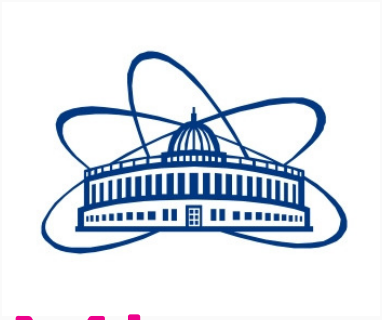



Microscopic-Macroscopic Models

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July, 2026

Joint Institute for Nuclear Research

Outline

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Macroscopic Model

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Wigner-Kirkwood Shell Corrections

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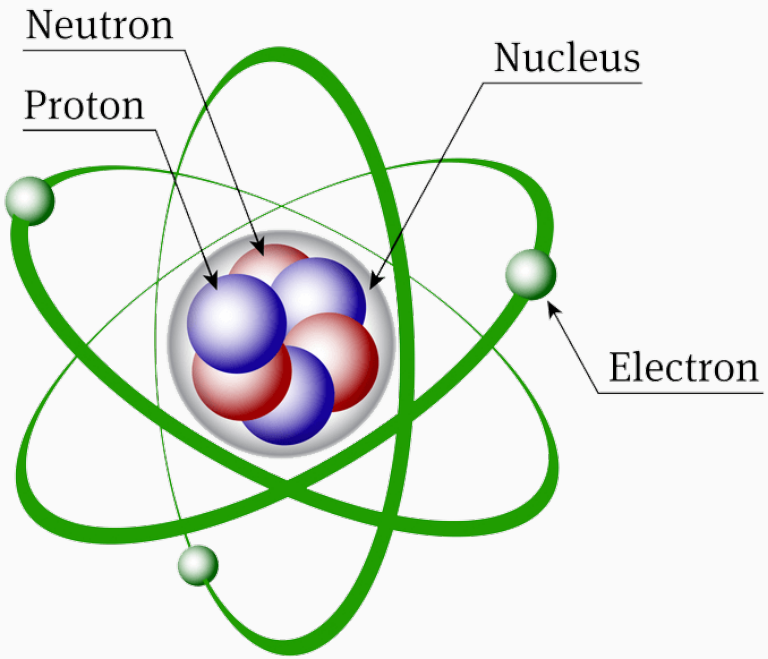
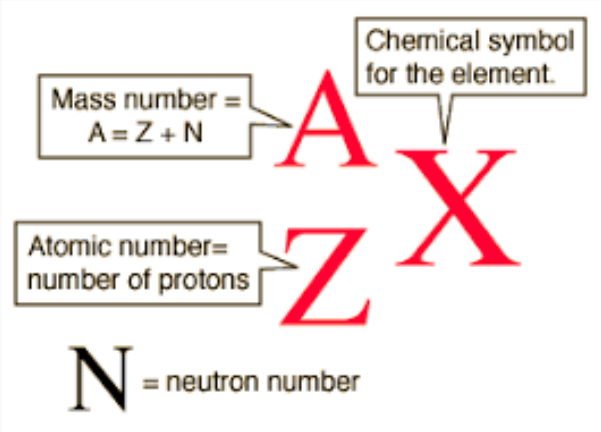
Mic-Mac vs Self-Consistent Mean-Field Models

Finite-Temperature PES

Introduction

Atomic nucleus





$M_p = 938.27\ \mathrm{MeV/c^2}$

$M_n = 939.56\ \mathrm{MeV/c^2}$

$M_e = 0.511\ \mathrm{MeV/c^2}$

Atom:

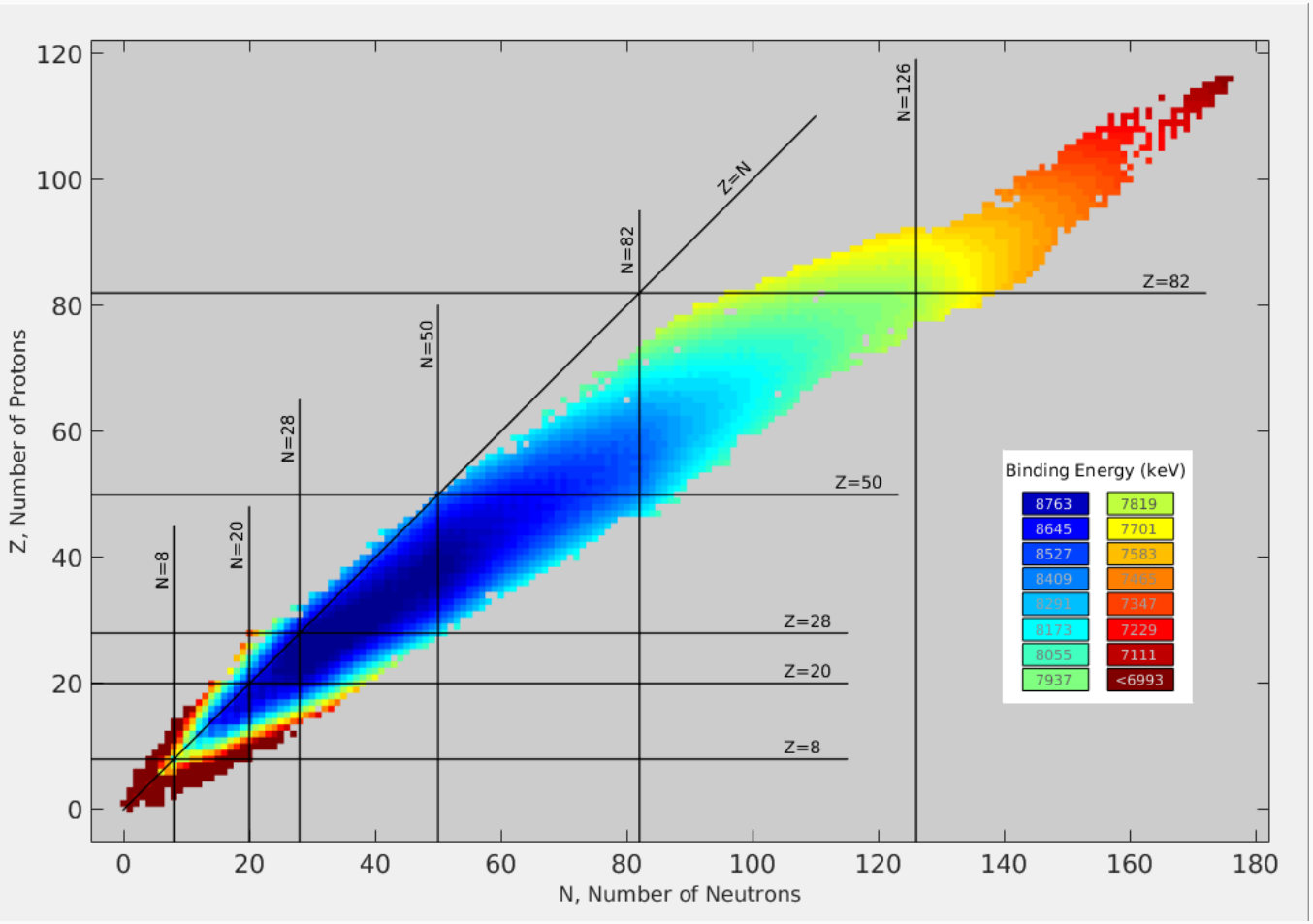
- Typical size $\sim 10^{-10}$ m (Å)
- Typical energies $\sim$ eV

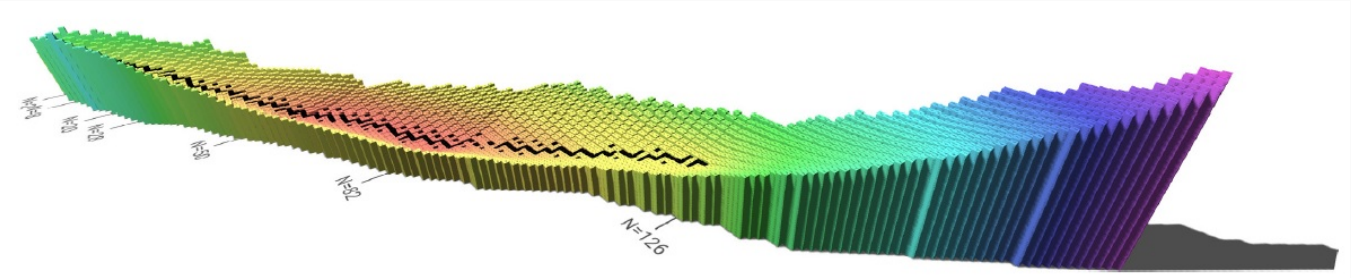
Nucleus:

- Typical size $\sim 10^{-15}$ m (fm)
- Typical energies $\sim$ MeV=10^6 eV

Binding energy: $B(Z,A) = N \times M_n + Z \times M_p - M(Z,A)$

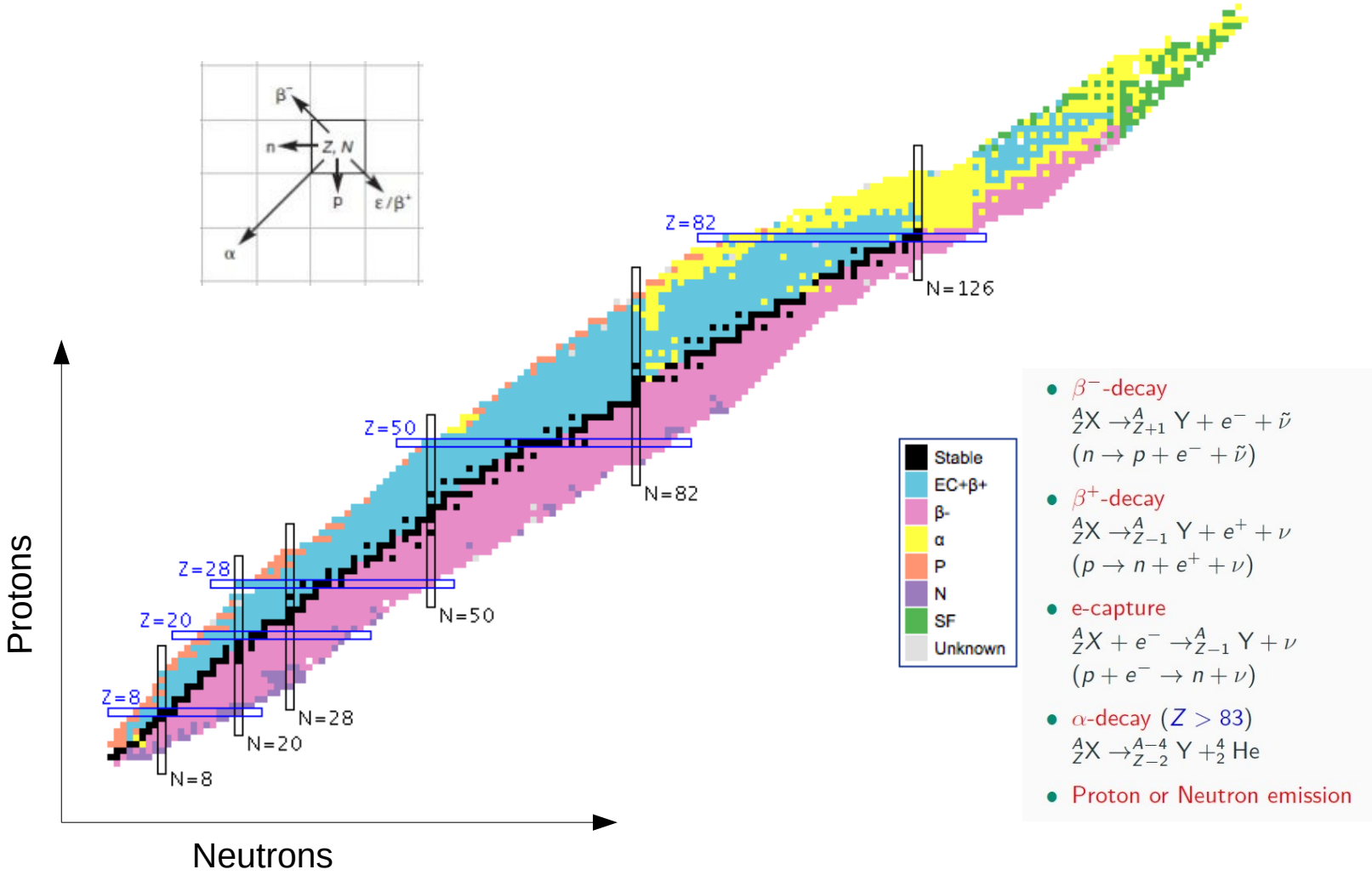
Nuclear chart





Spontaneous nuclear decay reactions

Nuclear decay reactions are spontaneous and occur at random, meaning that one cannot know exactly when or which radioactive nucleus will decay.



- β^--decay
  ${}^A_Z\mathrm{X} \rightarrow {}^A_{Z+1}\mathrm{Y} + e^- + \tilde{\nu}$
  $(n \rightarrow p + e^- + \tilde{\nu})$
- β^+-decay
  ${}^A_Z\mathrm{X} \rightarrow {}^A_{Z-1}\mathrm{Y} + e^+ + \nu$
  $(p \rightarrow n + e^+ + \nu)$
- e-capture
  ${}^A_Z\mathrm{X} + e^- \rightarrow {}^A_{Z-1}\mathrm{Y} + \nu$
  $(p + e^- \rightarrow n + \nu)$
- α-decay $(Z > 83)$
  ${}^A_Z\mathrm{X} \rightarrow {}^{A-4}_{Z-2}\mathrm{Y} + {}^4_2\mathrm{He}$
- Proton or Neutron emission

Nuclear models

"If binding energy determines stability, then the central question of nuclear structure is: Can we predict nuclear masses across the entire nuclear chart?"

Macroscopic-Microscopic models (Mic-Mac)

- One of the most successful approaches for predicting nuclear masses is the **Microscopic-Macroscopic (mic-mac) model**.
- Historically, its development can be understood in three stages:
  1. First, a purely **macroscopic** description was developed to reproduce the overall trend of measured nuclear masses.
  2. Later, **microscopic** corrections were introduced to explain the delicate effects that the macroscopic picture alone could not capture.
  3. Finally, both the macroscopic and microscopic ingredients were continuously refined, leading to the modern combined mic-mac models used today.

Macroscopic Model

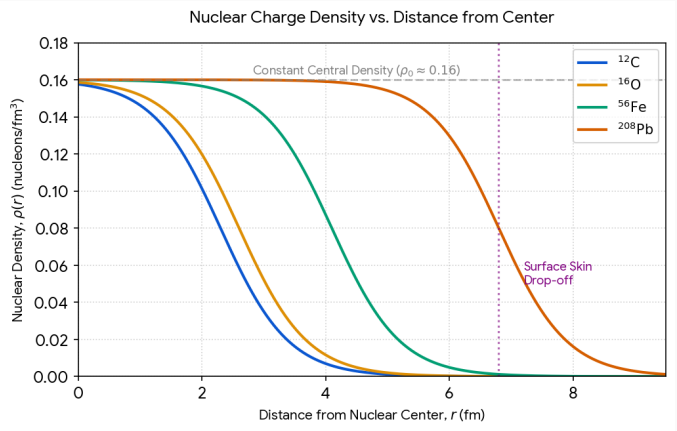
The Macroscopic Era: 1930s & The Liquid Drop Model

- **Experimental Clue:**

Nuclear radii were found to obey

$$R = r_0 A^{1/3},$$

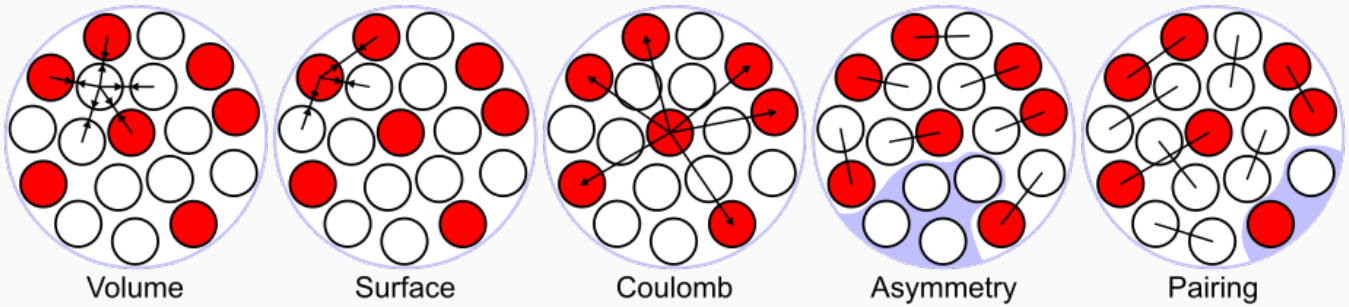
implying that the nuclear volume is proportional to A and the density is approximately constant.



- **Macroscopic Interpretation:** These observations suggested that nuclei behave like droplets of an incompressible quantum fluid.
- **The First Mass Model:** Based on this picture, Bethe and Weizsäcker developed the semi-empirical mass formula to reproduce the smooth trends of nuclear masses and binding energies.

The liquid-drop picture became the foundation of all later macroscopic models.

1935: Bethe–Weizsäcker Semi-Empirical Mass Formula



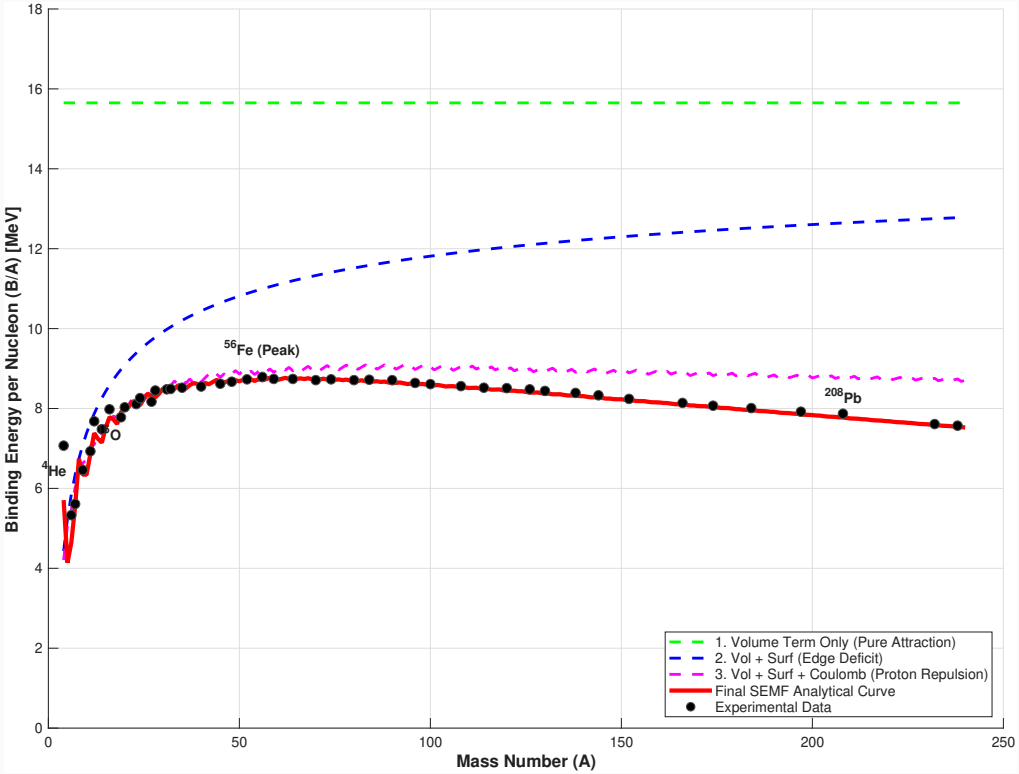
$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta(A,Z)$$

- **Volume Term ($a_V A$):** Uniform attractive energy from bulk nucleons.
- **Surface Term ($a_S A^{2/3}$):** Penalty for surface nucleons with fewer neighbors.
- **Coulomb Term (a_C):** Electrical repulsion between protons.
- **Asymmetry Term:** Penalty for neutron-proton imbalance.
- **Pairing Term (δ):** Extra stability boost for Even-Even nuclei.

Adjusted Coefficients:

- $a_V = 15.8$ MeV
- $a_S = 18.3$ MeV
- $a_C = 0.71$ MeV
- $a_A = 23.2$ MeV
- $\delta = \pm 11.2, 0$ MeV

Wigner term: $(E_W \propto |N-Z|)$ to force the model to capture the sharp, extra stability observed at $Z = N$.



From Liquid Drop to Shells: A New Hint

- The Bethe–Weizsäcker formula was remarkably successful: with only five terms, it reproduces the smooth global trend of nuclear binding energies to good accuracy.
- Some discrepancies could still be absorbed into the model by **parametrization**:
  - Pairing, asymmetry, and Wigner terms are all smooth corrections, fitted with one additional constant.

⇒ **Magic numbers ($N, Z = 2, 8, 20, 28, 50, 82, 126$) could not be reproduced this way.**

- Unlike pairing or asymmetry, magic numbers are not a smooth trend — they are sharp, localized jumps in stability at specific N or Z.
- Smooth correction term cannot reproduce sharp local peaks.

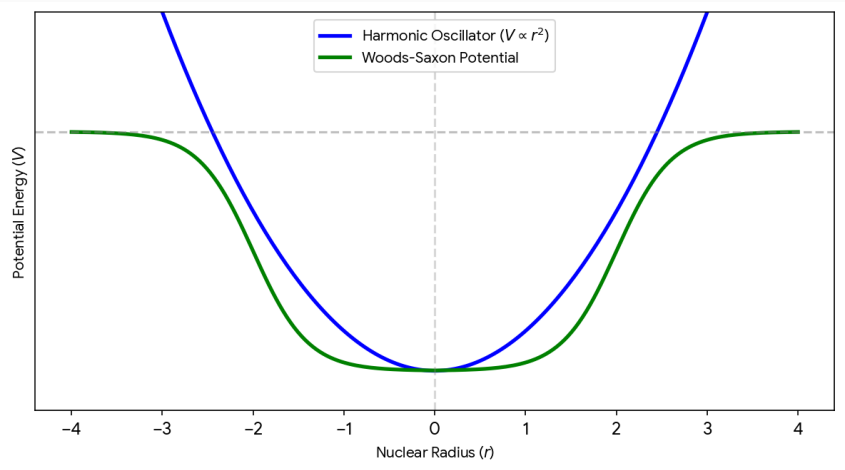
⇒ **Hypothesis:** nucleons, like electrons, might be arranged in discrete energy shells.

If true, nucleons should move in quantized orbits within an **average nuclear potential**.

Microscopic Models

The Nuclear Shell Model: Mean Field + Spin-Orbit

- **Mean-field idea:** Each nucleon moves independently in an average potential generated by all other nucleons (e.g. Woods–Saxon potential).
- A simple central potential reproduces only the first magic numbers reasonably well $(2, 8, 20)$, but fails for heavier nuclei due to incorrect level ordering.



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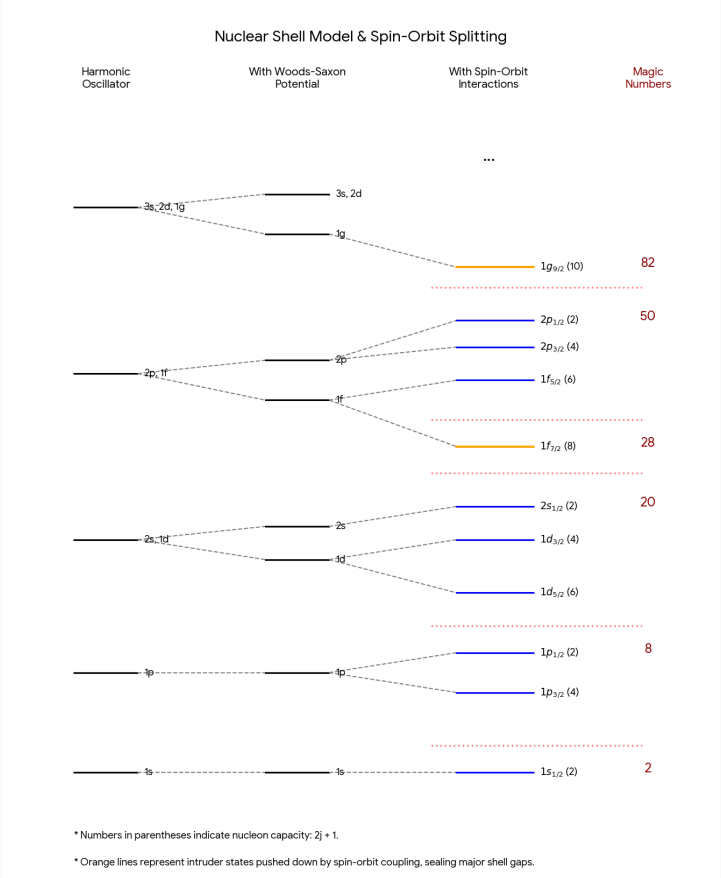
- A simple central potential reproduces only the first magic numbers reasonably well $(2, 8, 20)$, but fails for heavier nuclei due to incorrect level ordering.
- **Key breakthrough (Mayer & Jensen, 1949):** The inclusion of a strong **spin–orbit interaction** reorganizes the single-particle spectrum and produces the correct shell gaps.



$\Rightarrow$ All magic numbers are correctly reproduced $(28, 50, 82, 126)$.

The shell model succeeds exactly where the liquid-drop picture fails.

The Shell Model's Limitations

1. **The Absolute Energy Problem:** Simply summing the single-particle energies does **not** yield the total nuclear binding energy. It completely misses bulk saturation and overcounts interactions.
2. **The Shape Puzzle:**
   - Experimental data on nuclear γ-emissions revealed that many excited states display pure **rotational bands**.

   $\rightarrow$ Quantum mechanics dictates that a spherical ground state cannot have a permanent rotational band.

   $\rightarrow$ **Conclusion:** Many nuclei must have permanently **deformed ground states**.
   - **Macroscopic View (Liquid Drop):** Surface tension natively forces the nucleus to minimize its surface area $\rightarrow$ **Favors a spherical shape**.

The shell model gets local quantum structure right, but the absolute energy scale wrong.

Combining the Two: Birth of Mic-Mac model

- The natural idea: keep the macroscopic (liquid drop) energy for the smooth bulk trend, and add a microscopic **correction** for shell effects.
- This correction should capture only the **oscillating part** of the shell-model energy — not its absolute value.
- Early concrete realizations of this idea (e.g. **Seeger, 1961/1968**) combined the liquid drop with shell and deformation energies from the Nilsson model and BCS pairing.
- A systematic recipe for extracting this shell correction was later formalized by **Strutinsky (1967)**.

Strutinsky's Shell Correction

Splitting the Energy: Smooth + Oscillating

- The total energy of a nucleus can be separated into two physically distinct pieces:

$$E_{\text{total}} = \underbrace{\tilde{E}}_{\text{smooth, average}} + \underbrace{\delta E}_{\text{oscillating, shell}}$$

- $\tilde{E}$: the slowly varying trend with A — well approximated by the **liquid drop model**.
- δE: the local bunching/depletion of levels near the Fermi surface — the **shell effect**.

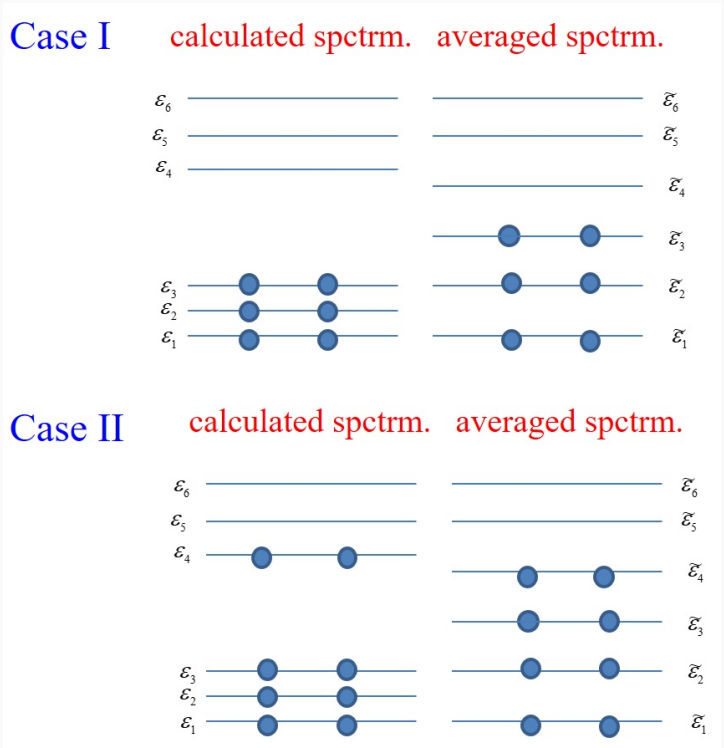


V. M. Strutinsky

Strutinsky's insight: calculate each part from the model best suited to it.

Strutinsky's Prescription (1967)

- Take the discrete single-particle spectrum ε_i from a shell-model (mean-field) calculation.
- Compute the actual summed energy $E_{\text{shell}} = \sum_i \varepsilon_i$.
- **Smooth** the level density $g(\varepsilon)$ over an energy window, replacing sharp levels with a smooth average $\tilde{g}(\varepsilon)$.
- From $\tilde{g}(\varepsilon)$, compute the smoothed energy $\tilde{E}$: $\delta E = E_{\text{shell}} - \tilde{E}$



$$E_{calc} - E_{av} < 0$$

Binding energy is increased due to shell structure

$$E_{calc} - E_{av} > 0$$

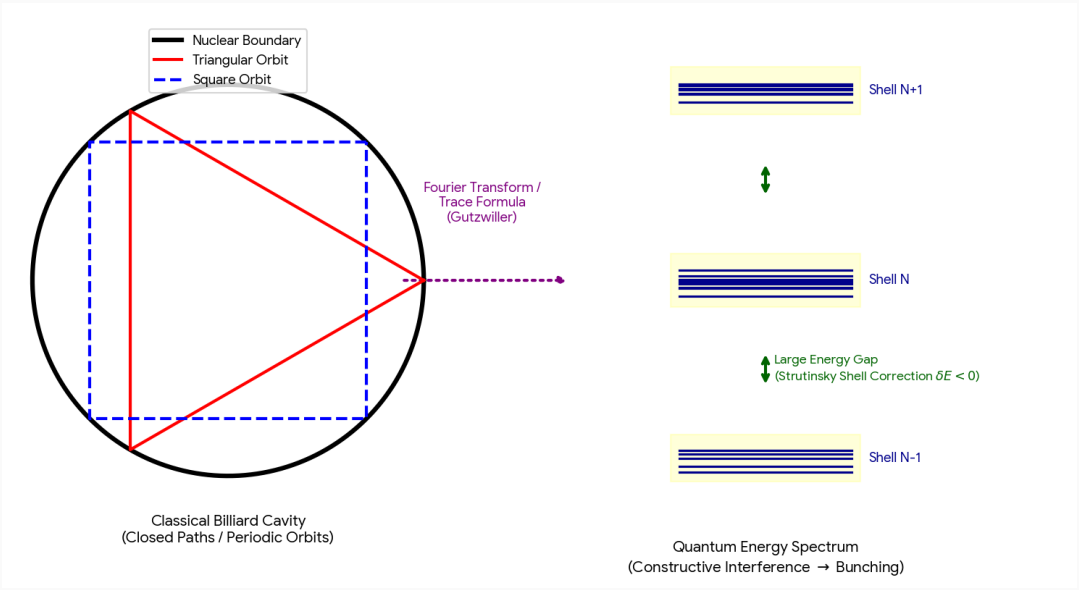
Binding energy is decreased due to shell structure

The Idea: A Nucleon as a Billiard Ball

- Picture a nucleon moving quasi-classically inside the nuclear mean-field potential — much like a ball bouncing inside a cavity (a **billiard**).
- Certain trajectories **close on themselves**: periodic orbits.
- These closed orbits cause constructive interference in the quantum spectrum $\Rightarrow$ **bunching of single-particle levels**.

$\Rightarrow$ **Shell structure is the quantum signature of classical periodic orbits.**

- This semiclassical picture (Gutzwiller; extended by Strutinsky) explains *why* the single-particle level density oscillates rather than being smooth.



The Deeper Foundation: Balian–Bloch & Gutzwiller

- **Balian & Bloch (1970–72):** studied quantum waves confined in a cavity (finite potential well) of arbitrary shape (a quantum billiard).
  - The smoothed level density depends only on simple geometric quantities: volume, surface area, curvature.
  - The leftover **oscillating part** can be written as a sum over **classical periodic orbits** inside the cavity.
- **Gutzwiller (1971):** independently derived the general semiclassical trace formula linking a quantum spectrum to the periodic orbits of its classical counterpart.

Strutinsky discussed his method with Balian and Bloch at Saclay — this is how the "billiard" picture became the rigorous justification for the shell-correction method.

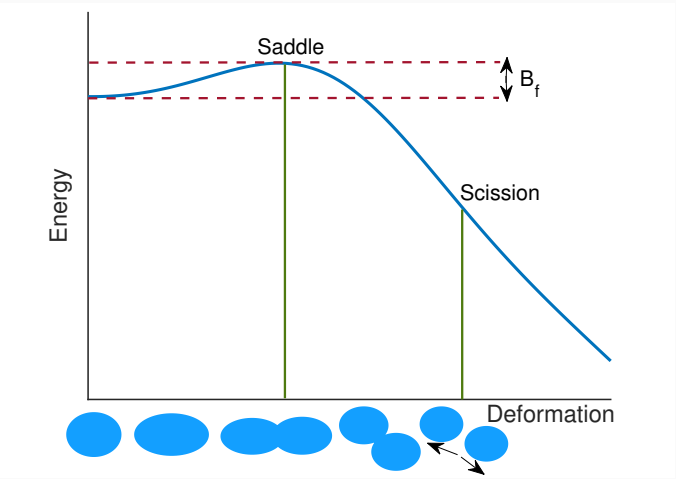
R. Balian, C. Bloch, *Ann. Phys.* **60**, 401 (1970); **69**, 76 (1972).
M. C. Gutzwiller, *J. Math. Phys.* **12**, 343 (1971).
Historical note: *Vilen Mitrofanovich Strutinsky's impact on nuclear and many particle physics*, arXiv:1006.5539.

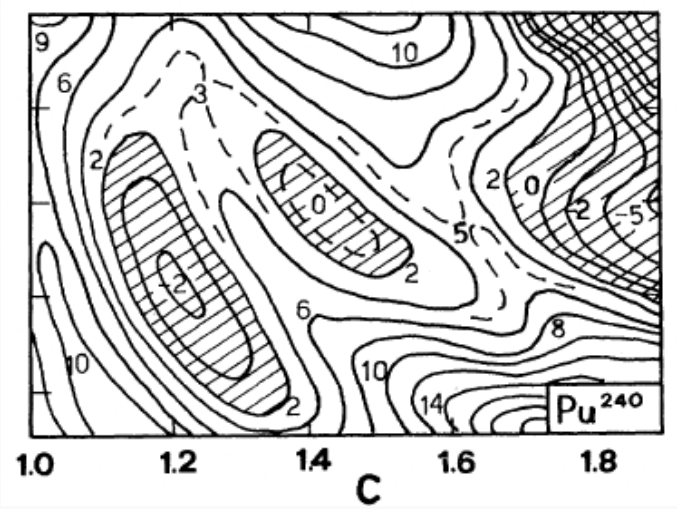
REVIEWS OF MODERN PHYSICS VOLUME 44, NUMBER 2 APRIL 1972

Funny Hills: The Shell-Correction Approach to Nuclear Shell Effects and Its Applications to the Fission Process

M. BRACK,* JENS DAMGAARD, A. S. JENSEN, H. C. PAULI,* V. M. STRUTINSKY,† C. Y. WONG‡
The Niels Bohr Institute, University of Copenhagen, Denmark

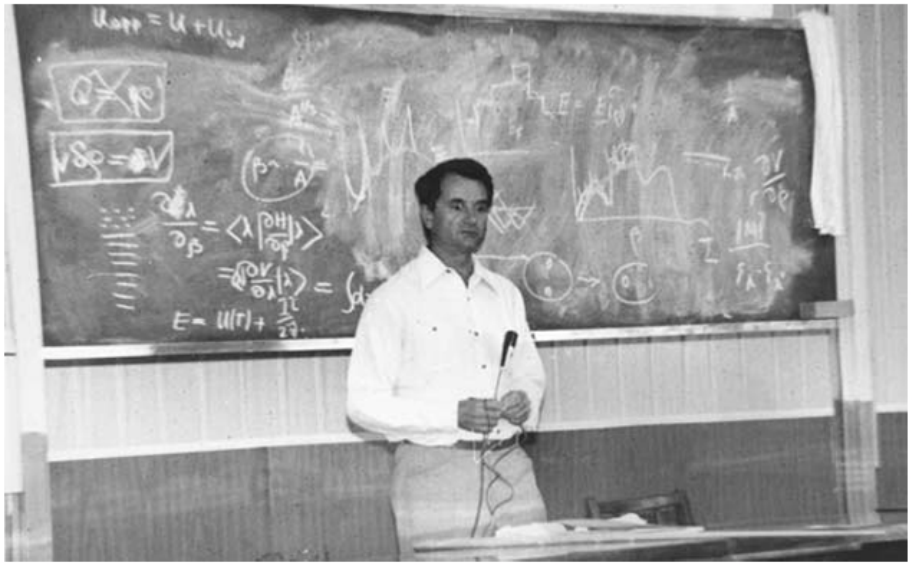
This paper reviews various results related to the single-particle structure in spherical and deformed nuclei, discussed from the viewpoint of the so-called shell-correction method. This method stresses the importance of large-scale nonuniformities in the energy distribution of the individual particles especially near the Fermi energy. The way in which these nonuniformities affect in an essential way many nuclear properties, such as the shape stiffness, the spatial density distribution, the total mass of the nucleus, the mass and inertia of the nuclear shape variations, etc. is also discussed. Against this background, the behavior of the nuclear deformation energy is described, in particular for larger distortions relevant to the fission process. In this connection, some qualitative singularities of the phenomenological liquid-drop deformation energy at large shape distortions are pointed out, and their possible implications for fission are discussed. As the problems considered cover a wide range of nuclear properties, this paper is not a review in the narrow sense of the word. Comparison with other approaches as well as historic references are given mainly to clarify specific points, because a complete review would be a monumental undertaking.





The results of this activity at the NBI were published in 1972 in a review article [2] which, upon Strutinsky's insistence (against the resistence of the editors), bears the title *"Funny Hills: The Shell-Correction Approach to Nuclear Shell Effects and Its Applications to the Fission Process"*. This title is characteristic of Strutinsky's humour which I came to like — in spite of the huge respect and fear which I initially had of him as a young student.

The following picture [3] was taken in 1972, on which he looks as I remember him from those years of scientific education and collaboration.



Report on the International School on Nuclear Structure, 1972

Vilen Mitrofanovich Strutinsky's impact on nuclear and many particle physics, arXiv:1006.5539.

The Smoothing Function

"Funny Hills," **Rev. Mod. Phys. 44, 320 (1972).**

$$E = \sum_i \varepsilon \delta(\varepsilon - \varepsilon_i) \longrightarrow \tilde{E} = \int_{-\infty}^{\tilde{\lambda}} \varepsilon\, \tilde{g}(\varepsilon)\, d\varepsilon, \qquad N = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\varepsilon)\, d\varepsilon.$$

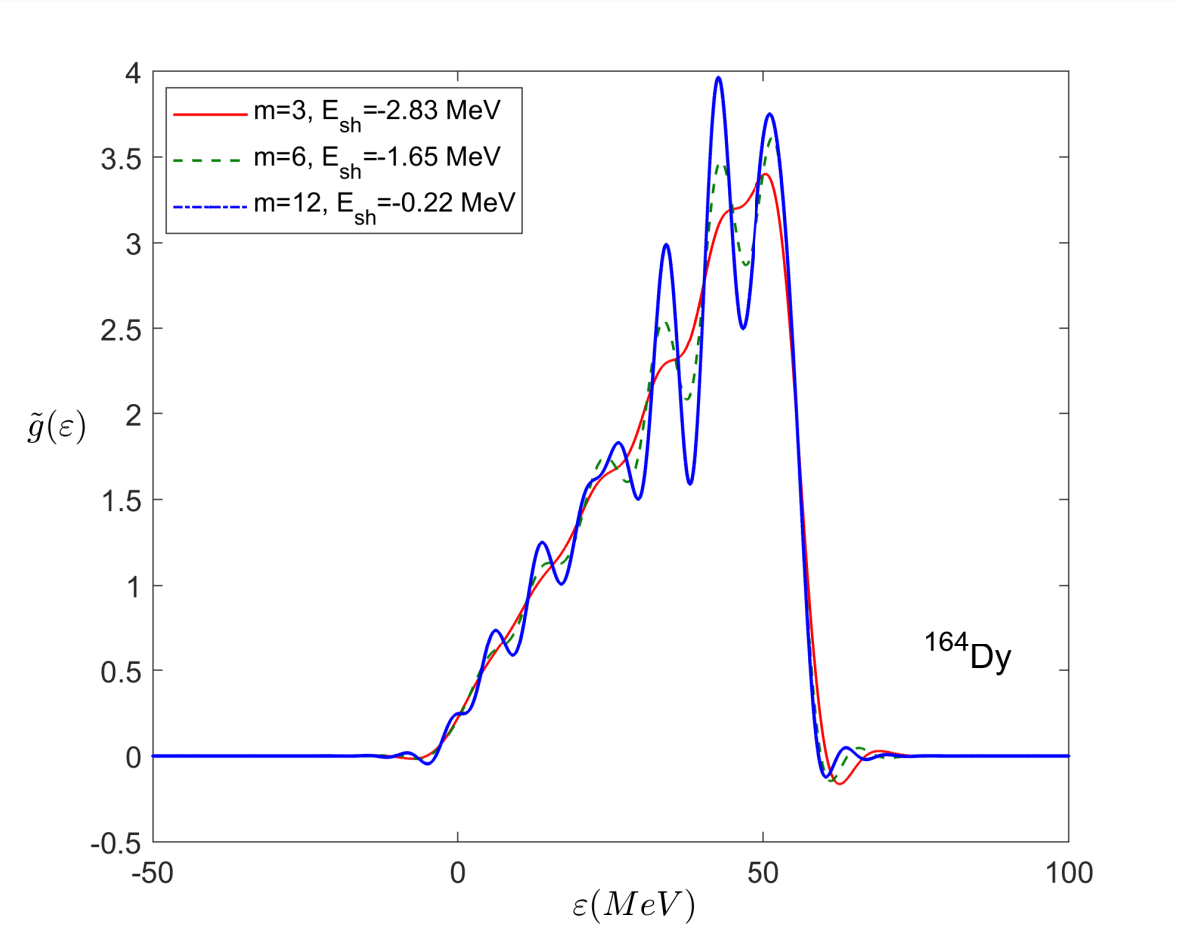
- To extract $\tilde{E}$, Strutinsky replaced each discrete level e_i by a smeared-out Gaussian of width γ:

$$\tilde{g}(\varepsilon) = \frac{1}{\gamma} \sum_i f\left(\frac{\varepsilon - \varepsilon_i}{\gamma}\right)$$

- A pure Gaussian alone is not quite enough—it slightly distorts the smooth trend.
- **A curvature correction** is added using Hermite polynomials H_{2n}:

$$f(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} \sum_{n=0}^{M} a_n H_{2n}(x)$$

- **The averaging width** γ is chosen so that $\tilde{E}$ becomes **insensitive to its exact values**—a stable "plateau" region.



$$E_{mic} = \delta E_{shell} + \delta E_{pair}$$
$$\delta E_{pair} = E_{pair} - \tilde{E}_{pair}$$
$$E_{pair} = E_{BCS} - E_{BCS}^{\Delta=0}$$
$$\tilde{E}_{pair} = \tilde{E}_{BCS} - \tilde{E}_{BCS}^{\Delta=0}$$

The Plateau Condition: Is the Result Physical?

The Strutinsky method introduces technical parameters:

- smoothing width $\gamma \approx \hbar\omega_0$
- curvature correction order $M = 6$

This raises a natural question:

Does the shell correction depend on these arbitrary choices?

The key requirement is that physical results must be stable:

$$\frac{d\,\delta E_{\text{shell}}}{d\gamma} \approx 0, \qquad \frac{d\,\delta E_{\text{shell}}}{dM} \approx 0$$

- The region where this stability is observed is called the **plateau region**.

The plateau condition ensures that shell effects are physical, not an artifact of smoothing.

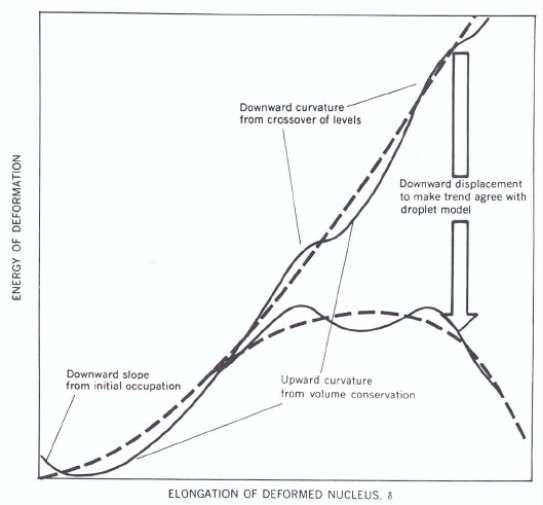
What Did the Shell Correction Achieve?

The introduction of microscopic shell effects on top of the macroscopic energy led to several major breakthroughs in nuclear structure:

$\Rightarrow$ The total binding energy in the **mic-mac** approach:

$$E_{\text{total}}(\text{shape}) = E_{\text{LDM}}(\text{shape}) + \delta E_{\text{shell}}(\text{shape}) + \delta E_{\text{pairing}}(\text{shape})$$

- **Magic numbers:** The observed extra stability at $N, Z = 2, 8, 20, 28, 50, 82, 126$ is naturally explained by shell gaps in the single-particle spectrum.
- **Deformed ground states:** Many nuclei are not spherical because deformation can lower the shell-correction energy, making non-spherical shapes energetically favorable.



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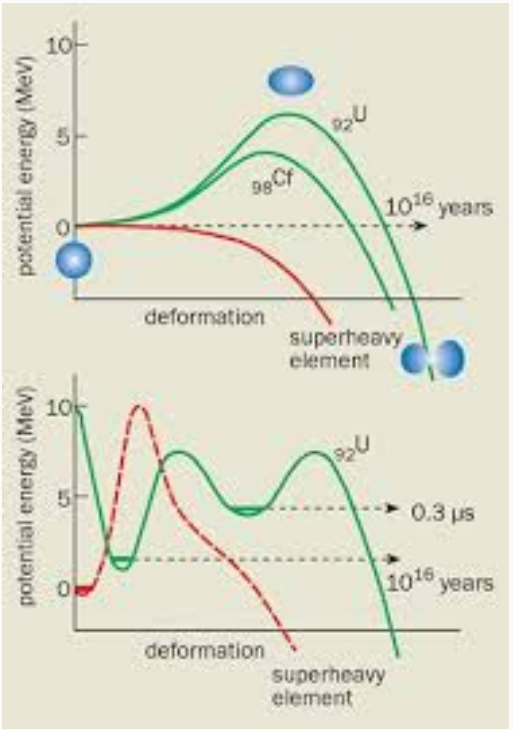
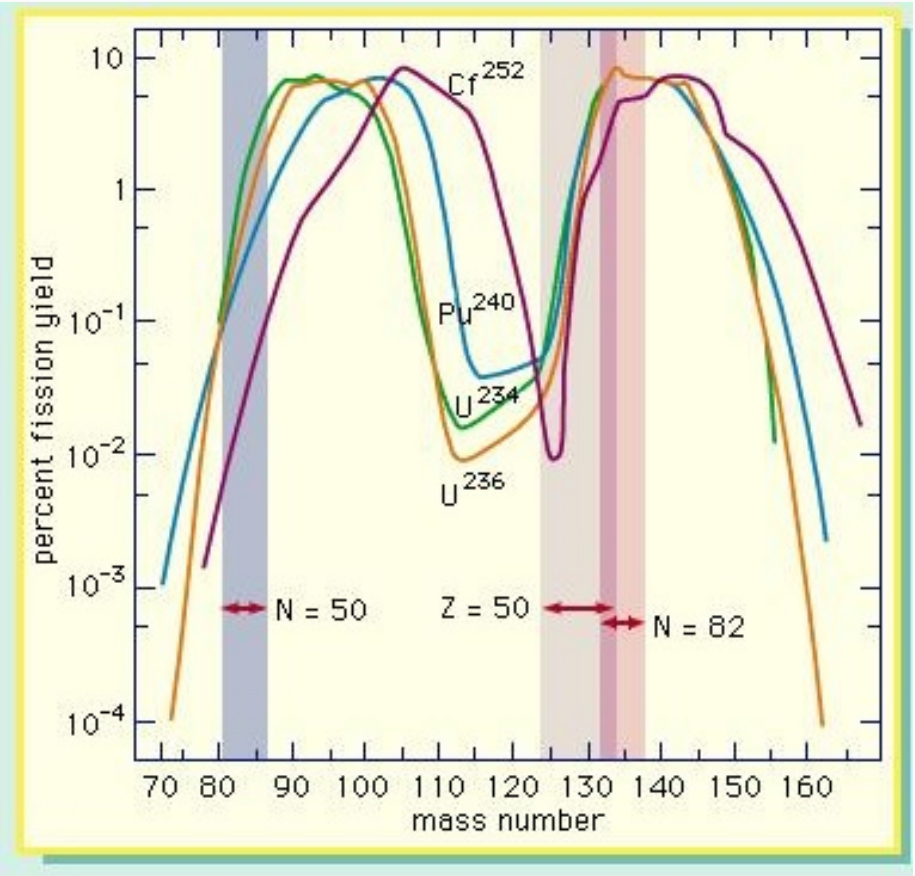
- **Magic numbers:** The observed extra stability at $N, Z = 2, 8, 20, 28, 50, 82, 126$ is naturally explained by shell gaps in the single-particle spectrum.
- **Deformed ground states:** Many nuclei are not spherical because deformation can lower the shell-correction energy, making non-spherical shapes energetically favorable.

- **Stability of heavy & superheavy nuclei:** Even though the macroscopic energy gives a fission barrier that can be very small or vanish in superheavy region, shell pockets create additional binding that physically stabilizes them.
- **Shape isomers:** Shell corrections can create a **second potential well** at large deformations, trapping the nucleus in a highly elongated, metastable isomeric state.



What Did the Shell Correction Achieve?

- Asymmetric mass/charge distributions of fission fragments



The light mass group shifts to higher masses as the mass of fissioning nucleus increases, while the heavy group remains nearly stationary. The shaded areas show the location of closed shells of 50 protons, 50 neutrons, and 82 neutrons.

Wigner-Kirkwood Shell Corrections

An Analytic Alternative: Wigner–Kirkwood Shell Corrections

- The goal is exactly the same as in the Strutinsky method but the smooth energy $\tilde{E}$ is obtained **analytically**, rather than by smoothing discrete levels.
- Instead of averaging the spectrum with $\tilde{g}$, the quantum partition function $Z(\beta) = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right)$ is expanded around its classical (Thomas–Fermi) limit as a power series in $\hbar$:

$$Z(\beta) \xrightarrow{\hbar\text{-expansion}} Z_{\mathrm{WK}}(\beta) \xrightarrow{\text{formal inverse Laplace}} g_{\mathrm{WK}}(E) \;\to\; \tilde{E}_{\mathrm{WK}}$$

$$\boxed{\tilde{E}_{\mathrm{WK}} = E^{(0)}_{\mathrm{TF}} + \hbar^2 E^{(2)} + \hbar^4 E^{(4)} + \cdots}$$

- Since the expansion contains only smooth functions of the potential, shell oscillations never appear in $\tilde{E}_{\mathrm{WK}}$.
- The shell correction is then obtained exactly as before:

$$\delta E_{\mathrm{shell}} = E - \tilde{E}_{\mathrm{WK}}.$$

A. Bhagwat *et al.*, Eur. Phys. J. A **59**, 299 (2023).

Comparison with Strutinsky

The quantum corrections depend explicitly on spatial derivatives of the mean-field potential:

$$E^{(2)},\, E^{(4)} \;\propto\; \nabla V,\; \nabla^2 V,\; (\nabla V)^2,\; \ldots$$

- $E^{(0)}_{\mathrm{TF}}$ describes the smooth bulk (volume) energy.
- Higher-order $\hbar$ corrections naturally generate surface and curvature contributions.
- The method therefore connects naturally with the macroscopic liquid-drop expansion.

Compared with Strutinsky:

- No smoothing width γ or polynomial order M.
- No plateau condition is required.
- Particularly reliable for very deformed nuclear shapes, where the Strutinsky plateau may become difficult to obtain.
- Requires analytical derivatives of the mean-field potential, making the implementation more involved.

Limitations of the Wigner–Kirkwood approach

Although conceptually elegant, the WK expansion has practical limitations:

- **Requires smooth mean-field potentials** $\rightarrow$ accuracy depends strongly on the differentiability of $V(\mathrm{r})$
- **Truncated $\hbar$ expansion** $\rightarrow$ only a finite number of semiclassical corrections can be included $\rightarrow$ may be less reliable in strongly quantal regimes
- **Algebraic complexity** $\rightarrow$ higher-order terms involve many spatial derivatives of V $\rightarrow$ becomes cumbersome for realistic deformed nuclei

WK is elegant and parameter-free, but less practical in large-scale applications compared to Strutinsky.

Applications of mic-mac models to fission

- **Parametrization of Nuclear Shape:**

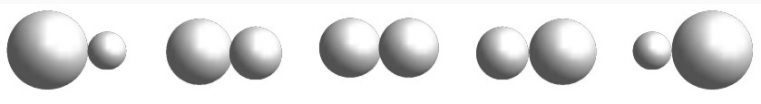
  $R(\theta,\phi) = c_{\text{vol}} R_0 \left[1 + \sum_{\lambda=2}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{+\lambda} \alpha^*_{\lambda,\mu} Y_{\lambda,\mu}(\theta,\phi)\right]$

  Where c_{vol} ensures volume conservation for any given deformation.

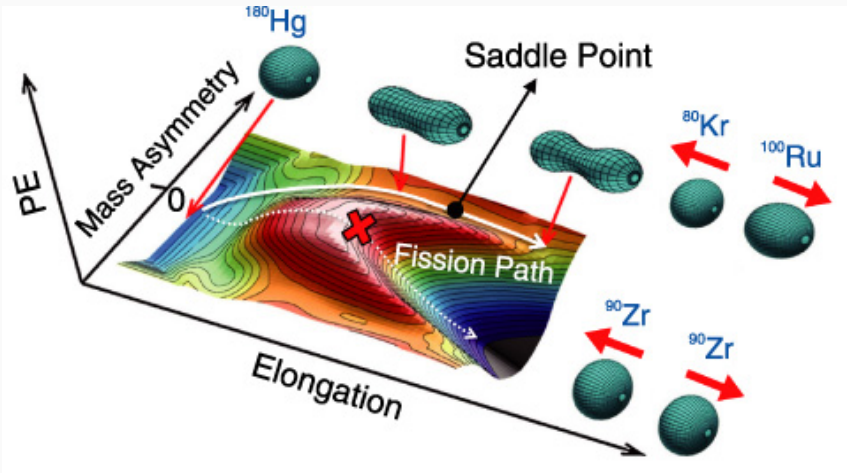
- **Potential Energy Surface (PES):** Calculated as a function of collective deformation parameters ($\beta_{\lambda,\mu}$).
  - **Elongation** (Quadrupole deformation, β, β_2, α_{20}, etc.)



  - **Asymmetry** (Octupole deformation, β_3, α_{30}, etc.)



- **Fission Dynamics:** Determination of the fission path, fission barrier height, and transition states (scission/saddle points).



Refinements of macroscopic models

The Droplet Model (Myers & Świątecki, 1974)

The Droplet Model extended the Liquid Drop Model by introducing shape dependence and a more realistic treatment of neutron-proton asymmetry.

$$E_{\mathrm{mac}}(A,Z,\beta) = a_v(1-k_v I^2)A - a_s(1-k_s I^2)A^{2/3}B_s(\beta) - E_C(A,Z,\beta)$$

where

$$E_C(A,Z,\beta) = \frac{3}{5}\frac{e^2Z^2}{r_0A^{1/3}}B_c(\beta) - C_{\mathrm{diff}}\frac{Z^2}{A} - C_{\mathrm{exch}}\frac{Z^{4/3}}{A^{1/3}}.$$

- $I = (N-Z)/A$: neutron-proton asymmetry.
- $B_s(\beta)$: deformation-dependent surface-energy factor.
- $B_c(\beta)$: deformation-dependent Coulomb-energy factor.
- Surface symmetry energy distinguishes between volume and surface contributions to the asymmetry energy.
- Diffuseness and exchange corrections improve the Coulomb energy.

The macroscopic energy is now a function of both the nuclear composition (A,Z) and its shape β.

The Droplet Model (Myers & Świątecki, 1974)

In the Liquid Drop Model the nucleus is assumed to be spherical. The Droplet Model introduces deformation by scaling the surface and Coulomb energies with shape-dependent factors:

$$B_s(\beta) = \frac{S(\beta)}{S_0}, \qquad B_c(\beta) = \frac{E_C(\beta)}{E_C(0)}$$

where S_0 and $E_C(0)$ correspond to a spherical nucleus with the same volume.

- $B_s(\beta)$: surface-energy factor
  - A deformation increases the nuclear surface area.
  - Therefore,

    $$B_s(\beta) > 1$$

    for deformed shapes, increasing the macroscopic energy.
- $B_c(\beta)$: Coulomb-energy factor
  - A deformation changes the average distance between protons.
  - For an elongated shape, protons are distributed over a larger region, reducing their electrostatic repulsion:

    $$B_c(\beta) < 1.$$

The Finite-Range Droplet Model (FRDM)

- The **Finite-Range Droplet Model (FRDM)** extends the Droplet Model by combining:
  - an improved macroscopic droplet energy,
  - Strutinsky shell corrections,
  - pairing corrections,
  - and a phenomenological single-particle potential.
- **Finite-range treatment:** The sharp-surface approximation of the Liquid Drop Model is replaced by a finite-range folding description of the nuclear interaction.
- **Macroscopic improvement:** The surface energy is calculated using the **Yukawa-plus-exponential folding function**, allowing a realistic description of strongly deformed and necked shapes.
- **Microscopic improvement:** Single-particle levels are generated from the **Folded-Yukawa potential**, providing deformation-dependent shell corrections.

FRDM combines a refined macroscopic description with a phenomenological microscopic shell structure.

FRDM: Finite-Range Surface Energy

The traditional surface term is replaced by a finite-range interaction between all volume elements:

$$E_s = -\frac{c_s}{8\pi^2 a^3} \iint_V \left(\frac{|\mathbf{r} - \mathbf{r}'|}{a} - 2 \right) \frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r} - \mathbf{r}'|} \, d^3r \, d^3r' .$$

where

- c_s is the surface-energy coefficient,
- $a \simeq 0.6$ fm is the range of the nuclear interaction,
- every volume element interacts with every other one through a **finite-range Yukawa-plus-exponential** kernel.

Physical consequence:

- Opposite sides of a necking nucleus already attract each other before scission.
- This removes the unrealistic behavior of sharp-surface liquid-drop models at large deformations.
- The model therefore describes fission barriers much more accurately.

FRDM: Folded-Yukawa Single-Particle Potential

The shell correction requires the single-particle spectrum $\{\epsilon_i\}$ for every nuclear deformation. In FRDM, these levels are obtained from the **Folded-Yukawa potential**:

$$V(\mathbf{r}) = -\frac{V_0}{4\pi a^3}\int_V \frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r}-\mathbf{r}'|}\,d^3r',$$

where V_0 is the potential depth and a is the range of the nuclear interaction.

- The complete single-particle Hamiltonian is $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + V_{\rm so} + V_C$, where $V_{\rm so}$ is the spin-orbit interaction and V_C is the Coulomb potential for protons.

Advantages

- The finite-range folding automatically generates a realistic diffuse nuclear surface for any chosen deformation.
- The same geometric shape used in the macroscopic energy is also used to generate the microscopic single-particle potential, providing a consistent description.

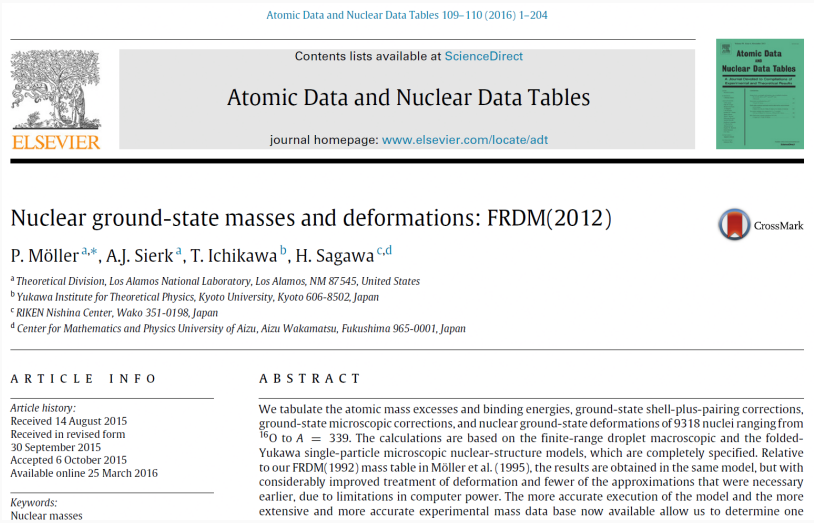
The Folded-Yukawa potential provides the microscopic input for the Strutinsky shell correction.

Predictive Power of Microscopic–Macroscopic Models

- Combining a macroscopic energy with microscopic shell and pairing corrections provides a quantitative description of nuclear masses throughout the chart of nuclides.
- Once calibrated to known nuclei, these models can be extrapolated into experimentally inaccessible regions.
- Microscopic–macroscopic models have been used to predict:
  - nuclear masses and binding energies,
  - ground-state deformations,
  - fission barriers,
  - decay properties,
  - the location of shell closures in superheavy nuclei.
- In particular, they predicted enhanced stability in the superheavy region long before many of these nuclei were synthesized.

The existence of superheavy nuclei is a direct manifestation of shell stabilization.

Global Predictions for Superheavy Nuclei



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Nuclear ground-state masses and deformations: FRDM(2012)

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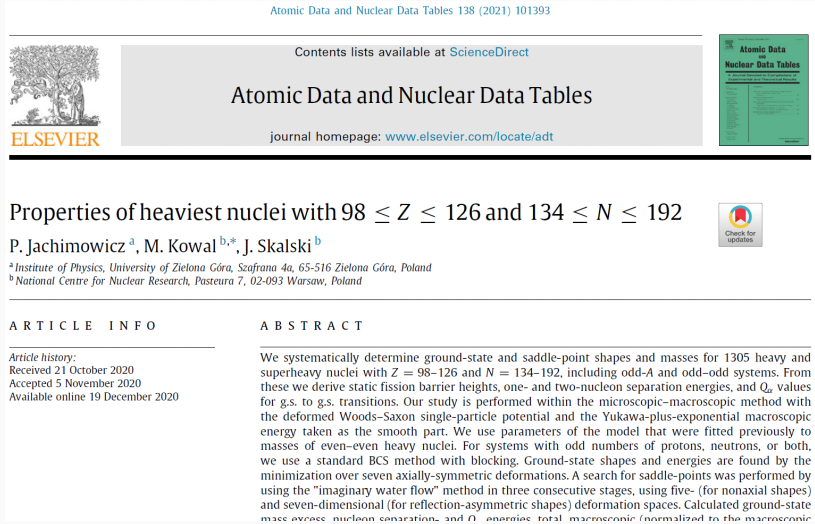
ABSTRACT

We tabulate the atomic mass excesses and binding energies, ground-state shell-plus-pairing corrections, ground-state microscopic corrections, and nuclear ground-state deformations of 9318 nuclei ranging from ^{16}O to $A = 339$. The calculations are based on the finite-range droplet macroscopic and the folded-Yukawa single-particle microscopic nuclear-structure models, which are completely specified. Relative to our FRDM(1992) mass table in Möller et al. (1995), the results are obtained in the same model, but with considerably improved treatment of deformation and fewer of the approximations that were necessary earlier, due to limitations in computer power. The more accurate execution of the model and the more extensive and more accurate experimental mass data base now available allow us to determine one



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Properties of heaviest nuclei with $98 \leq Z \leq 126$ and $134 \leq N \leq 192$

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ABSTRACT

We systematically determine ground-state and saddle-point shapes and masses for 1305 heavy and superheavy nuclei with $Z = 98$–126 and $N = 134$–192, including odd-A and odd–odd systems. From these we derive static fission barrier heights, one- and two-nucleon separation energies, and Q_α values for g.s. to g.s. transitions. Our study is performed within the microscopic–macroscopic method with the deformed Woods–Saxon single-particle potential and the Yukawa-plus-exponential macroscopic energy taken as the smooth part. We use parameters of the model that were fitted previously to masses of even–even heavy nuclei. For systems with odd numbers of protons, neutrons, or both, we use a standard BCS method with blocking. Ground-state shapes and energies are found by the minimization over seven axially-symmetric deformations. A search for saddle-points was performed by using the "imaginary water flow" method in three consecutive stages, using five- (for nonaxial shapes) and seven-dimensional (for reflection-asymmetric shapes) deformation spaces. Calculated ground-state

- Predictions extend far beyond experimentally known nuclei.
- Regions of enhanced stability appear due to shell effects.
- Different microscopic–macroscopic models predict similar global trends.

Mic-Mac vs Self-Consistent Mean-Field Models

Self-Consistent Mean-Field Models

Basic idea:

- The nuclear mean field is generated self-consistently by the nucleons themselves.
- The starting point is an effective nucleon–nucleon interaction (or energy density functional), rather than a prescribed potential.
- Shell structure, deformation, spin-orbit splitting, and pairing emerge self-consistently from the same effective interaction.

Classification of Self-Consistent Interactions:

- Non-Relativistic (Zero-Range): Skyrme-HFB (contact forces, computationally fast).
- Non-Relativistic (Finite-Range): Gogny-HFB (Gaussian forces, treats pairing natively).
- Relativistic Mean Field (RMF / RHB): Meson-exchange fields using the Dirac equation; yields spin-orbit forces naturally.

Self-consistent procedure:

- Start from an initial guess for the nucleon densities (or wave functions).
- Construct the corresponding mean-field potential.
- Solve the single-particle equations (e. g. Schrödinger/Dirac).
- Recalculate the densities from the new wave functions.
- Repeat until the input and output densities/potentials agree (**Self-Consistency**).

Why is the Mic-Mac Model NOT Self-Consistent?

Microscopic-Macroscopic models:

- The single-particle potential is chosen phenomenologically (e.g. Woods–Saxon, Folded-Yukawa).
- The potential parameters are fitted to experimental data rather than generated by the nucleons themselves.
- The shell correction is then extracted from this fixed spectrum.

Why is this not self-consistent?

- The nucleon density does not determine the potential.
- If the density changes, the potential is not recalculated.
- Therefore the input potential and the output density are not mutually consistent.

Although less fundamental than self-consistent approaches, Mic-Mac models remain highly competitive because of their excellent accuracy and computational efficiency, making them ideal for large-scale fission calculations.

Finite-Temperature PES

A Practical Advantage of the Mic-Mac Approach

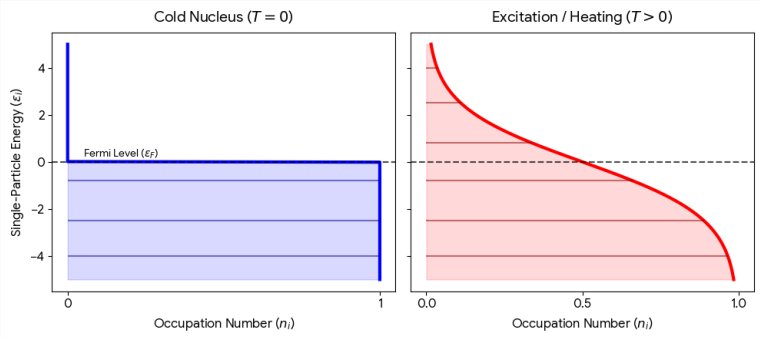
Despite the inconsistency, the Mic-Mac framework offers a major bonus:

- The macroscopic and microscopic contributions respond differently to excitation energy:
  - The macroscopic energy changes only slowly.
  - Shell and pairing effects are rapidly damped with increasing temperature.
- This allows finite-temperature potential-energy surfaces to be constructed by combining a nearly unchanged macroscopic energy with **temperature-dependent shell and pairing corrections**.
- The Mic-Mac models remain one of the most efficient tools for studying nuclear fission, shape evolution, and large-amplitude collective motion at **excited states**.

Why Do Shell Effects Fade out with Temperature?

The physical cause of shell-damping lies in the redistribution of nucleon **occupation numbers** (n_i) according to Fermi-Dirac statistics:

$$n_i = \frac{1}{1 + e^{(\epsilon_i - \lambda)/T}}$$



- **Cold Nucleus ($T = 0$):** Nucleons fill discrete levels from the bottom up ($n_i = 1$ or 0). This sharp boundary maximizes energy differences between magic shells, driving strong shell corrections (δE_{shell}).
- **Excited/Hot Nucleus ($T > 0$):** Thermal energy promotes nucleons across the Fermi surface. Occupation numbers become continuous fractions ($0 < n_i < 1$).
- **The Smoothing Effect:** This statistical blurring washes out the discrete shell gaps. Once T becomes comparable to the shell spacing around the Fermi surface ($\hbar\omega \approx 1-2$ MeV), the shell corrections become strongly damped.

Shell correction at finite temperature

$$\delta E \longrightarrow \delta F = E(T) - \tilde{E}(T) - T\left[S(T) - \tilde{S}(T)\right]$$

$$E(T) = 2\int_{-\infty}^{\infty} n(T)\varepsilon g(\varepsilon)d\varepsilon$$

$$S(T) = -\int_{-\infty}^{+\infty}[(1-n(T))\log(1-n(T)) + n(T)\log n(T)]g(\varepsilon)d\varepsilon$$

Discrete levels

$$g(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k)$$

$$n_k(T) = 1/(1+e^{(\varepsilon_k-\lambda)/T})$$

Smooth spectrum

$$\tilde{g}(\varepsilon) = \frac{1}{\gamma\sqrt{\pi}}\sum_{k=1} e^{-x^2}\sum_{n=0,2,\ldots}^{6} c_n H_n(x),$$

$$n_\varepsilon(T) = 1/(1+e^{(\varepsilon-\tilde{\lambda})/T})$$

$$N(Z) = 2\sum_k n_k(T) = 2\int_{-\infty}^{+\infty} n_\varepsilon(T)\tilde{g}(\varepsilon)d\varepsilon$$

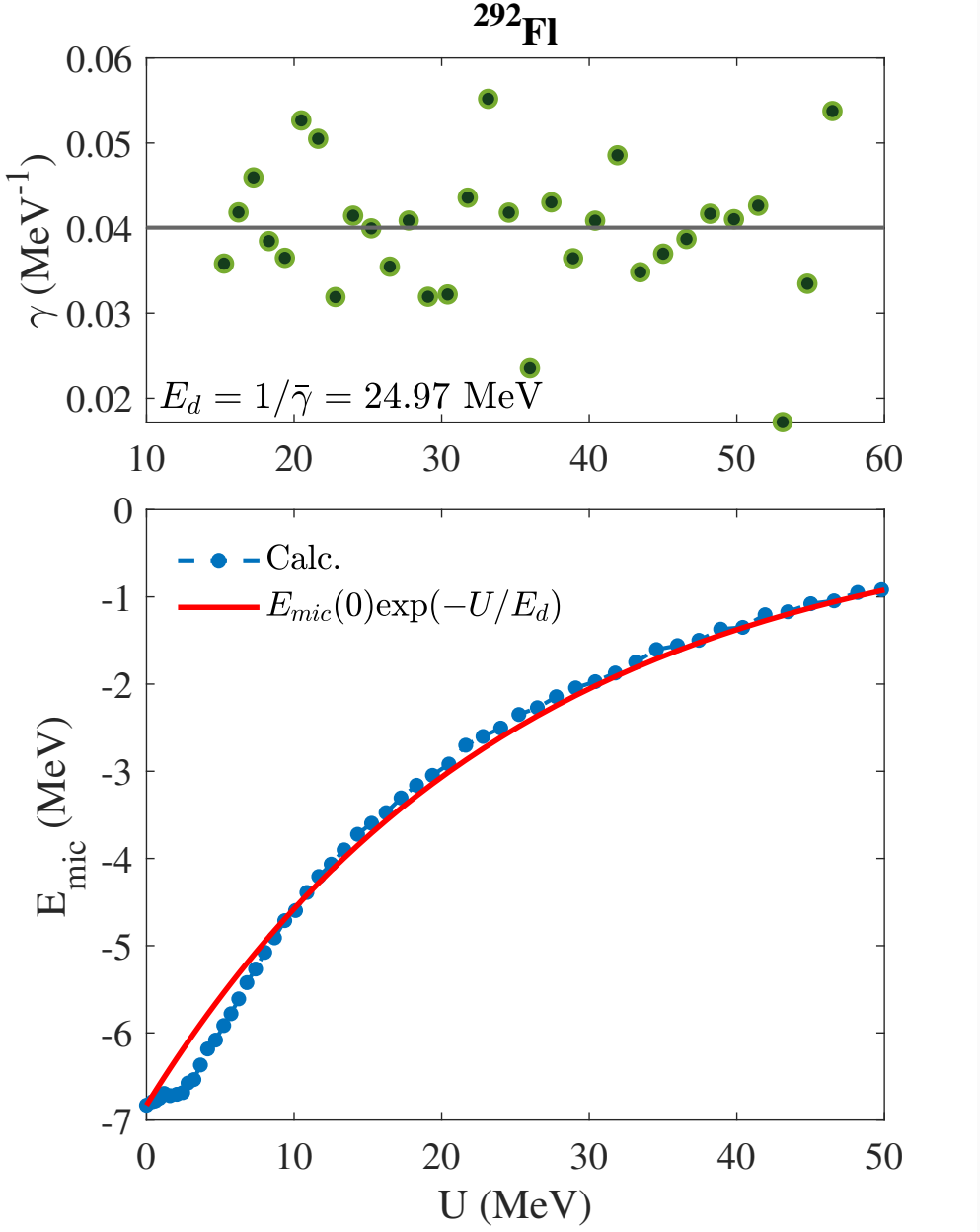
Excitation energy dependence of shell corrections

$$\gamma(U) = -\frac{E'_{mic}(U)}{E_{mic}(U)}$$

$$E_{mic}(U) = E_{mic}(0)e^{-\frac{U}{E_d}}$$

Damping parameter:

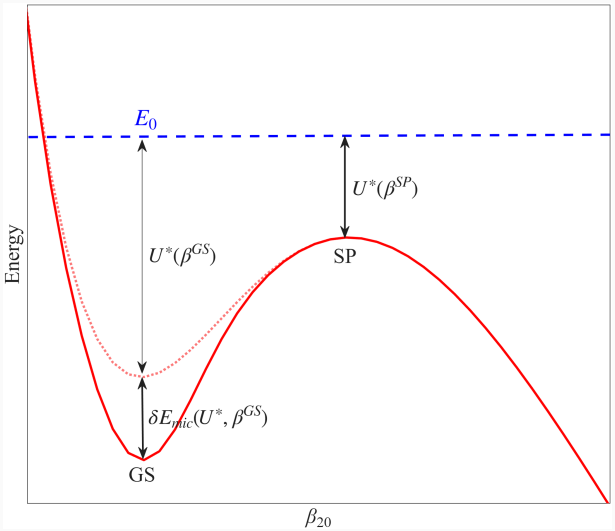
$$E_d = \frac{1}{\gamma}$$



Implications for survival probabilities: energy conservation

Since a portion of the excitation energy is consumed to "wash out" shell correlations, the effective thermal energy available to drive fission is reduced.

$$E_{\rm pot}(A-1,U^*) = E^{\rm GS}_{\rm pot}(A-1) + \delta E_{\rm mic}(A-1,U^*)$$
$$\delta E_{\rm mic}(A-1,U^*) = E_{\rm mic}(A-1,\beta^{\rm GS},U^*) - E^{\rm GS}_{\rm mic}(A-1)$$

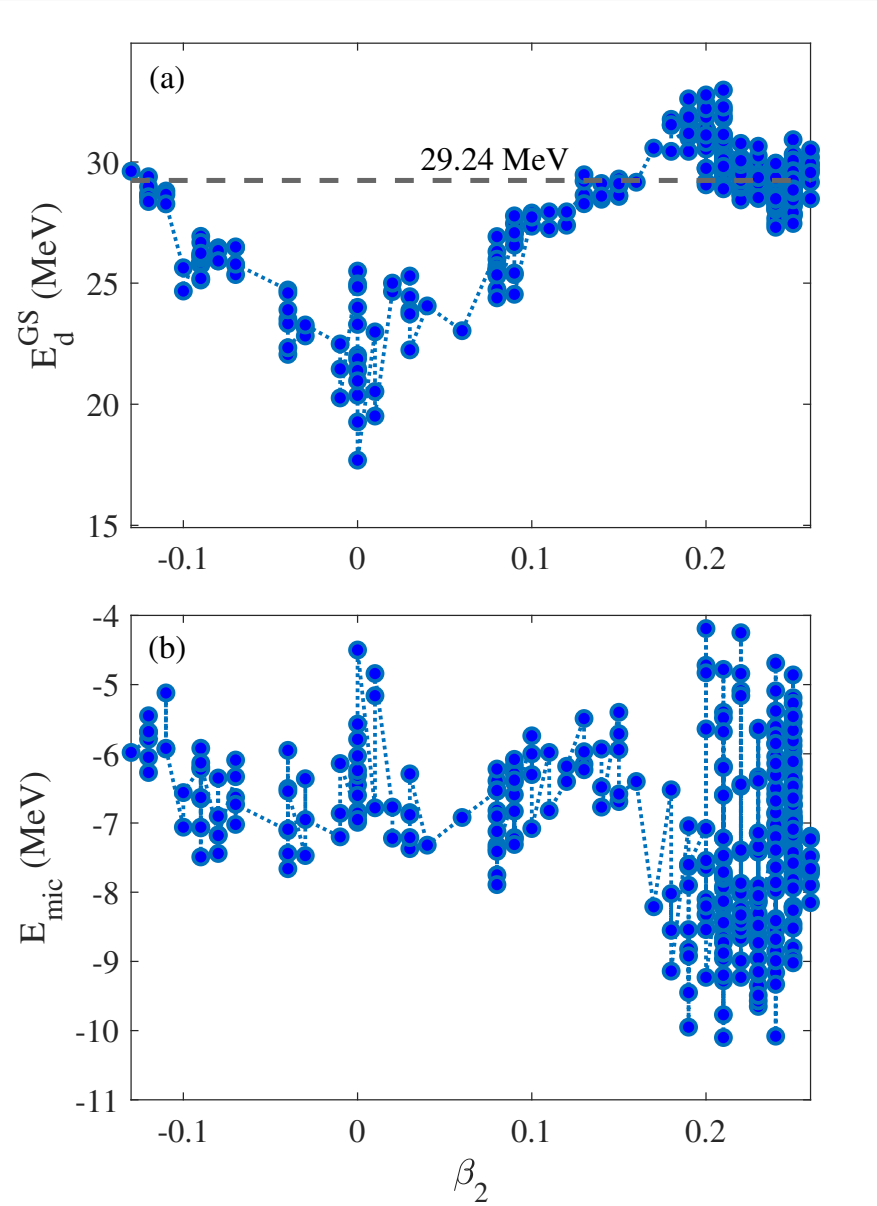


$$\frac{\Gamma_n}{\Gamma_f}(U^*) \propto \frac{\rho(A-1,\beta^{\rm GS},E_0 - E_{\rm pot}(A-1,U^*) - B_n)}{\rho(A,\beta^{\rm SP},E_0 - E^{\rm SP}_{\rm pot}(A))}$$

Suppression of the survival probability is driven by the reduction of the microscopic correction in the daughter nucleus, rather than by the modification of the fission barrier height

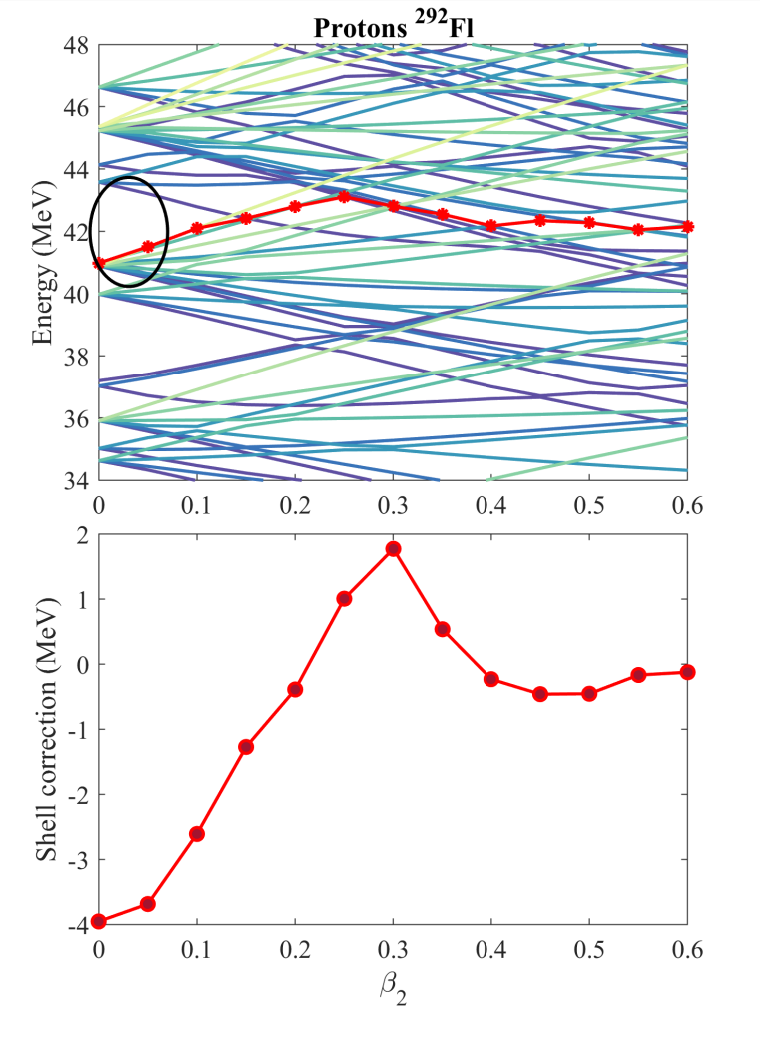
$$\frac{\Gamma_n}{\Gamma_f}(U^*) = \left(\frac{\Gamma_n}{\Gamma_f}\right)_0 e^{-\delta E_{\rm mic}(A-1,U^*)/T}$$

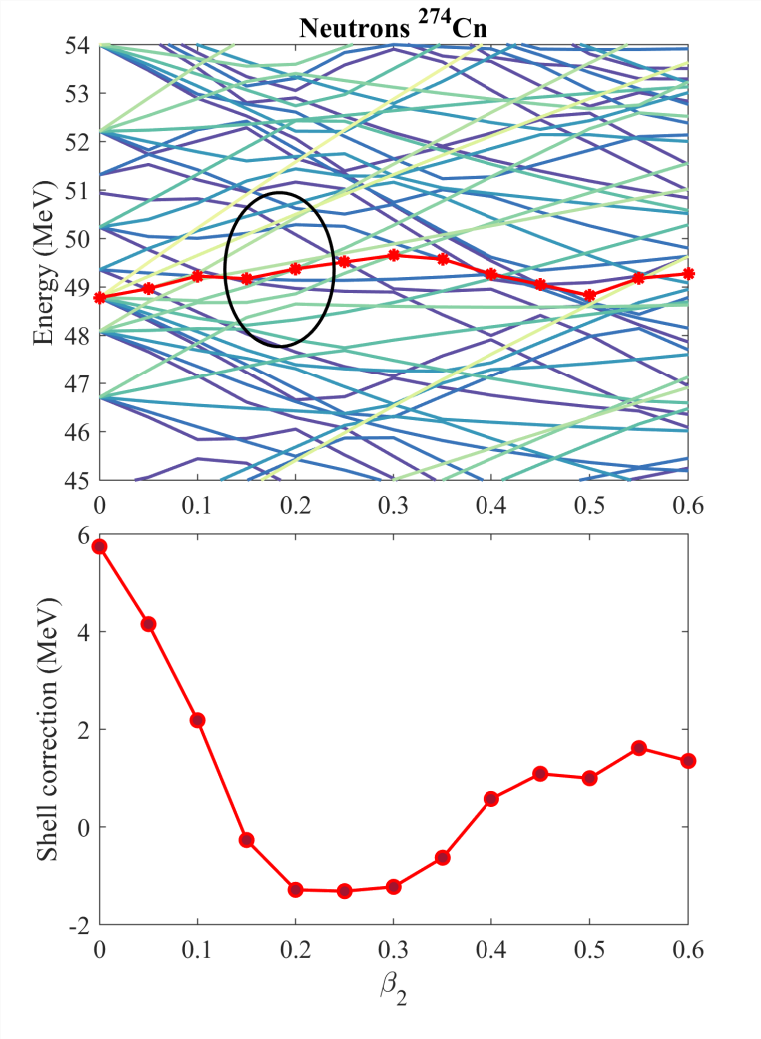
Deformation dependence of damping parameters



- E_d^{GS} exhibits a minimum at $\beta_2 = 0$.
  Shell effects fade out faster in spherical nuclei
- The damping parameter is influenced by the absolute value of deformation rather than the prolate or oblate nuclear shapes.
- The damping parameter remains relatively constant for nuclei with $|\beta_2| \geqslant 0.15$, despite significant variations in E_{mic} ranging from -10 to -4 MeV.

Distribution of single particle energy levels around the Fermi level

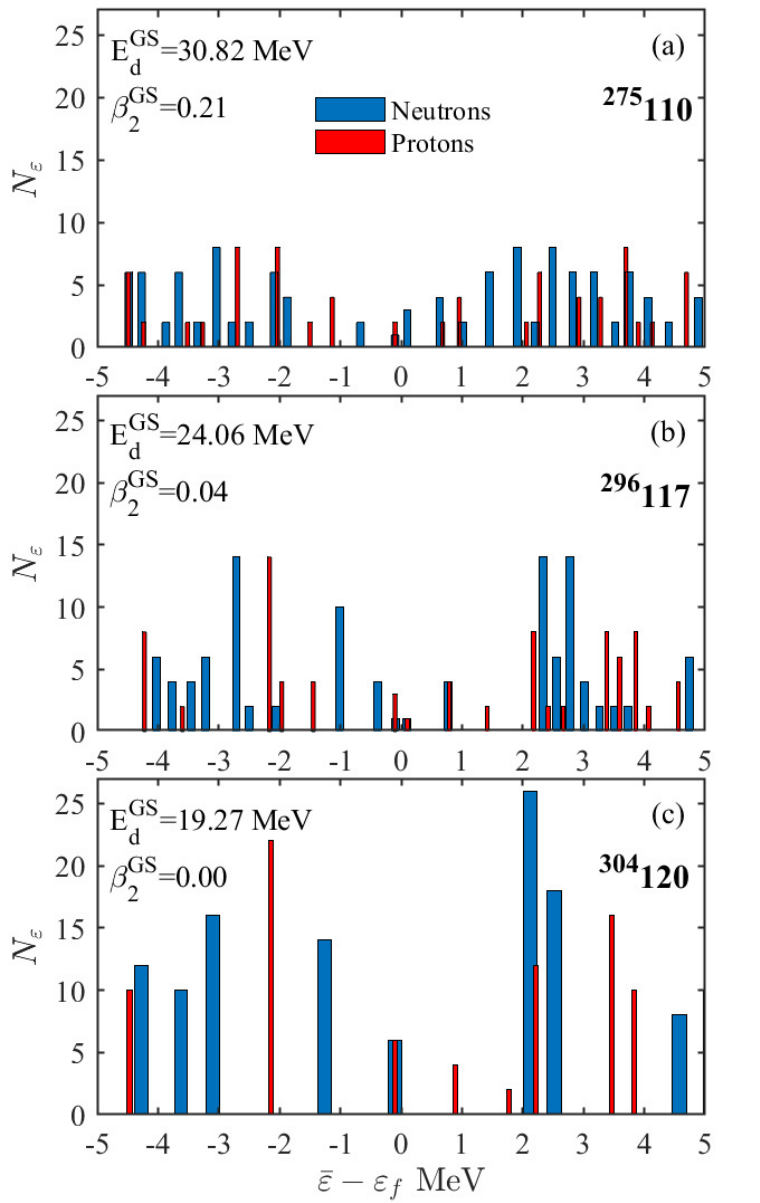


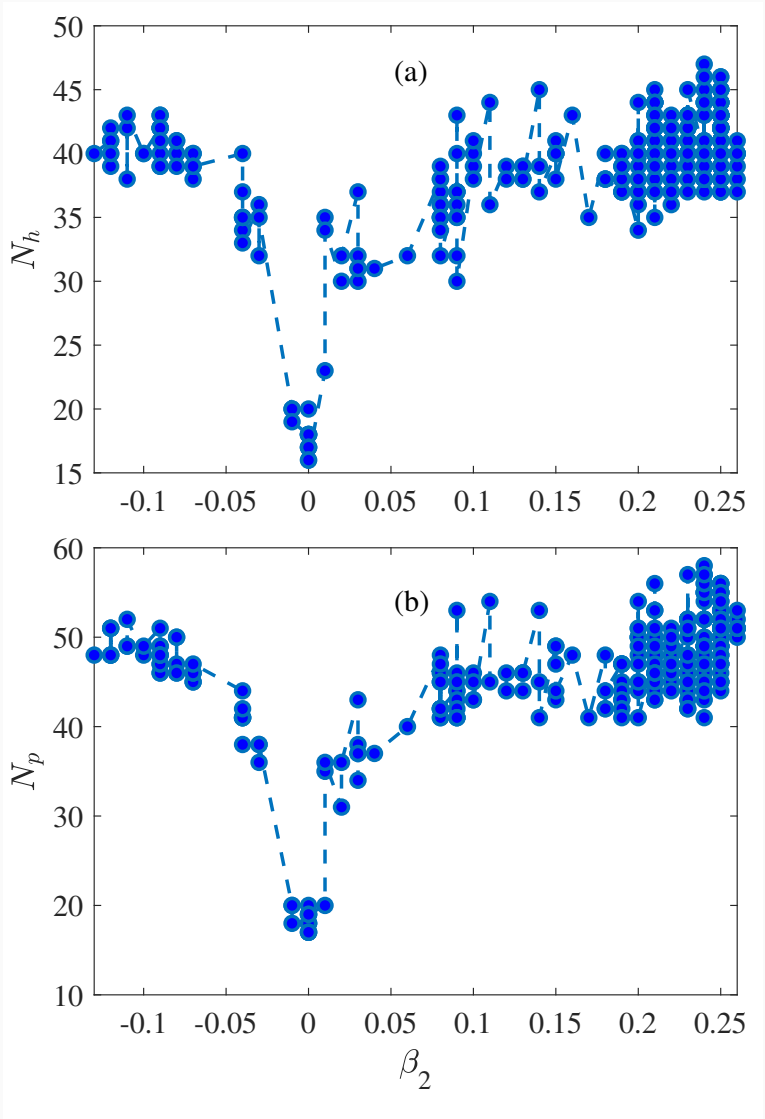


Spherical GS $\longrightarrow$ Degenerate energy levels above and below Fermi level

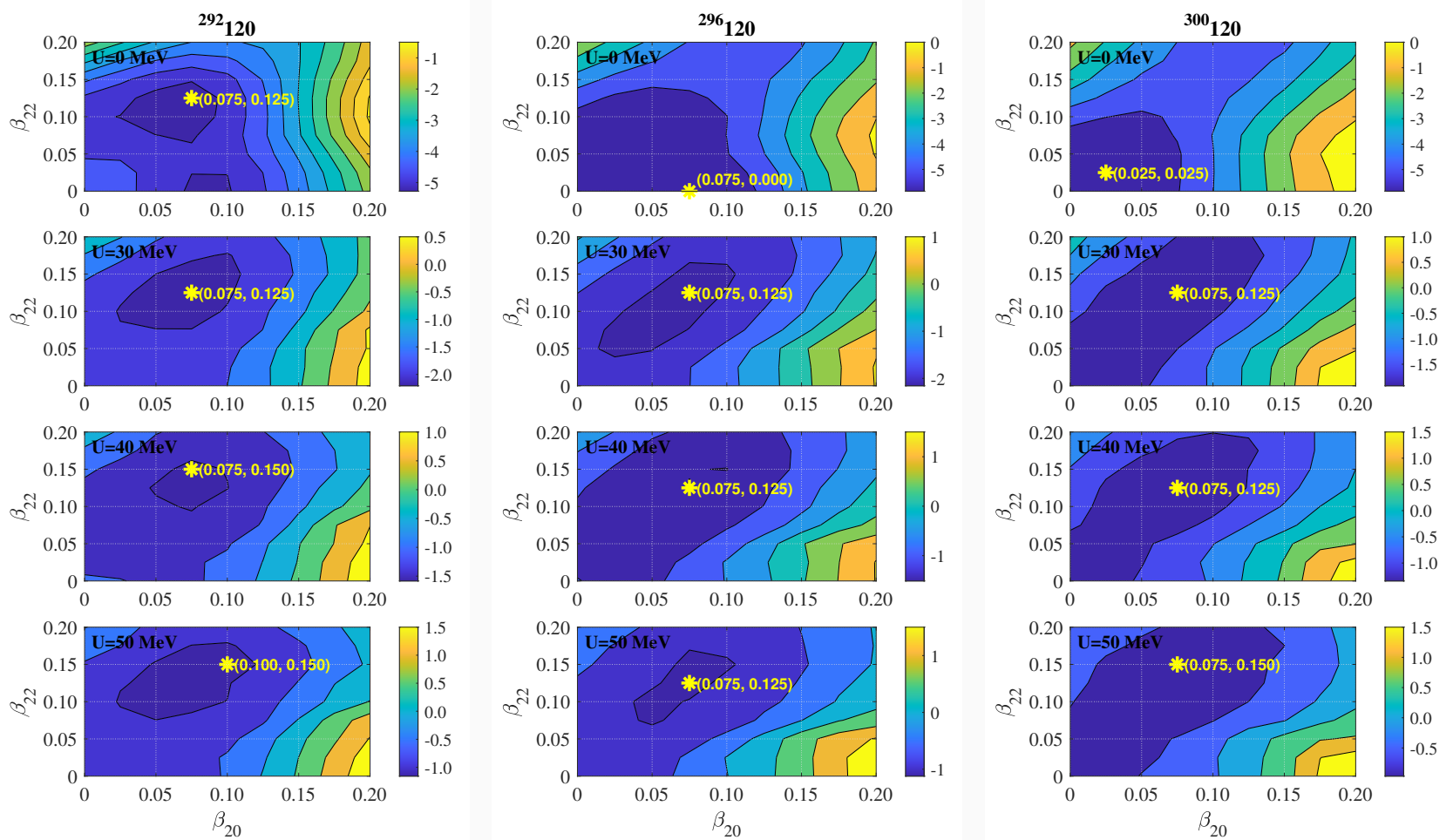
Deformed GS $\longrightarrow$ Uniformly distributed levels above and below Fermi level

Quasi-degenerate groups of energy levels





Evolution of PES with excitation energies



Shell effects fade out $\sim \beta \longrightarrow$ reshaping the energy landscape at higher excitation energies

Equilibrium shapes

Lighter nuclei:

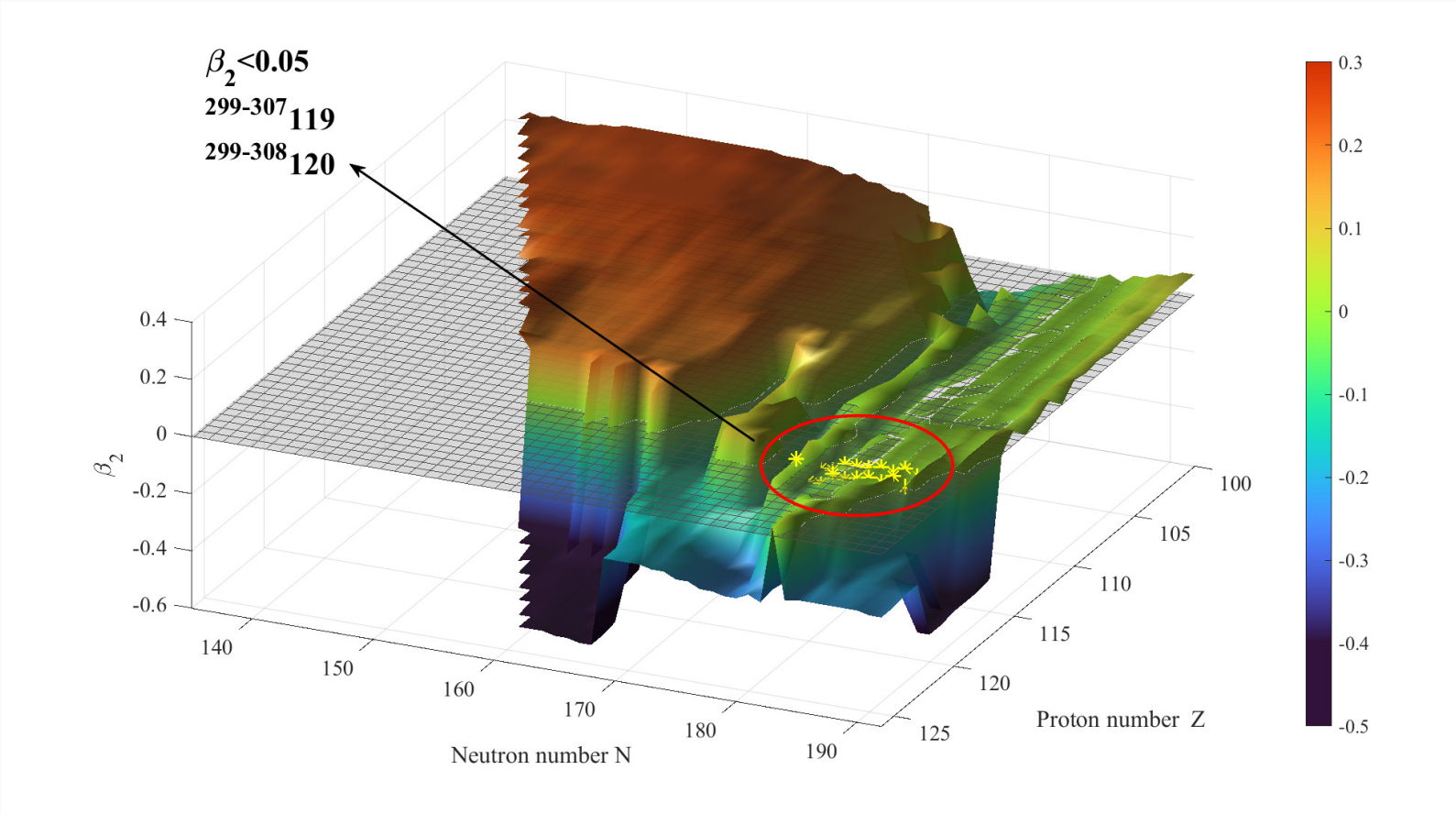
- Macroscopic PES has a spherical minimum ($\beta_2 \approx 0$)
- Deformed minimum due to shell effects
- Shell effects fade out with excitation $\longrightarrow$ shape changes from deformed to spherical.

Superheavy nuclei:

- Macroscopic PES lacks a strong minimum.
- The stability of superheavies is due to shell effects.
- Deformation-dependent reduction of shell effects can alter a spherical minimum into a deformed one.

Conclusions

Shell effects fade out differently for spherical and deformed minima, altering the PES and shifting the equilibrium shape from spherical to deformed — a feature **unique to the superheavy region**.



Candidates for the production of new superheavy elements are predicted to have spherical or near-spherical GS shapes

Thank You!