MeanField4Exp

Examples of Service Applications: Macroscopic-Microscopic Method (MMM) for Potential Energy Calculations in the User Chosen Formats

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Theory Service for the Low Energy Nuclear Physics Community: A Hands-On Workshop

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ECT*, Villazzano, Italy

EURO-LABS Project – MeanField4Exp

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MeanField4Exp

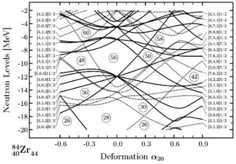
IFJ PAN, KRAKOW, POLAND and IPHC and UNIVERSITY OF STRASBOURG, FRANCE

Logged as Services About Theo4Exp

This website is based on an extensive research program
developed over many years by J. Dudek (IPHC and University of Strasbourg) and his collaborators;
it allows to explore elementary structure properties of atomic nuclei, including shapes, symmetries and excitations,
using **Realistic Phenomenological Nuclear Mean Field Theory Calculations.**

Single Particle Energies

Generating diagrams of single nucleon energies.



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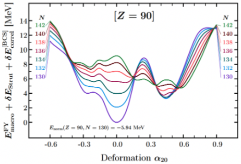
Nuclear Energy Diagrams

Generate Macroscopic-Microscopic Method nuclear energy diagrams.



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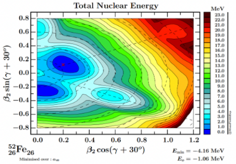
Macroscopic-Microscopic Energy

Generating total energy diagrams according to the Macroscopic-Microscopic approximation.



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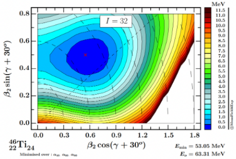
Shape Evolution with Spin

Generating diagrams of shape evolution with spin according to macroscopic energy models.



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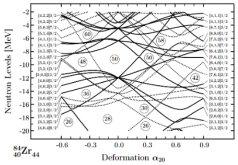

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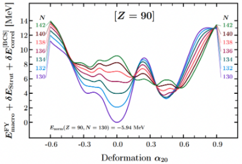

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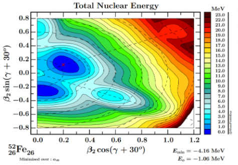

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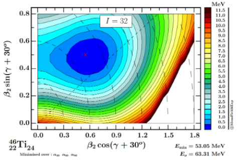

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Main Scope of Our Research

• Give the theoretical explanations to the experimental nuclear structure phenomena observed, as well as predicting the still unknown

How do we perform our studies?

• We describe the nuclear interior, i.e. *nuclear structure*, with a simple but very reliable and powerful theory called: **The Nuclear Mean-Field Theory**

• We combine contemporary **mathematical tools** of group theory, inverse problem theory and graph-theory with phenomenological nuclear mean-field theory

• One of the most important strategies: Making sure the theory we use is reliable, offering realistic, experiment comparable results for many nuclei.

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Deformed Universal Woods-Saxon Hamiltonian – Reminder

- **Given a nuclear surface Σ**

$$R(\vartheta,\varphi) = R_o\, c(\{\alpha\})\left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]$$

- **Phenomenological Woods-Saxon Hamiltonian with the so-called 'universal' parameterisation**

⇒ fixed set of parameters for thousands of nuclei!

- **Central Potential**

$$\mathcal{V}^{\rm WS}_{\rm cent} = \frac{V_c}{1+\exp\left[{\rm dist}_\Sigma(\vec{r};r_c)/a_c\right]}$$

- **Spin-Orbit Potential**

$$\mathcal{V}^{\rm WS}_{\rm SO} = \frac{2\hbar\lambda_{so}}{(2mc)^2}\left[(\vec{\nabla}V^{\rm WS}_{\rm SO})\wedge\hat{p}\,\right]\cdot\hat{s},\;\; \text{with } V^{\rm WS}_{\rm SO} = \frac{V_o}{1+\exp[{\rm dist}_\Sigma(\vec{r},r_{so})/a_{so}]}$$

- **This potential depends *only* on two sets of 6 parameters ↔ Mass Table ∼ 3 000 nuclei**

$$\boxed{\{V_c, r_c, a_c; \lambda_{so}, r_{so}, a_{so}\}_{\pi,\nu}} \Leftrightarrow \boxed{\{V_o, \kappa_c, r_c^{\pi,\nu}, a_c^{\pi,\nu}; \lambda_o, \kappa_{so}, r_{so}^{\pi,\nu}, a_{so}^{\pi,\nu}\}}$$

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Deformed Mean-Field Hamiltonian – Reminder

Mean-Field Potential: $\boxed{\hat{\mathcal{V}}_{\mathrm{m-f}} = \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{cent}} + \hat{\mathcal{V}}^{\mathrm{WS}}_{\mathrm{SO}} + \hat{\mathcal{V}}_{\mathrm{C}}}$

$\downarrow$

Hamiltonian: $\boxed{\hat{\mathcal{H}}_{\mathrm{m-f}} = \hat{\mathcal{T}} + \hat{\mathcal{V}}_{\mathrm{m-f}}}$

$\downarrow$

Schrödinger Equation: $\boxed{\hat{\mathcal{H}}_{\mathrm{m-f}}\,\psi_\nu = e_\nu\,\psi_\nu}$

$\downarrow$

SPE as functions of $\alpha_{\lambda\mu}$: $\boxed{e_\nu = e_\nu(\alpha_{\lambda\mu})}$

$\downarrow$

Total Energy as function of $\alpha_{\lambda\mu}$: $\boxed{E = E(\alpha_{\lambda\mu})}$

Total Nuclear Energy:

The Macroscopic-Microscopic Method

The Macroscopic-Microscopic Method

- Within the Macroscopic-Microscopic Method, the nuclear total energy is calculated following **Strutinsky Method***, as a function of the *proton number Z, neutron number N, and set of deformations* $\{\alpha_{\lambda\mu}\}$

$$
\begin{aligned}
E_{\mathrm{tot.}}(Z,N,\{\alpha_{\lambda\mu}\}) &= E_{\mathrm{Macro.}}(Z,N,\{\alpha_{\lambda\mu}\}) + E_{\mathrm{Micro.}}(Z,N,\{\alpha_{\lambda\mu}\}) \\
&= E_{\mathrm{Macro.}}(Z,N,\{\alpha_{\lambda\mu}\}) + \boxed{E_{\mathrm{shell}}(Z,N,\{\alpha_{\lambda\mu}\}) + E_{\mathrm{pair}}(Z,N,\{\alpha_{\lambda\mu}\})}
\end{aligned}
$$

- Macroscopic Energy $E_{\mathrm{Macro.}}(Z,N,\{\alpha_{\lambda\mu}\})$, based on finite range liquid drop model
- Microscopic Energy $E_{\mathrm{Micro.}}(Z,N,\{\alpha_{\lambda\mu}\})$, accounting for the shell+pairing correction

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References:

* M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky, C. Y. Wong, Rev. Mod. Phys. **44**, (1972) 320-405

* P. Möller, J. Nix, W. Myers, and W. Swiątecki, At. Data and Nucl. Data Tables **59** (1995) 185-381

* W. D. Myers and W. Swiątecki, Nucl. Phys. **81** (1966) 1-60

Comment About the Choice of $E_{\mathrm{Macro.}}$ and $E_{\mathrm{Micro.}}$

• The macroscopic energy depends on deformation through the surface and curvature integrals. In the present context, it appears in two variants

→ The ***Yukawa-Folded FYU***, Ref. [1];

→ The ***Lublin-Strasbourg-Drop LSD***, Ref. [2], which offers a better description to nuclei close to fission

• The microscopic energy depends on deformation through the single particle energies e_ν, obtained after solving the Schrödinger Equation. Regarding the pairing correction, it can be chosen from

→ The ***BCS*** "simple" correction, Ref. [3],

→ The ***Particle-Number-Projection PNP***, being a more advanced correction

– – –

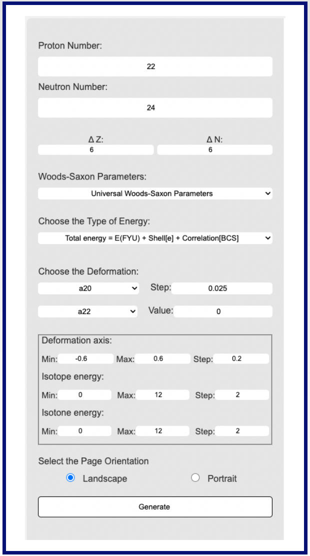
References:
1. P. Möller, J. Nix, W. Myers, and W. Swiątecki, At. Data and Nucl. Data Tables **59** (1995) 185-381
2. K. Pomorski and J. Dudek, Phys. Rev. C **67** (2003) 044316
3. M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Phys. Rev. C **5** (1972) 1050

Practical Example I:

Total Nuclear Energy Diagrams as functions of 1D deformation-space

(Total Nuclear Energy *Spaghetti*)

MeanField4Exp: Total Nuclear Energy Diagrams (1D)

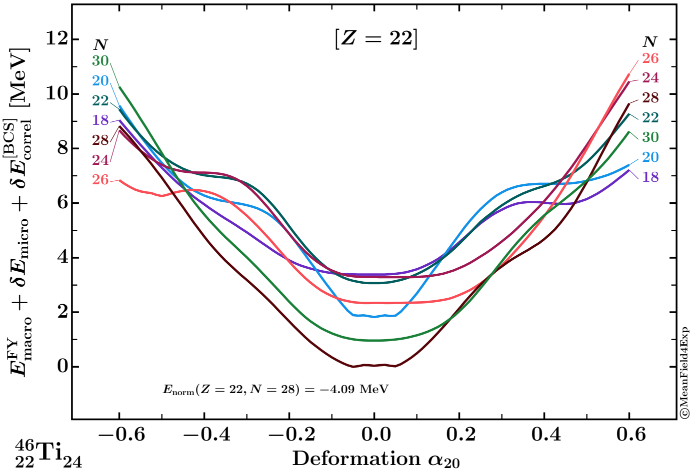


User Specifications:

- Central nucleus (Z_o, N_o) values
- Woods-Saxon Parametrisation
- Nuclei mesh: $(\Delta Z, \Delta N)$ around (Z_o, N_o)
- Choice of deformation:
  - selecting main x-axis $\alpha_{\lambda\mu} \in$ [min., max]
  - selecting a secondary $\alpha'_{\lambda\mu}$ kept at a fixed value for each value of $\alpha_{\lambda\mu}$
- Energy scale for isotope and isotone diagrams

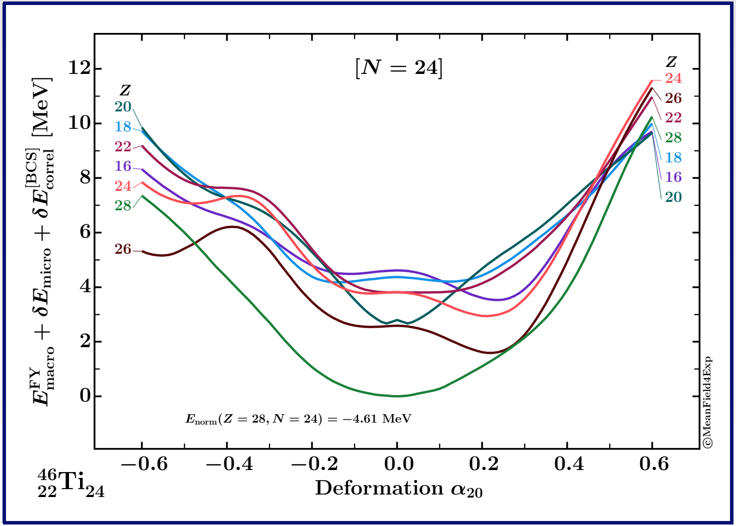
Total Nuclear Energies as functions of $\alpha_{\lambda\mu}$ – Isotopes

- Total nuclear energies for the $[Z_o = 22]$ isotopes for $N \in [18, 30]$ as functions of α_{20} deformation.



Total Nuclear Energies as functions of $\alpha_{\lambda\mu}$ – Isotones

- Total nuclear energies for the $[N_o = 24]$ isotones for $Z \in [16, 28]$ as functions of α_{20} deformation.



Total Nuclear Energies as functions of $\alpha_{\lambda\mu}$ – Comments

- The advantage of such graphical representation is allowing the user to see the total nuclear energy for several isotones or isotopes at one single glance

- The user can draw first conclusions on how a selected region of interest depends on a wide deformation range

- The disadvantage being that one can not perform (yet) energy minimisation over deformation

$\Rightarrow$ for this we need the **potential energy surfaces...**

Practical Example II:

Total Nuclear Energy Surfaces

Deformation Space in Analysis of Ground States

• Our deformation spaces are in 2D, 3D and 4D variants involving various combinations of the following shapes:

Deformation Space in Analysis of Ground States

- Our deformation spaces are in 2D, 3D and 4D variants involving various combinations of the following shapes:

→ quadrupole deformations: α_{20}, α_{22}

→ octupole deformations: α_{30}, α_{32}

→ hexadecapole deformations: α_{40}

Lund Convention: $(\alpha_{20}, \alpha_{22}) \leftrightarrow (\beta_2, \gamma)$

$$\begin{cases} \alpha_{20} = \beta_2 \cos\gamma \\ \alpha_{22} = \dfrac{1}{\sqrt{2}} \beta_2 \sin\gamma \end{cases} \leftrightarrow \begin{cases} \mathcal{X} = \beta_2 \cos(\gamma + 30^\circ) \\ \mathcal{Y} = \beta_2 \sin(\gamma + 30^\circ) \end{cases}$$

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- One 4D total nuclear energy calculation needs $\mathbf{10^6}$ deformation points

$\alpha_{20} \in [-1.00, 1.20]$, step 0.025

$\alpha_{22} \in [-0.80, 0.80]$, step 0.025

$\alpha_{3\mu} \in [-0.60, 0.60]$, step 0.025

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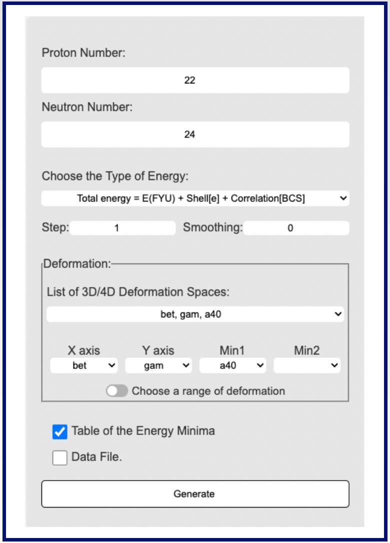
- Our 3D and 4D total nuclear energies are projected onto 2D deformation plane and minimised over the remaining deformation parameters

MeanField4Exp: Nuclear Energy Surfaces

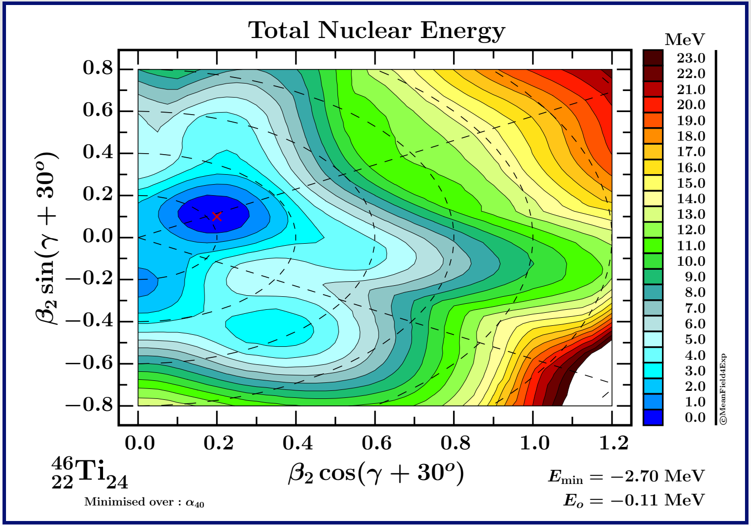


User Specifications:

- (Z, N) values
- Woods-Saxon Parametrisation
- Total Nuclear Energy contributions
- Deformation space projection and minimisation
  - select main deformation space
  - select projection (x, y)-axis
  - select minimisation deformations "Min1" and "Min2"
- The user can disable minimisation over deformation and simply plot pure 2D potential energy surface
- Possibility to download the table listing absolute and secondary minima and the source data file

MeanField4Exp: Nuclear Energy Surfaces – ^{46}Ti

- Nuclear energy surface for ^{46}Ti projected onto the quadrupole $(\mathcal{X},\mathcal{Y})$-plane, minimised over α_{40}



- **Spider web:**
  - Up-slopping dashed line means $\gamma = 0°$
  - Down-slopping dashed line means $\gamma = -60°$
  - Dashed circles have radius $r = \beta_2$
- $\boldsymbol{E_{\mathrm{min}}}$ is the energy minimum at the red-cross
- $\boldsymbol{E_{\mathrm{o}}}$ is the energy of the system at spherical deformation

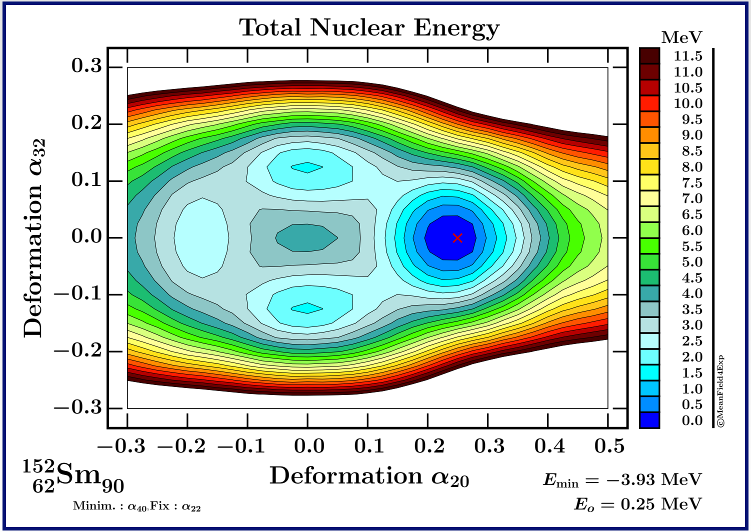
Practical Example III:

Hunting for Exotic Symmetries

Link with Experiment

MeanField4Exp: Nuclear Energy Surfaces – ^{152}Sm

- Total nuclear energy surface for ^{152}Sm projected on to the $(\alpha_{20}, \alpha_{32})$-plane, minimised over α_{40}

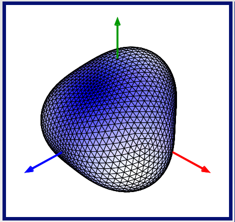


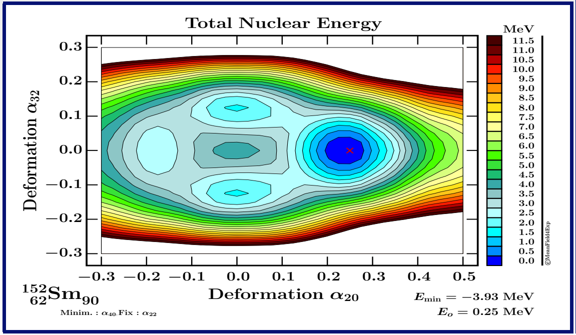
- Ground-state predicted at prolate $\boldsymbol{\alpha_{20} \approx 0.25}$
- Tetrahedral double minimum at $\boldsymbol{\alpha_{32} \neq 0}$ and $\boldsymbol{\alpha_{20} = 0}$
- Link with experiment was possible thanks to Group Theory

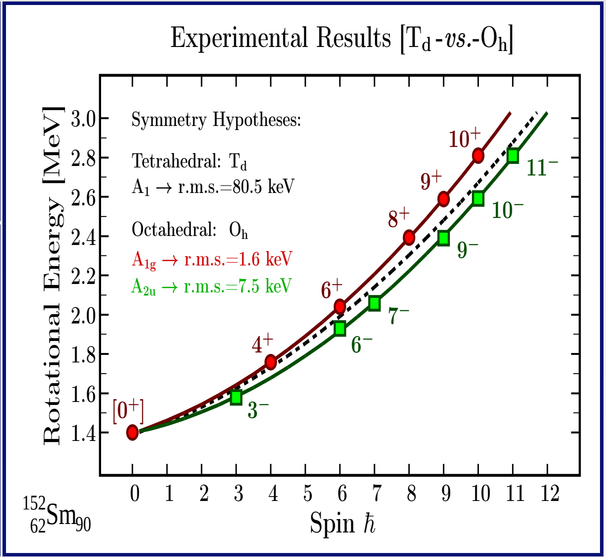
Link with Experiment: First Identification of Tetrahedral Symmetry

Investigations on ^{152}Sm

Phys. Rev. C**97**, 021302(R) (2018)







Experimental Advisory Team

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