Theoretical Proof of the Strutinsky Energy Theorem

Foundations of Nuclear DFT and Future Applications

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1. The Strutinsky method: sixty years of success and frustration

   The most successful and precise global model, still without a theoretical justification

2. A derivation from nuclear density functional theory

   The physical meaning of the “shell correction”

3. Extension to pairing and (future) applications to nuclear structure and fission

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Background: Binding energy in mean field approaches and double counting problem

The naive single-particle sum

$$E_{\text{sp}} = \sum_{i=1}^{N} \varepsilon_i = \int_{-\infty}^{\varepsilon_F} \varepsilon \, g(\varepsilon) \, d\varepsilon$$

This is *not* the total binding energy.

Why it fails:

- The mean-field potential U is generated by the nucleons themselves
- Each two-body interaction V_{ij} is counted **twice** — once for particle i, once for particle j
- The independent-particle picture is only an *effective representation* of a correlated many-body system

The Hartree–Fock correction:

$$E = \sum_i \langle t_i \rangle + \frac{1}{2}\langle V \rangle = \sum_i \varepsilon_i - \frac{1}{2}\langle V \rangle$$

Subtracting $\frac{1}{2}\langle V \rangle$ corrects the double counting — but requires explicit knowledge of the two-body force V.

For phenomenological potentials like Woods–Saxon: $\langle V \rangle$ is unavailable.

The Strutinsky Energy Theorem (1967–1968)



V. M. Strutinsky

$$\boxed{E = \tilde{E}^{(0)} + \delta E^{(1)}_{\text{shell}} + \delta E^{(2)}}$$

Shell correction

$$\delta E^{(1)}_{\text{shell}} = E_{\text{sp}} - \tilde{E}_{\text{sp}}$$

$$E_{\text{sp}} = \int_{-\infty}^{\varepsilon_F} \varepsilon\, g(\varepsilon)\, d\varepsilon$$

$\delta E^{(2)}$ is assumed small.

Smooth part

$$\tilde{E}_{\text{sp}} = \int_{-\infty}^{\tilde{\varepsilon}_F} \varepsilon\, \tilde{g}(\varepsilon)\, d\varepsilon, \qquad N = \int_{-\infty}^{\tilde{\varepsilon}_F} \tilde{g}(\varepsilon)\, d\varepsilon$$

$\tilde{g}$: Gaussian convolution with a curvature correction.

- **Golden standard** of the macroscopic–microscopic framework for over 50 years
- Family of "semi-classical physics" (or more exactly the *leading-order approximation*) © 2003 by M. Brack and R.K. Bhaduri
- Still among the most **precise and practical tools** for global nuclear structure calculations; Reproduces **binding energies** and **fission barriers**
- But in practice it functions essentially as a controlled *"black box"*

Strutinsky's original justification (reformulated)

Strutinsky attempted to justify the energy theorem based on the perturbative Hartree-Fock argument:

Assuming an averaged density $\tilde{\rho}$ with smooth potential $\tilde{U}$:

$$E \approx \sum_i \tilde{\varepsilon}_i - \frac{1}{2}\langle \tilde{V} \rangle_{\tilde{\rho}} + O\big[(\delta\rho)^2\big]$$

with $\delta\rho = \rho - \tilde{\rho}$, $\delta U = U - \tilde{U}$, and to first order:

$$\varepsilon_i = \tilde{\varepsilon}_i + \langle \delta U \rangle + O\big[(\delta\rho)^2\big]$$

Strutinsky explicitly acknowledged the resulting expression may not be of practical use and it is a *perturbative reorganization*.

A fundamental inconsistency in the HF argument

▸ The SP energies $\{\tilde{\varepsilon}_i\}$ are identified with eigenvalues of an **averaged non-self-consistent** potential — distinct from those in the original self-consistent solution.

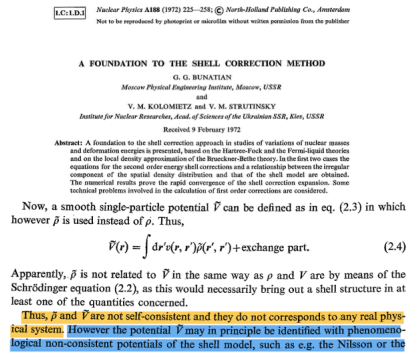
In other words, HF and phenomenological shell model are based on **different Hamiltonians** or *two inequivalent mean-field descriptions*.

▸ The shell correction emerges as the fluctuating part of the SP energy sum — but **no prescription** is given for subtracting a suitably smoothed average

A fundamental inconsistency in the HF argument

Bunatian, Kolomietz & Strutinsky (1972):

*"$\tilde{\rho}$ and $\tilde{U}$ are not self-consistent and **they do not correspond to any real physical system**. However, the potential $\tilde{U}$ may in principle be identified with phenomenological non-consistent potentials of the shell model."*



I.C.T.P.

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A FOUNDATION TO THE SHELL CORRECTION METHOD

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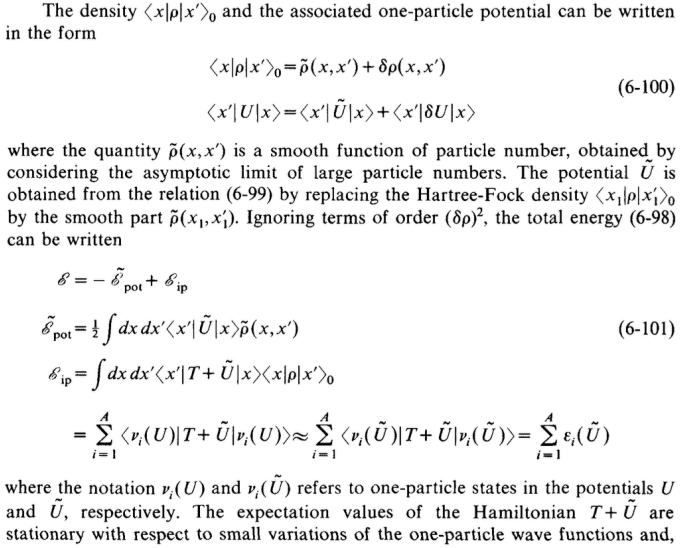
Abstract: A foundation to the shell correction approach in studies of variations of nuclear masses and deformation energies is presented, based on the Hartree-Fock and the Fermi-liquid theories and on the local density approximation of the Brueckner-Bethe theory. In the first two cases the equations for the second order energy shell corrections and a relationship between the irregular component of the spatial density distribution and that of the shell model are obtained. The numerical results prove the rapid convergence of the shell correction expansion. Some technical problems involved in the calculation of first order corrections are considered.

Now, a smooth single-particle potential $\tilde{V}$ can be defined as in eq. (2.3) in which however $\tilde{\rho}$ is used instead of ρ. Thus,

$$\tilde{V}(r) = \int \mathrm{d}r' v(r, r') \tilde{\rho}(r', r') + \text{exchange part.} \qquad (2.4)$$

Apparently, $\tilde{\rho}$ is not related to $\tilde{V}$ in the same way as ρ and V are by means of the Schrödinger equation (2.2), as this would necessarily bring out a shell structure in at least one of the quantities concerned.

Thus, $\tilde{\rho}$ and $\tilde{V}$ are not self-consistent and they do not corresponds to any real physical system. However the potential $\tilde{V}$ may in principle be identified with phenomenological non-consistent potentials of the shell model, such as e.g. the Nilsson or the



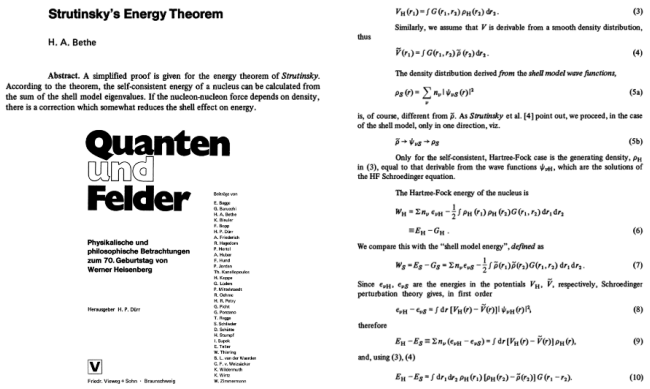
The density $\langle x|\rho|x'\rangle_0$ and the associated one-particle potential can be written in the form

$$\langle x|\rho|x'\rangle_0 = \tilde{\rho}(x,x') + \delta\rho(x,x')$$
$$\langle x'|U|x\rangle = \langle x'|\tilde{U}|x\rangle + \langle x'|\delta U|x\rangle \qquad (6\text{-}100)$$

where the quantity $\tilde{\rho}(x,x')$ is a smooth function of particle number, obtained by considering the asymptotic limit of large particle numbers. The potential $\tilde{U}$ is obtained from the relation (6-99) by replacing the Hartree-Fock density $\langle x_1|\rho|x_1'\rangle_0$ by the smooth part $\tilde{\rho}(x_1, x_1')$. Ignoring terms of order $(\delta\rho)^2$, the total energy (6-98) can be written

$$\mathscr{E} = -\tilde{\mathscr{E}}_{\text{pot}} + \mathscr{E}_{\text{ip}}$$
$$\tilde{\mathscr{E}}_{\text{pot}} = \tfrac{1}{2}\int dx\, dx' \langle x'|\tilde{U}|x\rangle\tilde{\rho}(x,x') \qquad (6\text{-}101)$$
$$\mathscr{E}_{\text{ip}} = \int dx\, dx' \langle x'|T+\tilde{U}|x\rangle\langle x|\rho|x'\rangle_0$$
$$= \sum_{i=1}^{A} \langle \nu_i(U)|T+\tilde{U}|\nu_i(U)\rangle \approx \sum_{i=1}^{A} \langle \nu_i(\tilde{U})|T+\tilde{U}|\nu_i(\tilde{U})\rangle = \sum_{i=1}^{A} \varepsilon_i(\tilde{U})$$

where the notation $\nu_i(U)$ and $\nu_i(\tilde{U})$ refers to one-particle states in the potentials U and $\tilde{U}$, respectively. The expectation values of the Hamiltonian $T+\tilde{U}$ are stationary with respect to small variations of the one-particle wave functions and,



Strutinsky's Energy Theorem

H. A. Bethe

Abstract. A simplified proof is given for the energy theorem of *Strutinsky*. According to the theorem, the self-consistent energy of a nucleus can be calculated from the sum of the shell model eigenvalues. If the nucleon-nucleon force depends on density, there is a correction which somewhat reduces the shell effect on energy.

Quanten und Felder

Physikalische und philosophische Betrachtungen zum 70. Geburtstag von Werner Heisenberg

Herausgeber H. P. Dürr

Vieweg

$$V_{\mathrm{H}}(r_1) = \int G(r_1, r_2)\, \rho_{\mathrm{H}}(r_2)\, \mathrm{d}r_2. \qquad (3)$$

Similarly, we assume that V is derivable from a smooth density distribution, thus

$$\tilde{V}(r_1) = \int G(r_1, r_2)\, \tilde{\rho}(r_2)\, \mathrm{d}r_2. \qquad (4)$$

The density distribution derived *from the shell model wave functions,*

$$\rho_{\mathrm{g}}(r) = \sum_{\sigma} n_\sigma |\psi_{\sigma\mathrm{g}}(r)|^2 \qquad (5a)$$

is, of course, different from $\tilde{\rho}$. As *Strutinsky* et al. [4] point out, we proceed, in the case of the shell model, only in one direction, viz.

$$\tilde{\rho} \to \psi_{\sigma\mathrm{g}} \to \rho_{\mathrm{g}} \qquad (5b)$$

Only for the self-consistent, Hartree-Fock case is the generating density, ρ_{H} in (3), equal to that derivable from the wave functions $\psi_{\sigma\mathrm{H}}$, which are the solutions of the HF Schroedinger equation.

The Hartree-Fock energy of the nucleus is

$$W_{\mathrm{H}} = \Sigma n_\sigma\, \epsilon_{\sigma\mathrm{H}} - \tfrac{1}{2}\int \rho_{\mathrm{H}}(r_1)\, \rho_{\mathrm{H}}(r_2) G(r_1, r_2)\, \mathrm{d}r_1 \mathrm{d}r_2$$
$$\equiv E_{\mathrm{H}} - G_{\mathrm{H}}. \qquad (6)$$

We compare this with the "shell model energy", *defined* as

$$W_{\mathrm{g}} = E_{\mathrm{g}} - G_{\mathrm{g}} = \Sigma n_\sigma \epsilon_{\sigma\mathrm{g}} - \tfrac{1}{2}\int \tilde{\rho}(r_1)\tilde{\rho}(r_2) G(r_1, r_2)\, \mathrm{d}r_1 \mathrm{d}r_2. \qquad (7)$$

Since $\epsilon_{\sigma\mathrm{H}}$, $\epsilon_{\sigma\mathrm{g}}$ are the energies in the potentials V_{H}, $\tilde{V}$, respectively, Schroedinger perturbation theory gives, in first order

$$\epsilon_{\sigma\mathrm{H}} - \epsilon_{\sigma\mathrm{g}} = \int \mathrm{d}r\, [V_{\mathrm{H}}(r) - \tilde{V}(r)]\, |\psi_{\sigma\mathrm{H}}(r)|^2, \qquad (8)$$

therefore

$$E_{\mathrm{H}} - E_{\mathrm{g}} \equiv \Sigma n_\sigma (\epsilon_{\sigma\mathrm{H}} - \epsilon_{\sigma\mathrm{g}}) = \int \mathrm{d}r\, [V_{\mathrm{H}}(r) - \tilde{V}(r)]\, \rho_{\mathrm{H}}(r), \qquad (9)$$

and, using (3), (4)

$$E_{\mathrm{H}} - E_{\mathrm{g}} = \int \mathrm{d}r_1 \mathrm{d}r_2\, \rho_{\mathrm{H}}(r_1) [\rho_{\mathrm{H}}(r_2) - \tilde{\rho}(r_2)] G(r_1 - r_2). \qquad (10)$$

Strutinsky (1967, 1968, 1972); Nilsson et al. (1969); Brack et al. (1972); Bohr & Mottelson, Vol. II, p. 370. The same argument appears in Ring & Schuck (1980) and Bethe.

Kohn–Sham scheme for nuclei

Hohenberg–Kohn (1964)

The ground-state density $\rho(\mathbf{r})$ fixes all properties. $E[\rho]$ is minimal at the exact density:

$$\frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} = \mu$$

Kohn–Sham

$$h[\rho] = -\frac{\hbar^2}{2m}\nabla^2 + U[\rho](\mathbf{r}), \qquad h[\rho]\,\phi_i = \varepsilon_i\,\phi_i$$

$$\rho(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

Example: local two-body force

$$E[\rho] = T[\rho] + \tfrac{1}{2}\iint V(\mathbf{r},\mathbf{r}')\rho(\mathbf{r})\rho(\mathbf{r}')$$

$$= \sum_i \varepsilon_i - \tfrac{1}{2}\iint V(\mathbf{r},\mathbf{r}')\rho(\mathbf{r})\rho(\mathbf{r}')$$

- Kohn–Sham links the density to a single-particle spectrum.
- This is exactly the link the shell-correction method needs.

Strictly, Hohenberg–Kohn DFT does not exist for nuclei since there is no external potential, and the laboratory density of the exact ground state carries no structure. Nuclear DFT is mostly used as an energy density functional framework.

Perturbation expansion of the energy functional

Starting point: Given a reference density $\tilde{\rho}$, expand $E[\rho]$ as a functional Taylor series:

$$\boxed{E[\rho] = E[\tilde{\rho}] + \int \frac{\delta E}{\delta \rho(\mathbf{r})}\bigg|_{\tilde{\rho}} \big(\rho(\mathbf{r}) - \tilde{\rho}(\mathbf{r})\big) d^3r + O(\delta\rho^2)}$$

The zeroth-order term:

$$\tilde{E} = E[\tilde{\rho}] = \int t\,\tilde{\rho}(\mathbf{r})\, d^3r + \frac{1}{2}\iint V(\mathbf{r},\mathbf{r}')\tilde{\rho}(\mathbf{r})\tilde{\rho}(\mathbf{r}')\, d^3r\, d^3r'$$

This is the energy evaluated at the reference density which takes exactly the same DFT form.

Key condition on $\tilde{\rho}$:

- For higher-order terms to be negligible, $\tilde{\rho}$ cannot be arbitrary. It must be a **variational density** that remains in the neighborhood of the true ground-state density ρ.
- $\tilde{E}$ and $\tilde{\rho}$ serve as a baseline for the perturbation need not represent a real or observable physical system by itself.

The first-order correction

The first-order term is governed by the effective single-particle Hamiltonian evaluated at the reference density:

$$\tilde{h} = \left.\frac{\delta E}{\delta \rho(\mathbf{r})}\right|_{\tilde{\rho}}$$

So the first-order correction is:

$$\delta E^{(1)} = \int \left.\frac{\delta E}{\delta \rho(\mathbf{r})}\right|_{\tilde{\rho}} \big(\rho(\mathbf{r}) - \tilde{\rho}(\mathbf{r})\big)\, d^3r = \int \tilde{h}\, \delta\rho(\mathbf{r})\, d\mathbf{r}$$

Physical interpretation of $\tilde{h}$:

$$\tilde{h}[\tilde{\rho}] = t + \tilde{U}[\tilde{\rho}](\mathbf{r}), \qquad \tilde{U}[\tilde{\rho}](\mathbf{r}) = \int V(\mathbf{r}, \mathbf{r}')\tilde{\rho}(\mathbf{r}')\, d\mathbf{r}'$$

$\tilde{h}$ is the mean-field generated by the reference density. In the shell-correction context, this provides the **link between macroscopic bulk energy and microscopic shell fluctuations**.

The Strutinsky "correction": DFT form

We can now write the energy theorem in its rigorous form:

$$\boxed{E[\rho] = E[\tilde{\rho}] + \delta E^{(1)} + O(\delta\rho^2)}$$

where

- $\tilde{E}[\tilde{\rho}]$ is a **smooth functional** of the smoothed density $\tilde{\rho}$
- $\delta E^{(1)}$ captures **all oscillatory energy contributions** arising from density fluctuations about $\tilde{\rho}$, and consequently from the discrete single-particle spectrum of $\tilde{h}$
- $O(\delta\rho^2)$ is generally negligible

This simple expansion provides a rigorous mathematical foundation for evaluating the shell correction. It establishes a formal link between a self-consistent DFT calculation and the **phenomenology** (empirical studies on the decomposition)

But it is still not of practice use so far as we don't really know how to calculate $E[\tilde{\rho}]$ or $\delta E^{(1)}$

Orbital-level decomposition

Let the reference density be generated by a set of reference orbitals $\{\phi_i^0\}$:

$$\tilde{\rho}(\mathbf{r}) = \sum_i |\phi_i^0(\mathbf{r})|^2$$

Solving $\tilde{h}[\tilde{\rho}]$ yields a **new set** of eigenstates and eigenvalues:

$$\tilde{h}[\tilde{\rho}]|\phi_i^1\rangle = \varepsilon_i^1|\phi_i^1\rangle, \qquad \rho^1(\mathbf{r}) = \sum_i |\phi_i^1(\mathbf{r})|^2$$

The density variation is:

$$\delta\rho(\mathbf{r}) = \rho^1 - \tilde{\rho} = \sum_i \left[|\phi_i^1|^2 - |\phi_i^0|^2\right]$$

Key assumption: $\delta\rho$ is **small** — $\tilde{\rho}$ is a reasonable approximation to the true ground-state density.

Note on self-consistency:

We are generally *not* at self-consistency: ϕ_i^0 are not eigenstates of $\tilde{h}[\tilde{\rho}]$ in general.

Self-consistency is recovered only when $\phi_i^1 = \phi_i^0$ and $\rho^1 = \tilde{\rho} = \rho$.

Evaluating the first-order term explicitly

Substituting the orbital expansion into $\delta E^{(1)}$:

$$\delta E^{(1)} = \sum_i \int \tilde{h}[\tilde{\rho}] \left[\phi_i^{1*}\phi_i^1 - \phi_i^{0*}\phi_i^0\right] d\mathbf{r} = \sum_i \left[\langle\phi_i^1|\tilde{h}|\phi_i^1\rangle - \langle\phi_i^0|\tilde{h}|\phi_i^0\rangle\right]$$

The first term gives SP energies $\{\varepsilon_i^1\}$ by construction. For the second term, expand $|\phi_i^0\rangle$ in the eigenbasis of $\tilde{h}$:

$$|\phi_i^0\rangle = \sum_j c_{ij}|\phi_j^1\rangle, \quad c_{ij} = \langle\phi_j^1|\phi_i^0\rangle \implies \langle\phi_i^0|\tilde{h}|\phi_i^0\rangle = \sum_j |c_{ij}|^2 \varepsilon_j^1$$

- This is a **weighted average** of eigenvalues ε_j^1. As $\tilde{\rho}$ approaches the self-consistent solution: $\phi_i^0 \approx \phi_i^1$, so $|c_{ij}|^2 \approx \delta_{ij}$ — and $\delta E^{(1)} \to 0$ as required.
- The conventional "shell correction" = first-order functional derivative correction governed by $\tilde{h}$
- "Smoothness" is redefined as a **density property**, not a spectral one
- Phenomenological potentials are given rigorous justification

A new perspective on nuclear DFT

The first-order correction:

$$\delta E^{(1)} = \sum_i \varepsilon_i^1 - T[\tilde{\rho}] - \int \tilde{U}[\tilde{\rho}](\mathbf{r})\tilde{\rho}(\mathbf{r})\, d\mathbf{r}$$

Substituting $\delta E^{(1)}$ into $E[\tilde{\rho}]$:

$$E[\rho'] = \underbrace{T[\tilde{\rho}] + V[\tilde{\rho}]}_{\tilde{E}[\tilde{\rho}]} + \sum_i \varepsilon_i^1 - T[\tilde{\rho}] - \int \tilde{U}[\tilde{\rho}]\tilde{\rho}\, d\mathbf{r}$$

$$\boxed{E[\rho'] = \sum_i \varepsilon_i^1 + V[\tilde{\rho}] - \int \frac{\delta V}{\delta \tilde{\rho}(\mathbf{r})}\tilde{\rho}(\mathbf{r})\, d\mathbf{r}}$$

Remarkable simplification: The kinetic energy functional $T_s[\tilde{\rho}]$ **cancels exactly**. The total energy depends only on:

1. The single-particle eigenvalues $\{\varepsilon_i^1\}$ — computable from any mean-field potential
2. The interaction functional $V[\tilde{\rho}]$ — the target for machine learning
3. Its functional derivative — automatically obtained from the variational structure

Future Applications: Energy Functional, Pairing and Fission

Learning $V[\rho]$ from data

$$V_\theta[\rho] = \int \mathcal{F}_\theta\big(\rho, \nabla\rho, \nabla^2\rho, \ldots\big)\, d\mathbf{r}, \qquad \tilde{U} = \frac{\delta V_\theta}{\delta \rho}$$

$$\mathcal{L}(\theta) = \sum_{A,Z} \big(E_\theta^{A,Z} - E_{\text{exp}}^{A,Z}\big)^2$$

Symbolic regression (PySR) gives explicit expressions. Energy and potential are consistent by construction.

Potential energy/Fission barriers

$$E(q) = E[\tilde{\rho}_q] + \sum_i \varepsilon_i^1(q) - \int \tilde{h}_q\, \tilde{\rho}_q\, d\mathbf{r} + O(\delta\rho^2)$$

q: elongation, asymmetry, neck. $\tilde{\rho}_q$ is the smooth density constrained to shape q. One functional from ground state to scission.

Pairing in the spectrum of $\tilde{h}$

$$H_{\text{pair}} = \sum_i \varepsilon_i^1 \big(a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}\big) - G \sum_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

$$E \approx E[\tilde{\rho}] + E_0\big(\{\varepsilon_i^1\}, G\big) - \int \tilde{h}\, \tilde{\rho}\, d\mathbf{r}$$

E_0 replaces $\sum_i \varepsilon_i^1$. It is the exact ground-state energy (diagonalization, Richardson) or the particle-number-projected BCS/HFB energy. Formal basis: reduced density matrix functional theory, $\rho \to \gamma$. Open point: the smooth pairing part of $E[\tilde{\rho}]$.

Summary

The Strutinsky shell-correction method, despite its remarkable empirical success for six decades, has lacked a rigorous theoretical foundation. This work provides that foundation through density functional theory.

Theorem:

$$E[\rho'] = \tilde{E}[\tilde{\rho}] + \sum_i \varepsilon'_i - \int \tilde{h}\,\tilde{\rho}\,d\mathbf{r} + O(\delta\rho^2)$$

The decomposition is exact to first order in $\delta\rho = \rho - \tilde{\rho}$.

Reinterpretation:

- The shell energy is governed by the mean field $\tilde{h}$ generated by the smooth reference density — not by the smoothed level density $\tilde{g}(\varepsilon)$.
- One can state that the **Shell correction** is a fundamentally wrong concept.

Outlook:

- Variational, ML-driven construction of the nuclear DFT functional $V_\theta[\rho]$;
- Extension to pairing and second order correction
- Potential energy and fission barrier.

Thank you!!谢谢！