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

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1. Introduction
   a) The kinetic energy functionals $T_s[\rho]$ and $\tau[\rho]$
   b) Smooth and oscillating components
   c) Two kinds of semiclassical expansions

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

3. Periodic orbit theory (POT) for oscillating components
   of energy and level density (short)

4. Oscillations in spatial densities
   a) A surprise
   b) Closed orbit theory (COT) for oscillating parts of densities
   c) Local virial theorems
   d) A note about Friedel oscillations

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 $\rho(r)$:

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

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

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

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

and solve the Kohn-Sham equations for the $\psi_n(r)$ and $E_n$. 
The **Kohn-Sham (KS) equations**:

\[
\begin{aligned}
\left\{-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + V_{\text{KS}}[\rho(r)]\right\} \psi_n(r) &= E_n \psi_n(r),
\end{aligned}
\]

where \( V_{\text{KS}}[\rho(r)] \) is given by the variational derivative

\[
V_{\text{KS}}[\rho(r)] = \frac{\delta(E_H[\rho] + E_{xc}[\rho])}{\delta \rho(r)} = V_H(r) + V_{xc}(r).
\]

We define a **kinetic-energy density** \( \tau(r) \) by

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

Then, \( T_s[\rho] \) is given exactly by the integral \( T_s[\rho] = \int \tau(r) \, dr \).

(The crux: \( E_{xc}[\rho] \) and hence \( V_{xc}[\rho(r)] \) are not exactly known!)

In this talk, we shall discuss semiclassical approximations to \( T_s[\rho] \) and \( \tau(r) \) as explicit functionals of \( \rho(r) \).
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; $\delta E =$”shell correction”)
- $g(E) = \tilde{g}(E) + \delta g(E)$ (cf. Gutzwiller, Berry & Tabor, Balian & Bloch)
- $\rho(r) = \tilde{\rho}(r) + \delta \rho(r)$ 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 $V(r)$, an expansion in gradients of $V(r)$ (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 $\rho(r)$ and $\tau(r)$ for non-interacting fermions in a potential $V(r)$ in $D$ dimensions:

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

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

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

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

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

Historically, Weizsäcker (1935) derived an “inhomogeneity correction”: 

$$
\tau_W[\rho(r)] = \frac{\hbar^2}{8m} \frac{(\nabla \rho)^2}{\rho} \quad \text{(for } D = 3)\]
$$

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

Under the integral $\int d^3r \, \tau_{ETF}[\rho(r)] = T_{ETF}[\rho]$ many terms vanish.
ETF kinetic energy functional in $D = 3$ dimensions:

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

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

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 $\tilde{\rho}(r)$ and compare the results to the selfconsistently averaged quantum-mechanical kinetic energies $\tilde{T}_s$ in terms of the eigenfunctions $\psi(r)$ of the selfconsistently averaged potential $\tilde{V}(r)$
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.

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

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

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

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 ($PO$s) of the classical system $H(p, r) = p^2/2m + V(r)$

Ingredients:
- $S_{PO} = \oint_{PO} p \cdot dq =$ action integral along $PO$
- $A_{PO} =$ amplitude (related to stability and degeneracy)
- $\sigma_{PO} =$ 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”):

$$E_{tot} = \tilde{E}_{tot} + \delta E \quad \text{(and} \quad N = \tilde{N} + \delta N)$$

[Average $\tilde{E}_{tot}(\tilde{N})$ e.g. from selfconsistent ETF model]

Trace formulae for $\delta E$ and $\delta N$ (Strutinsky et al., 1975):

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

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

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

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

\[
\rho(x) = \sum_{n \leq n_{\text{max}}} |\psi_n|^2
\]

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 $\tau_{TF}[\rho(r)]$ with the exact quantum-mechanical $\rho(r)$? 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 $\tau(r)$ 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 $V(r)$ in $D$ dimensions:  
\[ \hat{H}_r \psi_n(r) = [\hat{T} + V(r)] \psi_n(r) = E_n \psi_n(r) \]

We define the following spatial densities

- Particle density:
  \[ \rho(r) = \sum_{E_n \leq \lambda} \psi_n^*(r) \psi_n(r) \]

- Kinetic-energy density:
  \[ \tau(r) = -\frac{\hbar^2}{2m} \sum_{E_n \leq \lambda} \psi_n^*(r) \nabla^2 \psi_n(r) \]

- Another kinetic-energy density:
  \[ \tau_1(r) = \frac{\hbar^2}{2m} \sum_{E_n \leq \lambda} |\nabla \psi_n(r)|^2 \]

- Still another kinetic-energy density:
  \[ \xi(r) = \frac{1}{2} [\tau(r) + \tau_1(r)] \]
The Fermi energy is a function of the particle number \( N \):

\[
N = \int \, d\mathbf{r} \, \rho(\mathbf{r}) = \int \, \lambda \, g(E) \, dE \quad \implies \quad \lambda = \lambda(N)
\]

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 \( T_s[\rho] \):

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

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

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

\(G(E, r, r')\) in terms of eigenfunctions:

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

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

\[g(E) = -\frac{1}{\pi} \Im \int \text{d}r \ G(E, r, r' = r)\]

(trace integral over space)
and the spatial densities:

\[ \rho(N, r) = -\frac{1}{\pi} \Im \int_0^{\lambda(N)} dE \, G(E, r, r') |_{r' = r} \]

\[ \tau(N, r) = \frac{\hbar^2}{2\pi m} \Im \int_0^{\lambda(N)} dE \, \nabla^2_{r'} G(E, r, r') |_{r' = r} \]

\[ \tau_1(N, r) = -\frac{\hbar^2}{2\pi m} \Im \int_0^{\lambda(N)} dE \, \nabla_r \nabla_{r'} G(E, r, r') |_{r' = r} \]

(energy integral up to Fermi energy)

Note: no integral over space variables \( r \)!
Semiclassical approximation

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

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

Ingredients:

- sum over all classical trajectories $\gamma$ from $r$ to $r'$
- $D_{\gamma}$ is the Van Vleck determinant (related to stability)
- $S_{\gamma}(E, r, r') = \int_{r}^{r'} p \cdot dq$ is the action integral along $\gamma$
- $\mu_{\gamma}$ is the classical Morse index (number of conjugate points)
- $\alpha_D = 2\pi(2i\pi\hbar)^{-\frac{D+1}{2}}$
Now we use leading-order terms in $1/\hbar$:

- $\nabla_r G_{\text{scl}}(\tilde{\lambda}, r, r') \approx \frac{i}{\hbar} \nabla_r S(\tilde{\lambda}, r, r')$
- $\nabla_r S(\tilde{\lambda}, r, r') = -p(\tilde{\lambda}, r) =: -p_\lambda$ (initial momentum)
- $\nabla_{r'} S(\tilde{\lambda}, r, r') = p(\tilde{\lambda}, r') =: p'_{\lambda}$ (final momentum)

- the local Fermi momentum is $p(\tilde{\lambda}, r) = |p(\tilde{\lambda}, r)| = \{2m [\tilde{\lambda} - V(r)]\}^{1/2}$
- hereby: $\lambda(N) = \tilde{\lambda} + \delta\lambda$, with $\int^{\tilde{\lambda}} \tilde{g}(E) \, dE = N$
- $\tilde{g}(E) = \text{smooth (ETF or Weyl) part of level density}$
Since we always need \( r' = r \), only closed orbits \( \gamma \) (in coordinate space) contribute to the spatial densities!

For the **level density**, we need the **spatial trace integral**:

\[
\int \mathrm{d}r \ G_{\text{scl}}(E, r, r' = r)
\]

Doing it in **stationary-phase approximation** yields \( p_\lambda = p'_\lambda \)

\( \Rightarrow \) only **periodic orbits** (PO) contribute (to leading order in \( \hbar \)):

\[
\sum_{\gamma} = \sum_{\text{PO}}
\]

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:

$$\rho(\mathbf{r}) = \frac{m\hbar}{\pi} \Re \alpha_D \sum_\gamma \frac{\sqrt{|D_\perp|}}{p(\tilde{\lambda}, \mathbf{r})} \frac{\sqrt{p(\tilde{\lambda}, \mathbf{r})}}{T_\gamma(\tilde{\lambda}, \mathbf{r})} \exp\left[\frac{i}{\hbar} \frac{S_\gamma(\tilde{\lambda}, \mathbf{r})}{\mu - \frac{\hbar}{\pi}} \right]$$

with

$$T_\gamma(\tilde{\lambda}, \mathbf{r}) = \frac{d}{dE} S_\gamma(E, \mathbf{r}, \mathbf{r}) \big|_{E=\tilde{\lambda}} \quad \text{(running time)}$$

- Under the sum over closed orbits $\gamma$:
  - periodic orbits (POs) 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 (NPOs) 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 $\hbar$)

\[
\delta \rho(r) = \frac{m\hbar}{\pi} \Re \alpha_D \sum_{NPO} \frac{\sqrt{|D_\perp|}}{p(\tilde{\lambda}, r) T_{NPO}(\tilde{\lambda}, r)} e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]

\[
\delta \tau(r) = \frac{\hbar}{2\pi} \Re \alpha_D \sum_{NPO} \frac{p(\tilde{\lambda}, r) \sqrt{|D_\perp|}}{T_{NPO}(\tilde{\lambda}, r)} e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]

\[
\delta \tau_1(r) = \frac{\hbar}{2\pi} \Re \alpha_D \sum_{NPO} \frac{\{(p_\lambda \cdot p'_\lambda) \sqrt{|D_\perp|}\}}{p(\tilde{\lambda}, r) T_{NPO}(\tilde{\lambda}, r)} e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]

- $NPO = \text{nonperiodic (closed) orbits}$
- $\Phi_{NPO}(\tilde{\lambda}, r) = S_{NPO}(\tilde{\lambda}, r, r)/\hbar - \mu_{NPO} \frac{\pi}{2}$ (phase function)
- $T_{NPO}(\tilde{\lambda}, r) = \frac{d}{dE} S_{NPO}(E, r, r)|_{E=\tilde{\lambda}}$ (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 $r$)
The circular billiard \((D = 2, \text{ radius } R)\) for \(N = 606\):

Density \(\rho(r)\):

\[\begin{array}{cccccc}
0.0 & 0.2 & 0.4 & 0.6 & 0.8 & 1.0 \\
\end{array}\]

\(\begin{array}{cccccc}
0 & 50 & 100 & 150 & 200 & \\
\end{array}\)

\((\text{solid: qm, dotted: scl}) \quad [\sum_{NPO} \text{ converged}]\)
The circular billiard \((D = 2, \text{ radius } R)\) 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 $\hbar$

\[
\delta \rho(r) = \frac{m\hbar}{\pi} \Re \alpha_D \sum_{NPO} \frac{\sqrt{|D_{\bot}|}}{p(\tilde{\lambda}, r)} T_{NPO}(\tilde{\lambda}, r) e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]
\[
\delta \tau(r) = \frac{\hbar}{2\pi} \Re \alpha_D \sum_{NPO} \frac{p(\tilde{\lambda}, r) \sqrt{|D_{\bot}|}}{T_{NPO}(\tilde{\lambda}, r)} e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]
\[
\delta \tau_1(r) = \frac{\hbar}{2\pi} \Re \alpha_D \sum_{NPO} \frac{(p_{\lambda} \cdot p'_{\lambda}) \sqrt{|D_{\bot}|}}{p(\tilde{\lambda}, r) T_{NPO}(\tilde{\lambda}, r)} e^{i\Phi_{NPO}(\tilde{\lambda}, r)}
\]

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

But $p(\tilde{\lambda}, r) = \{2m[\tilde{\lambda} - V(r)]\}^{1/2}$ does not!
4.c) A Local Virial Theorem (LVT)

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

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

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

[LVT is exact in the limit $N \to \infty$ for the quantum-mechanical densities of harmonic [M.B. and M.V.N.M., J. Phys. A 36, 1111 (2003)]


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

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

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

$$\tau_{TF}[\rho(r)] \approx \tau_{TF}[\rho_{TF}(r)] + \frac{d\tau_{TF}}{d\rho_{TF}}|_{\rho_{TF}(r)} \delta\rho(r) + O[\delta\rho(r)]^2$$

$$= \tau_{TF}(r) + [\tilde{\lambda} - V(r)] \delta\rho(r) + O[\delta\rho(r)]^2$$

$$\approx \tau_{TF}(r) + \delta\tau(r) + O[\delta\rho(r)]^2$$

Follows: $\tau_{TF}[\rho(r)] \approx \tau(r)$ 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 \( N = 100068 \)

\[
\begin{align*}
\tau(r), & \quad \tau_{TF}[\rho(r)] \\
\tau_T & \quad \rho(r)
\end{align*}
\]

*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!), \( N = 632 \)

\[
\begin{array}{c|c|c|c|c|c}
\tau(x, y) & \text{black: exact q.m. } \tau(x, y) & \text{red: } \tau_{TF}[\rho(x, y)] & \text{using exact q.m. } \rho(x, y) & \text{taken along } x = y \\
\hline
0 & 600 & 600 & 600 & 600 \\
0.5 & 400 & 400 & 400 & 400 \\
1 & 200 & 200 & 200 & 200 \\
1.5 & 100 & 100 & 100 & 100 \\
2 & 50 & 50 & 50 & 50 \\
2.5 & 25 & 25 & 25 & 25 \\
3 & 12.5 & 12.5 & 12.5 & 12.5 \\
3.5 & 6.25 & 6.25 & 6.25 & 6.25 \\
\end{array}
\]

So far, so good! ... BUT
We have some problems:

- The functional $\tau_{TF}[\rho(r)]$, used in the density-varitional equation
  $$\frac{\delta}{\delta \rho(r)} \int dr \{ \tau_{TF}[\rho] + V\rho - \lambda \rho \} = 0,$$
  yields the TF density $\rho_{TF}(r)$ without oscillations!

- Can some kind of constraint “stabilize” the solution $\rho(r)$ including the oscillations?

- The integral $\int dr \tau_{TF}[\rho(r)]$ does not reproduce the exact kinetic energy $\int dr \tau(r)$
  (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 \[ T_+(\tilde{\lambda}, r) \to 0 \text{ at t.p.} \]

For smooth potentials: Airy solution for linearized potential

3D isotropic harmonic oscillator, M=40 filled shells (h\omega=m=1)
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 \[ T_+ (\tilde{\lambda}, r) \to 0 \text{ at t.p.}! \]

For billiards: use regularized short-time propagator

![Graph showing contribution of '+' orbit in a 2D disk billiard, N=606.](image)
Analytical result for spherical billiards (radius $R$) in $D$ dimensions:

Regularized contribution of the primitive “+” orbit to density:

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

with $\nu = D/2$, $z = 2 (R - r) \rho_\lambda/\hbar$.

Take integral over whole space:

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

This turns out to be exactly the surface correction to the Weyl expansion of the particle number!

E.g. for $D = 3$:

$$
N_{\text{Weyl}}(k) = c_V k^3 V + c_s k^2 S + c_c k C + \ldots
$$

($V =$ 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!