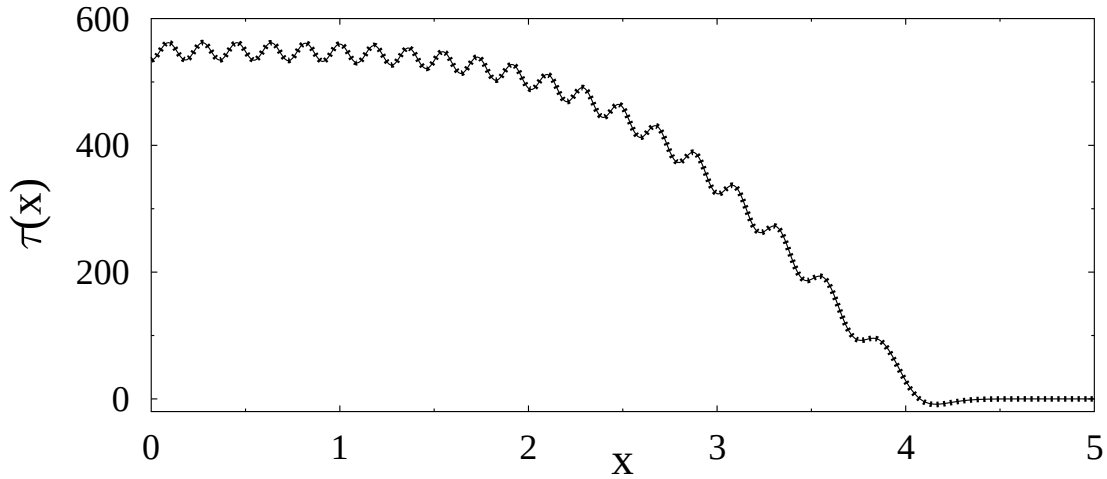
- No such relation for $\delta\tau_1(\mathbf{r})$!
- For the total densities, generalized LVTs are available (also in the surface region)

A generalized LVT

$$\tau(\mathbf{r}) \approx [\tilde{\lambda} - V(\mathbf{r})]\,\rho(\mathbf{r}) - \frac{2}{D}\,\xi(\mathbf{r})$$

(see J. Phys. A **43**, 255204 (2010) for details about surface region; exact equality holds for linear and harmonic potentials)

Numerical test for the 1D potential $V(x) = \frac{1}{2}x^4$ with $N = 40$:



Solid line: exact $\tau(x)$
crosses: generalized LVT using exact $\rho(x)$ and $\xi(x)$

A consequence of the LVT

Taylor expand $\tau_{TF}[\rho(\mathbf{r})]$ around $\tilde{\rho}(\mathbf{r})$ using $\rho(\mathbf{r}) = \tilde{\rho}(\mathbf{r}) + \delta\rho(\mathbf{r})$, assuming $|\tilde{\rho}(\mathbf{r})| = |\rho_{TF}(\mathbf{r})| \gg |\delta\rho(\mathbf{r})|$:

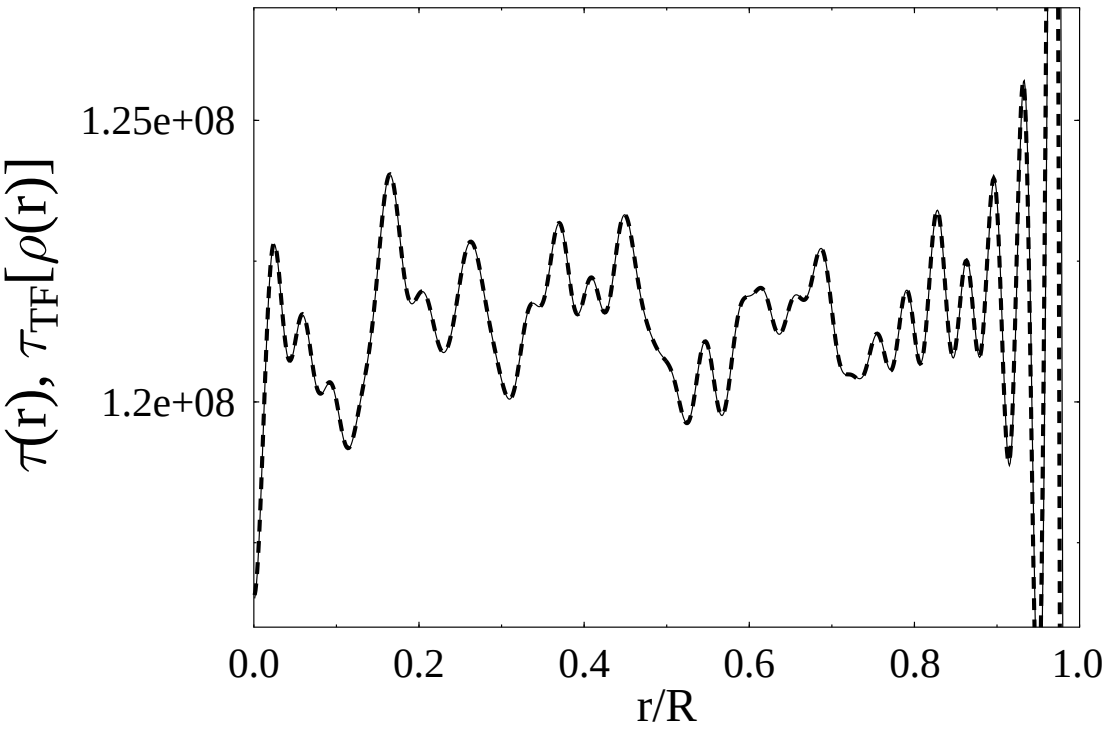
$$\begin{aligned}
\tau_{TF}[\rho(\mathbf{r})] &\simeq \tau_{TF}[\rho_{TF}(\mathbf{r})] + \left.\frac{\mathrm{d}\tau_{TF}}{\mathrm{d}\rho_{TF}}\right|_{\rho_{TF}(\mathbf{r})} \delta\rho(\mathbf{r}) + \mathcal{O}[\delta\rho(\mathbf{r})]^2 \\
&= \tau_{TF}(\mathbf{r}) + [\tilde{\lambda} - V(\mathbf{r})]\,\delta\rho(\mathbf{r}) + \mathcal{O}[\delta\rho(\mathbf{r})]^2 \\
&\simeq \tau_{TF}(\mathbf{r}) + \delta\tau(\mathbf{r}) + \mathcal{O}[\delta\rho(\mathbf{r})]^2
\end{aligned}$$

Follows: $\boxed{\tau_{TF}[\rho(\mathbf{r})] \simeq \tau(\mathbf{r})}$ to first order in $\delta\rho$!

Thus:

- The TF functional reproduces the shell effects to first order in $\delta\rho$ and $\delta\tau$! (except near surface)
- This was known empirically for some time, but not understood. Let's see two more numerical examples ...

Test example: $3D$ spherical billiard (integrable) with $N = 100068$

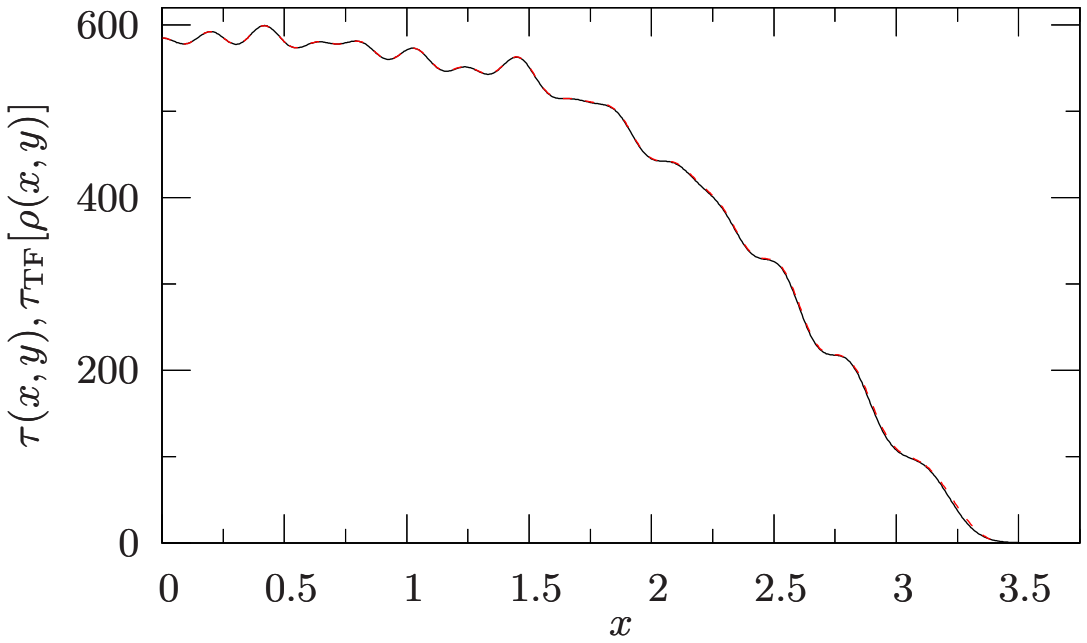


solid: exact quantum-mechanical $\tau(r)$,

dashed: $\tau_{TF}[\rho(r)]$ using exact quantum-mechanical $\rho(r)$

Test example: 2D potential $V(x,y) = \frac{1}{4}(x^4 + y^4) - \kappa x^2 y^2$

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



black: exact q.m. $\tau(x,y)$, *red:* $\tau_{TF}[\rho(x,y)]$ using exact q.m. $\rho(x,y)$ (taken along $x = y$)

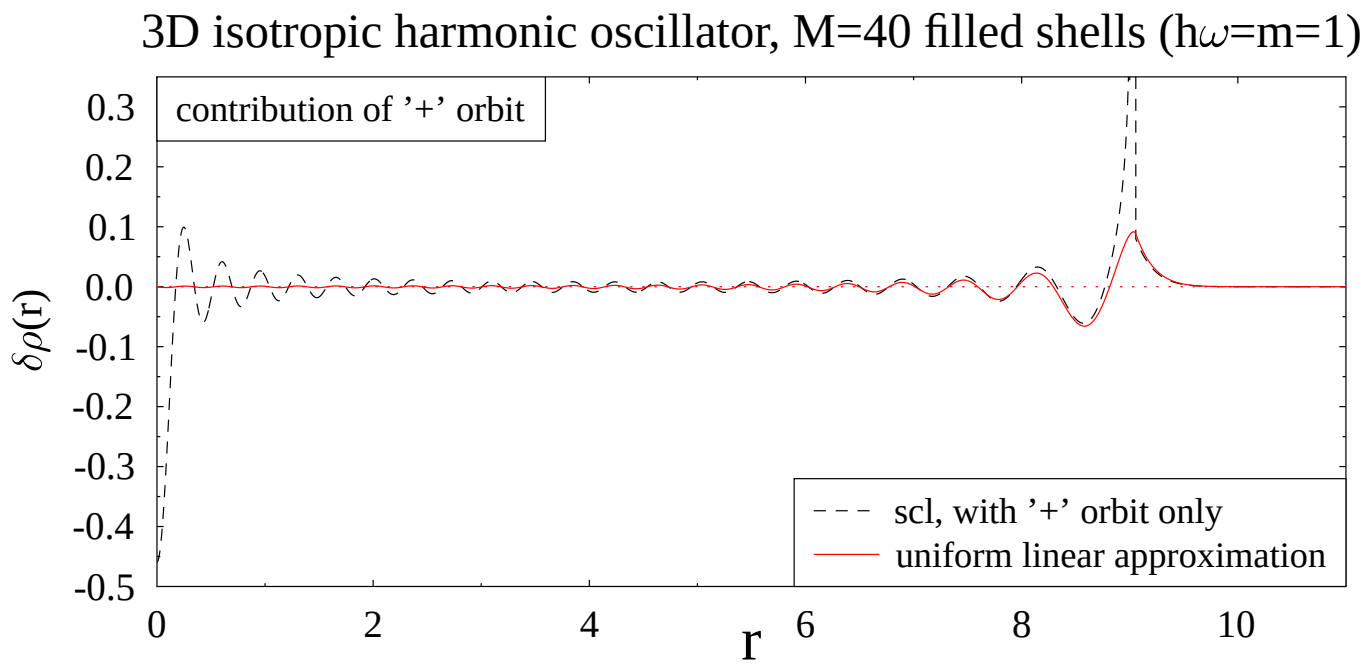
So far, so good! **... BUT**

We have some problems:

- The functional $\tau_{TF}[\rho(\mathbf{r})]$, used in the density-varitional equation $\frac{\delta}{\delta\rho(\mathbf{r})}\int \mathrm{d}\mathbf{r}\,\{\tau_{TF}[\rho] + V\rho - \lambda\rho\} = 0$, yields the TF density $\rho_{TF}(\mathbf{r})$ without oscillations!
- Can some kind of constraint "stabilize" the solution $\rho(\mathbf{r})$ including the oscillations?
- The integral $\int \mathrm{d}\mathbf{r}\,\tau_{TF}[\rho(\mathbf{r})]$ does **not** reproduce the exact kinetic energy $\int \mathrm{d}\mathbf{r}\,\tau(\mathbf{r})$ (except for the isotropic harmonic oscillator in $D = 2$)!
- A challenge to DFT?

4.d) Friedel oscillations

- Friedel oscillations near the surface come from the shortest linear *NPO* (one single reflection) orthogonal to the plane touching the turning point (the '+' orbit)
- uniform approximation required $[T_+(\tilde{\lambda}, \mathbf{r}) \to 0$ at t.p.!]
  For smooth potentials: Airy solution for linearized potential



4.d) Friedel oscillations

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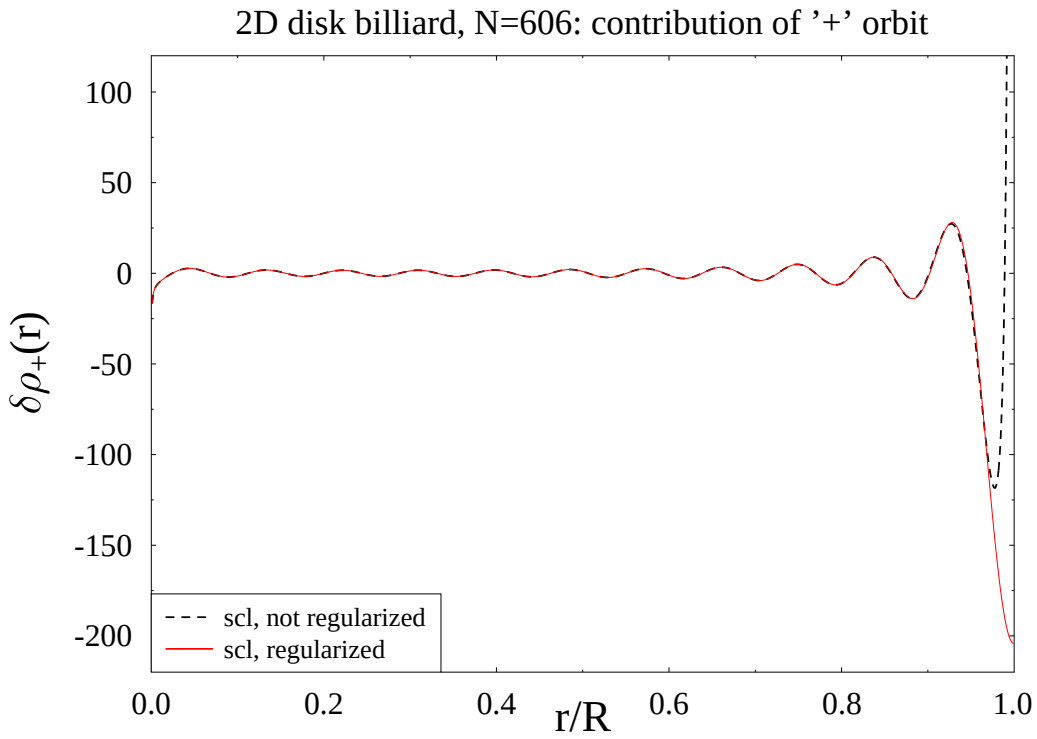
  For billiards: use regularized short-time propagator



Analytical result for spherical billiards (radius R) in D dimensions:

Regularized contribution of the primitive "+" orbit to density:

$$\delta\rho_+^{(\mathrm{un})}(r) = -\rho_{\mathrm{TF}}^{(D)}\, 2^\nu \Gamma(\nu+1) \left(\frac{R}{r}\right)^{\nu-1/2} \frac{J_\nu(z)}{z^\nu}$$

with $\nu = D/2$, $z = 2\,(R-r)\,p_\lambda/\hbar$.
Take integral over whole space:

$$\int \delta\rho_+^{(\mathrm{un})}(r)\,\mathrm{d}^D r = \delta N_+\,.$$

This turns out to be exactly the surface correction to the Weyl expansion of the particle number!
E.g. for $D = 3$: $N_{\mathrm{Weyl}}(k) = c_V k^3 V + c_s k^2 S + c_c k C + \ldots$
(V = volume, S = surface, C = mean curvature, etc. of billiard, $k = p/\hbar = \sqrt{2mE}/\hbar$) $c_s k^2 S = \delta N_+$

Thanks for your attention!