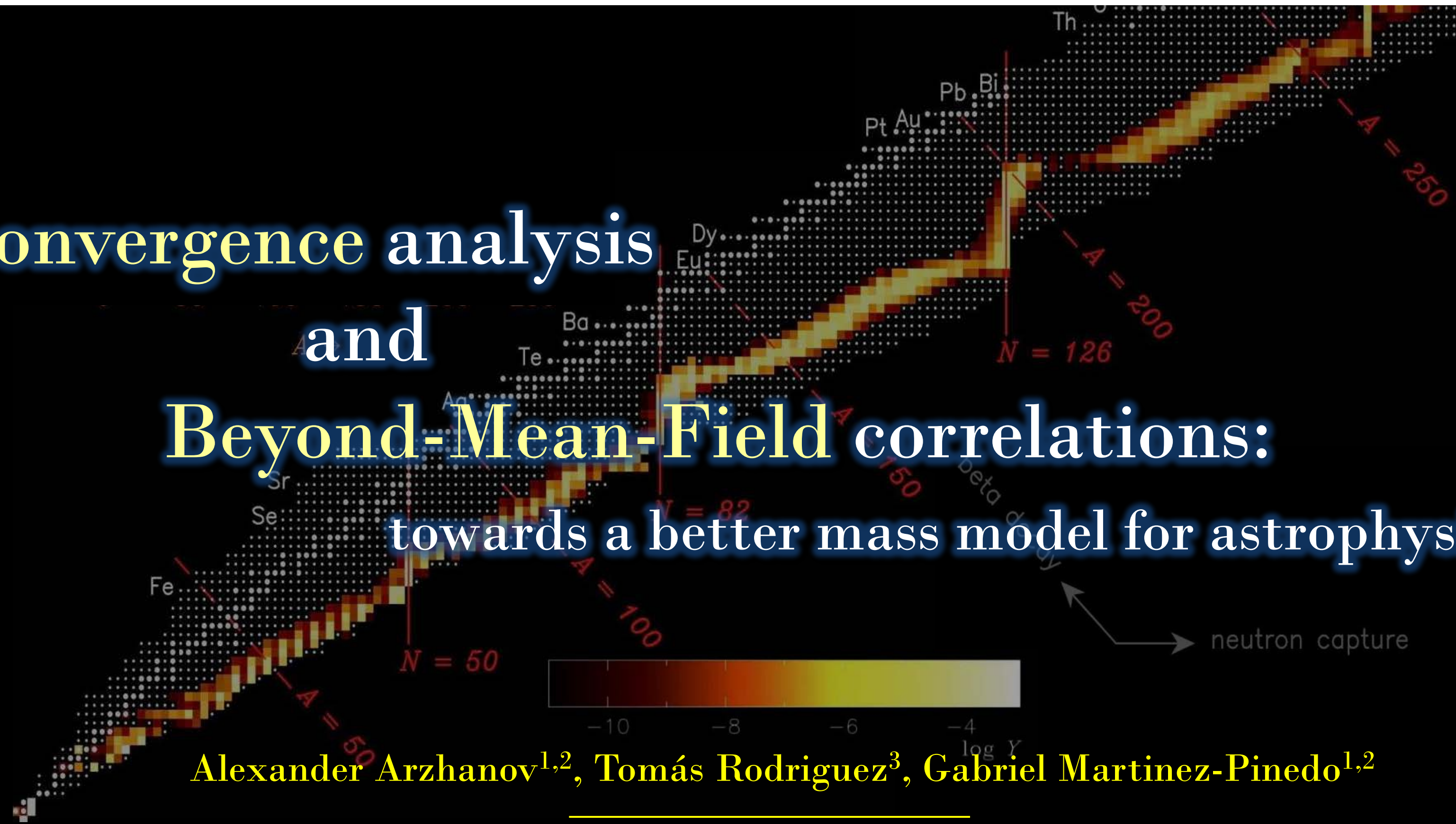
NAVI physics days

Convergence analysis and Beyond-Mean-Field correlations:

towards a better mass model for astrophysics



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[3]Departamento de Física Teórica, Universidad Autónoma de Madrid, Spain

Outline

Introduction

τ_0

Convergence of masses and
IR-Extrapolation to infinite basis

τ_1

Large-scale HFB calculation
and **Beyond-Mean-Field corrections**

τ_2

Summary and Outlook

τ_{end}

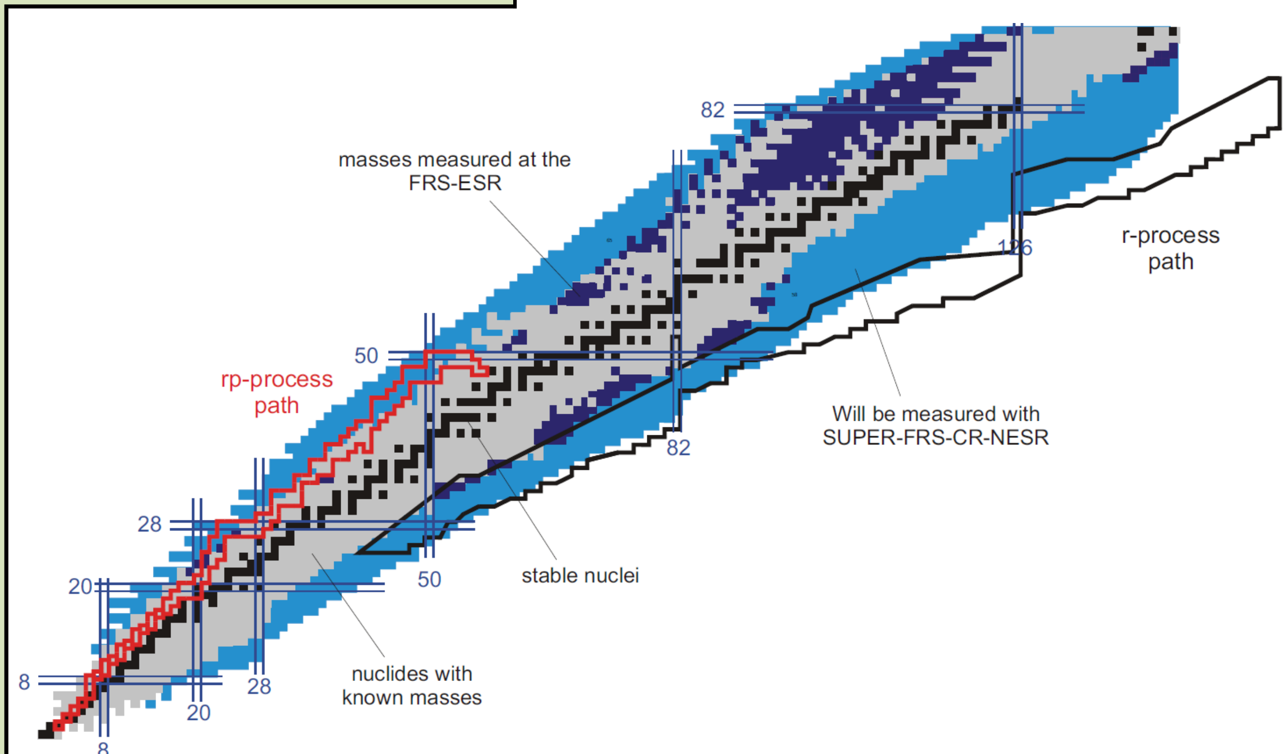
Presentation evolution

t

Introduction

- Astrophysical models require as an input thousands of **nuclear masses** → beyond experimental reach

most relevant input are the extracted
→ **neutron-separation energies S_n**
→ **beta-decay energies Q_β**
which determine thresholds of all nuclear reactions



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- Astrophysical models require as an input thousands of **nuclear masses** beyond experimental reach
- Need accurate predictions from theoretical **global mass models** →

→ Modern mass market:

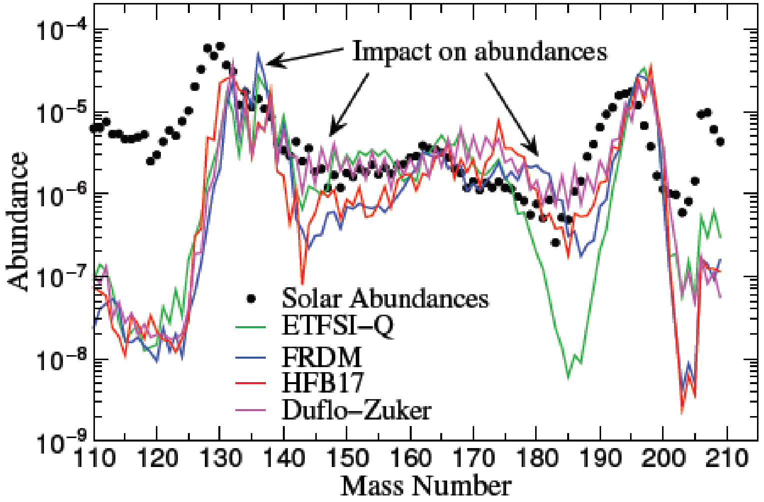
Finite Range Droplet Model (FRDM)
rms = 0.57 MeV

Extended Thomas-Fermi + Strutinsky Integral (ETFSI)
0.69 MeV

Duflo-Zuker (DZ)
0.36 MeV

Weizsäcker-Skyrme (WS)
0.298 MeV

Hartree-Fock-Bogolyubov (HFB)
(Skyrme) 0.51 MeV
(Gogny) 0.798 MeV



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Modern mass market:

(more microscopic ↓)

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self-consistent mean field models based on **Energy Density Functionals**:

- **Skyrme HFB-*** *(Goriely S. et al., PRC**88**, 2013)*
- **Gogny D1S/D1M** *(Goriely S. et al., PRL**102**, 2009)*
- **UNEDF** *(Erler J. et al., Nature **486**, 2012)*

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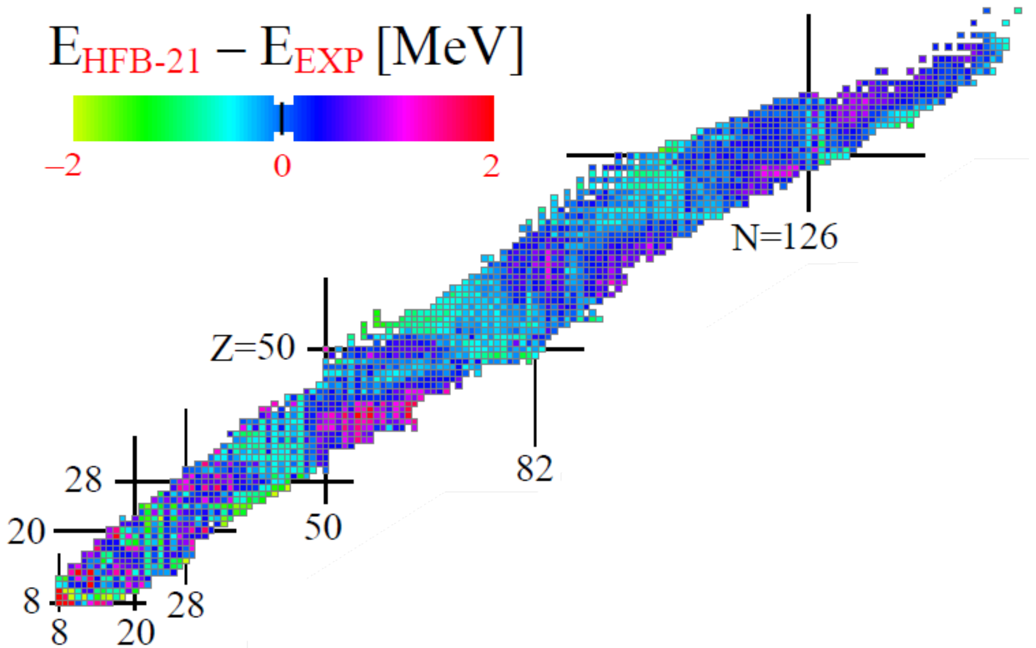
- All models have similar rms, but more fundamental **HFB models** *should provide* greater confidence in describing unknown isotopes
- **Still some problems with HFB models:**
  I) **Issue of convergence** due to truncated model space
  II) Missing some physics without **Beyond-Mean-Field** correlations
  III) **Odd-mass nuclei** are not treated on the same footing



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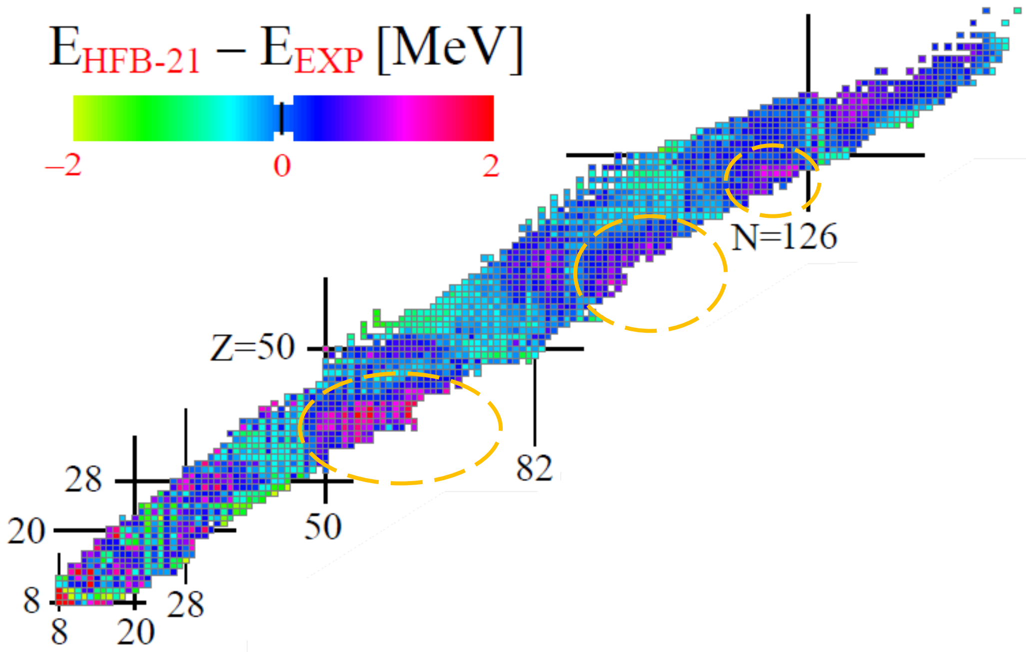

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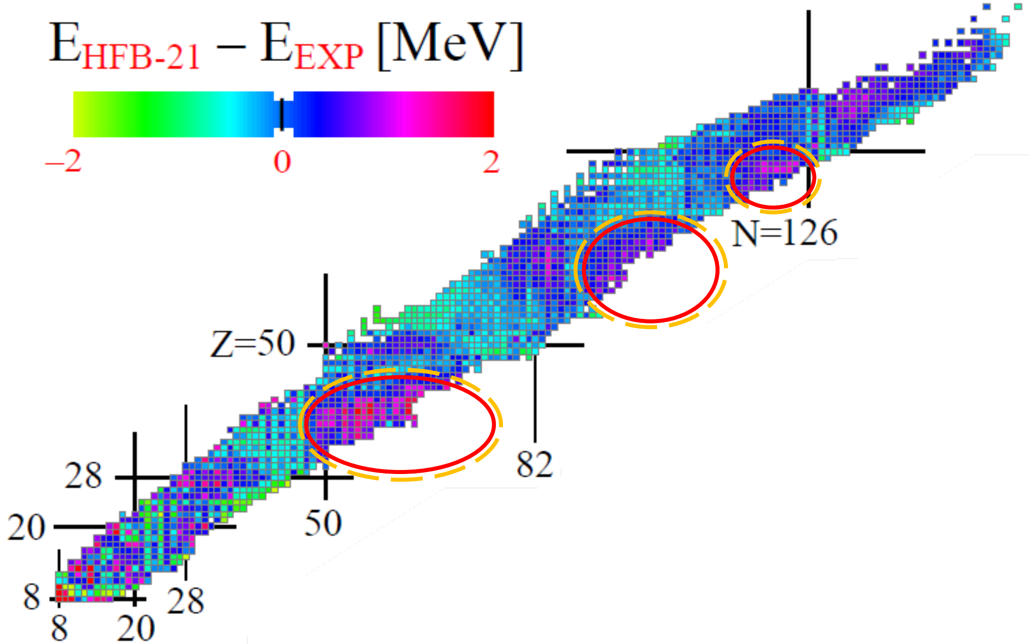
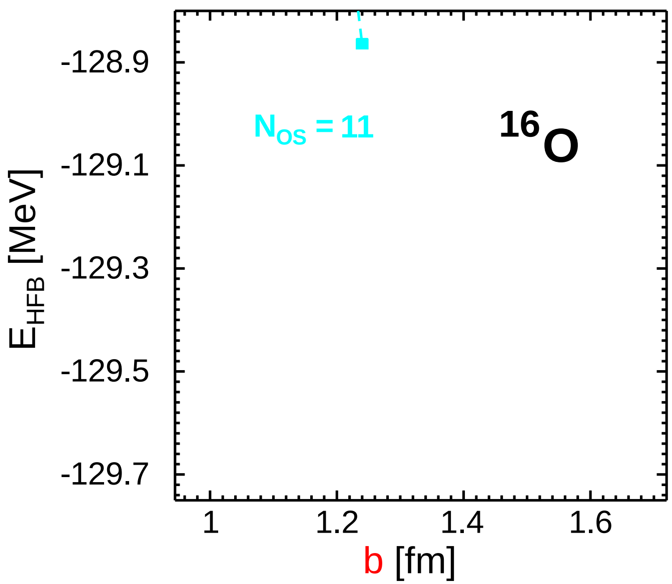


Convergence of masses and **IR-Extrapolation** to infinite basis



Convergence in finite oscillator space

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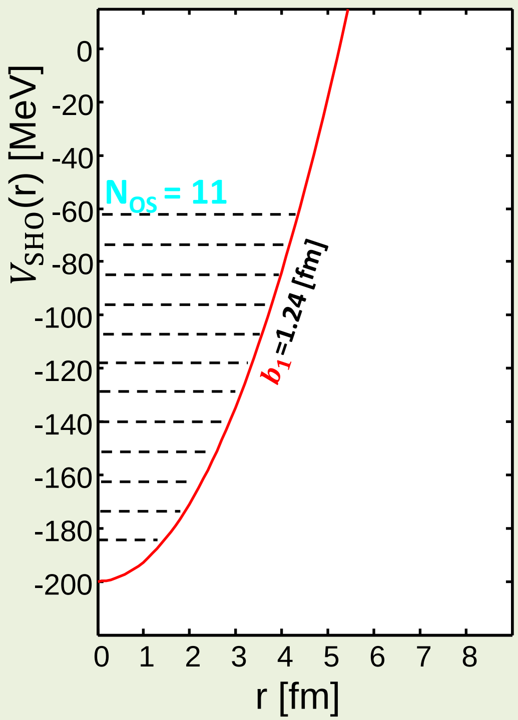
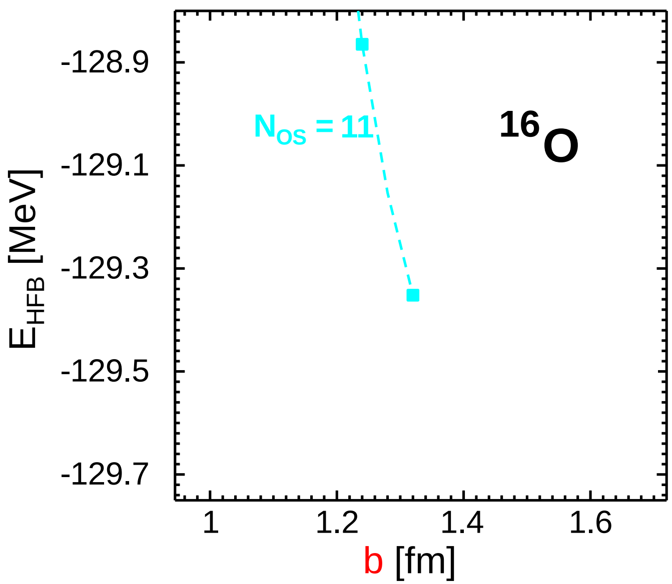
  - N_{OS} - *number of major oscillator shells*
  - b - *length of SHO wavefunctions*





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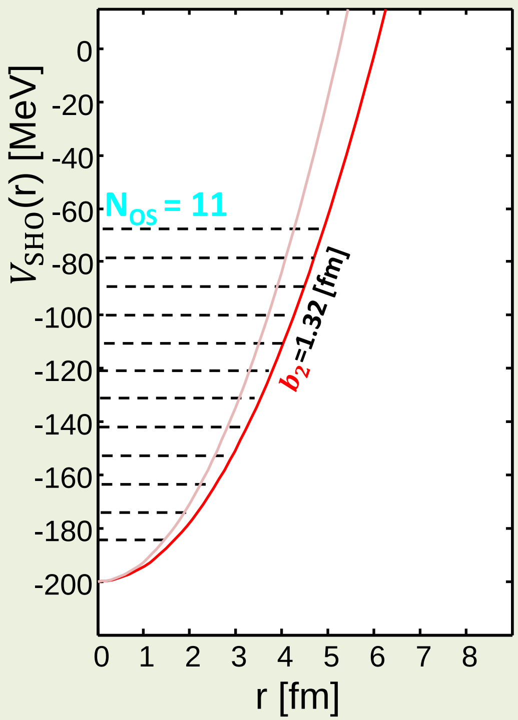

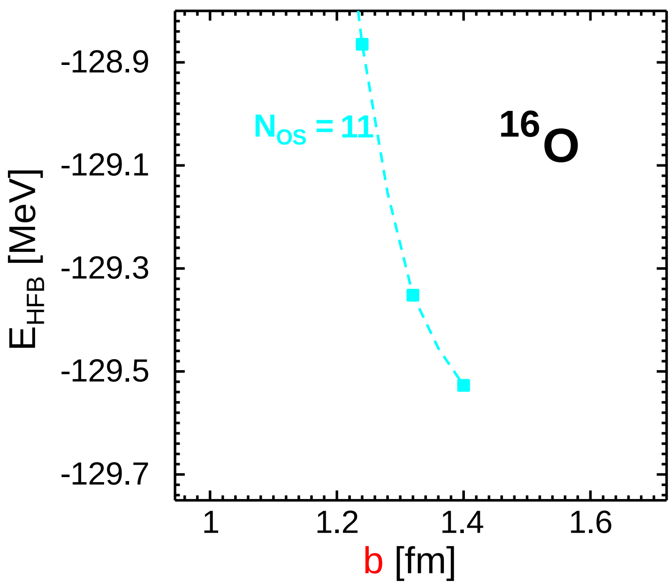

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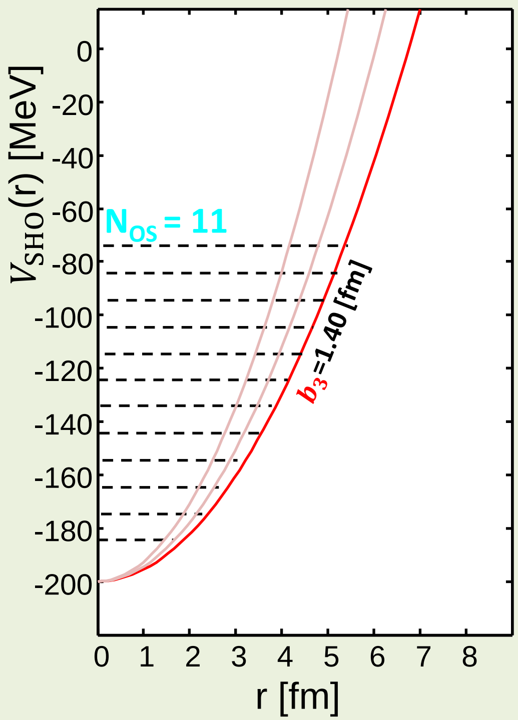

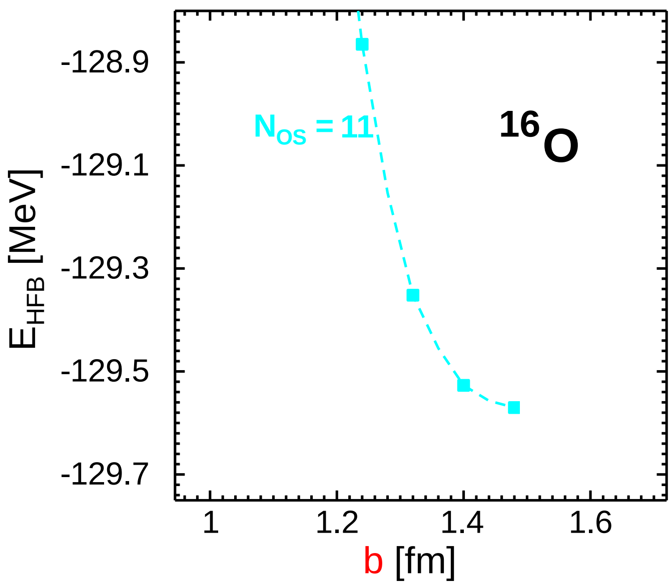

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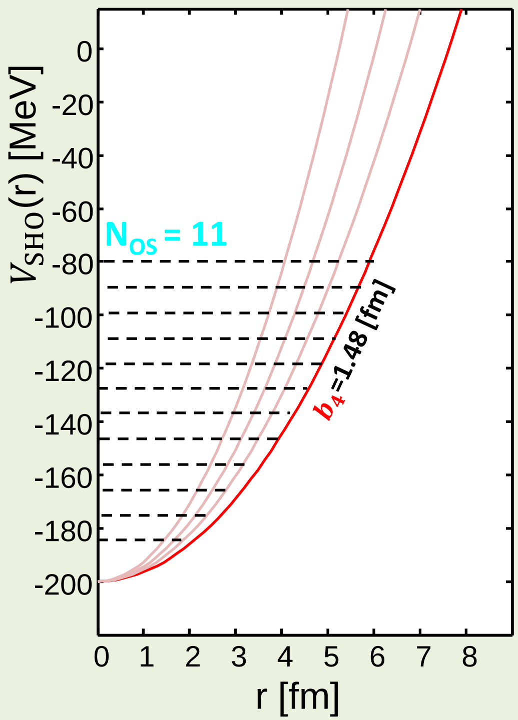

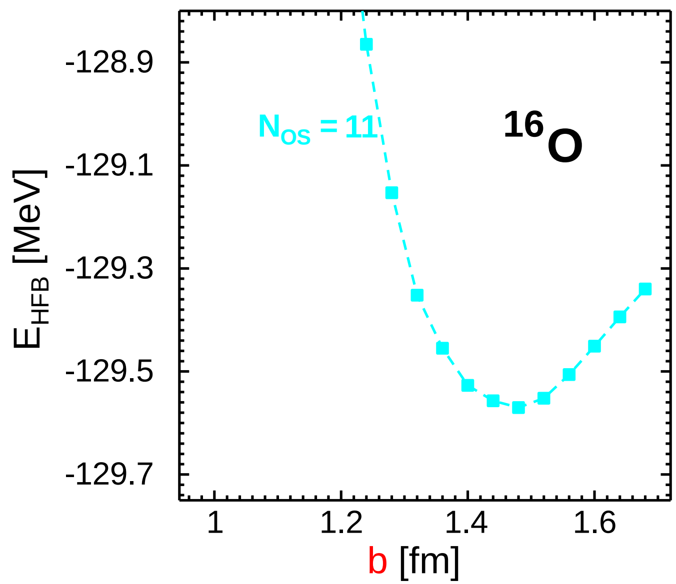

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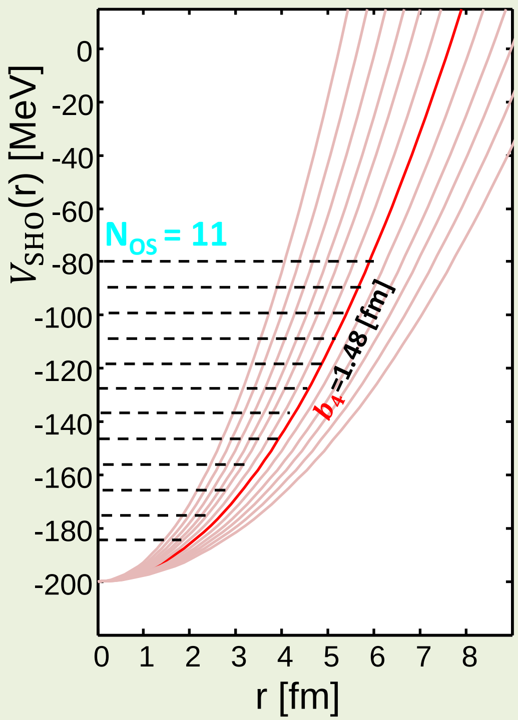

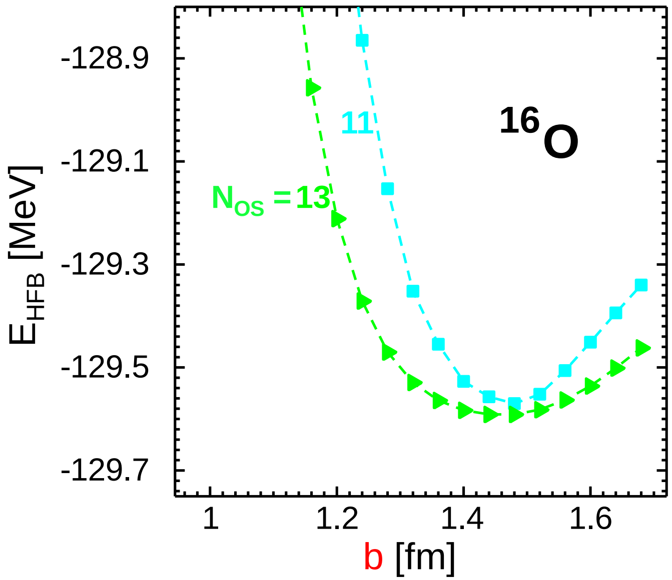

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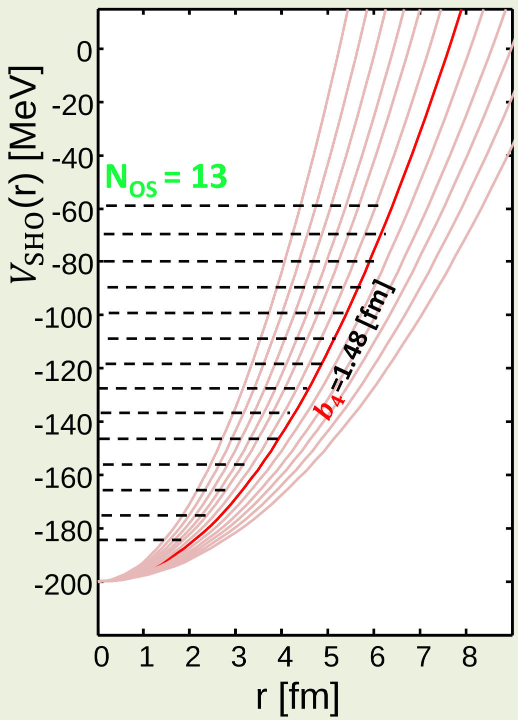

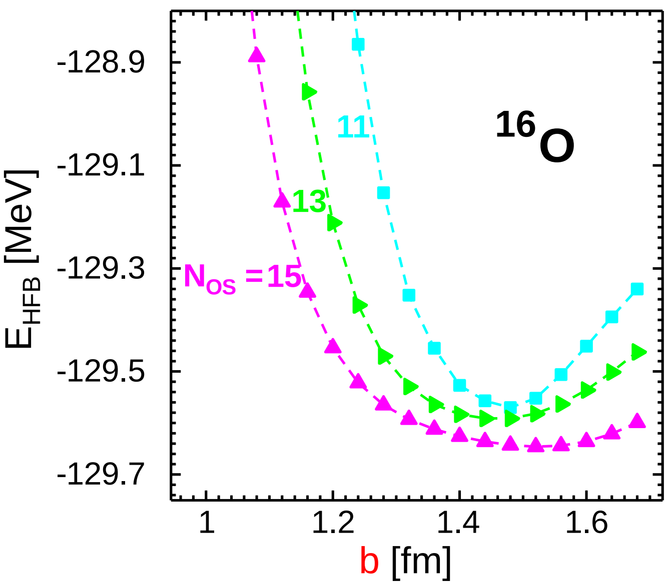

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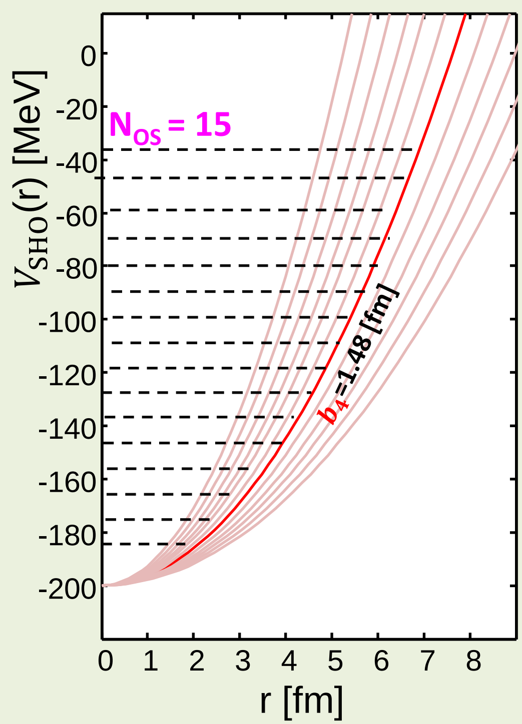

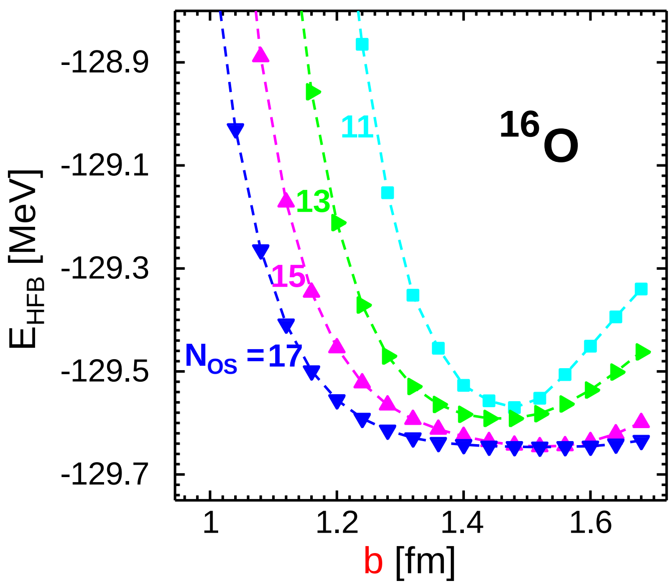

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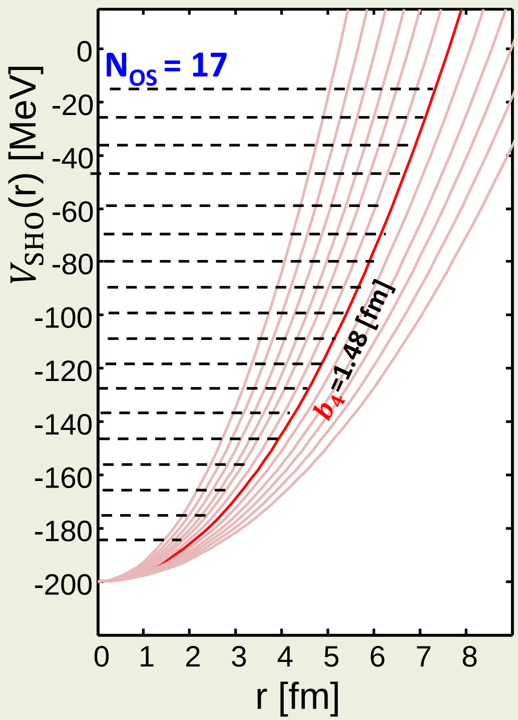

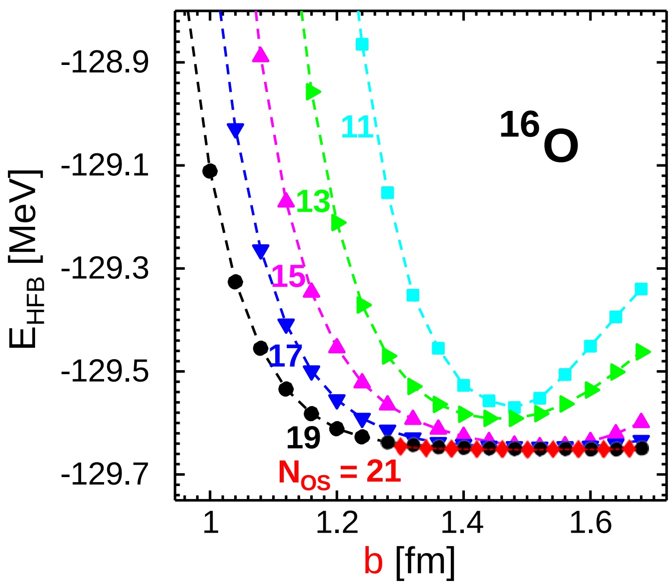

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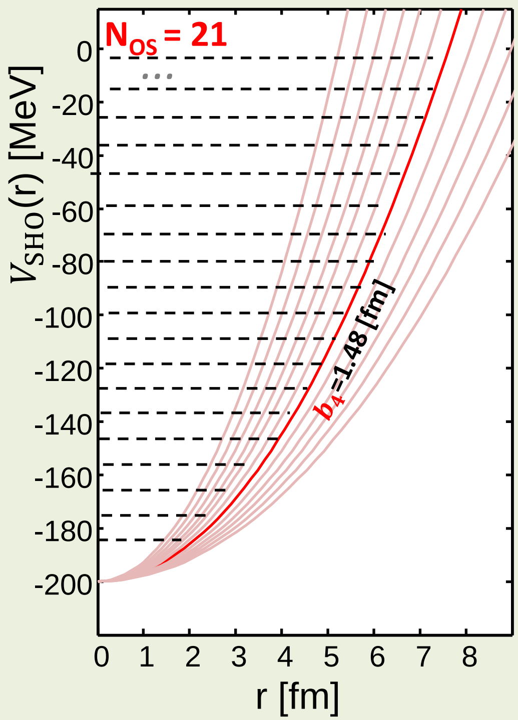

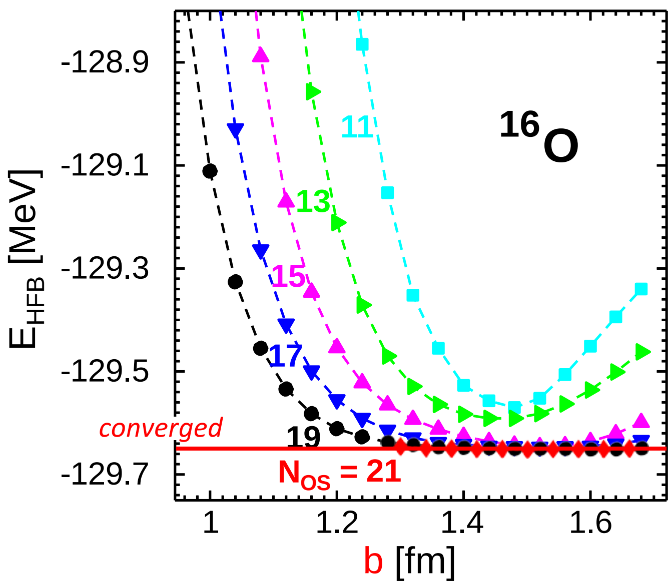

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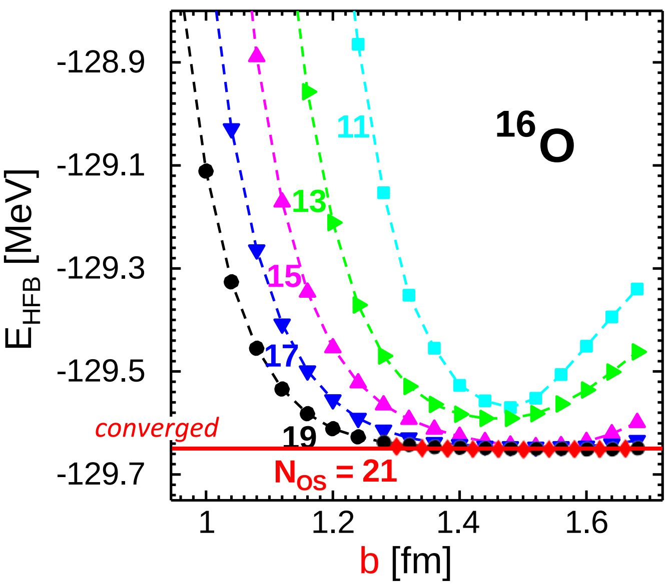

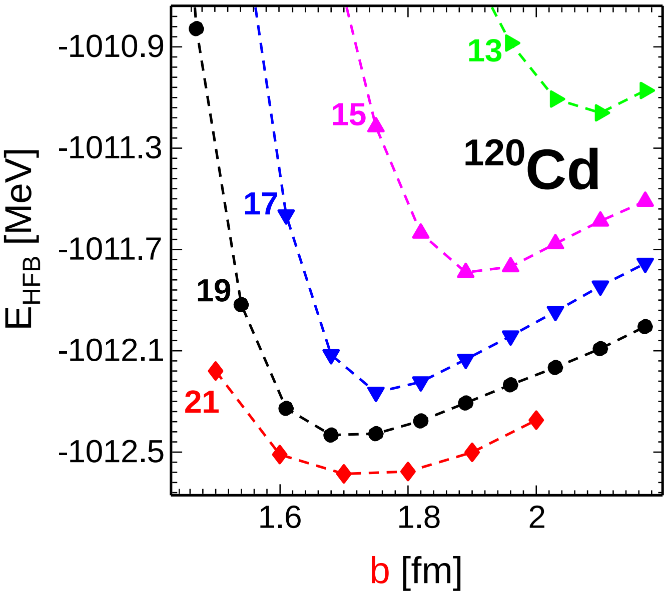

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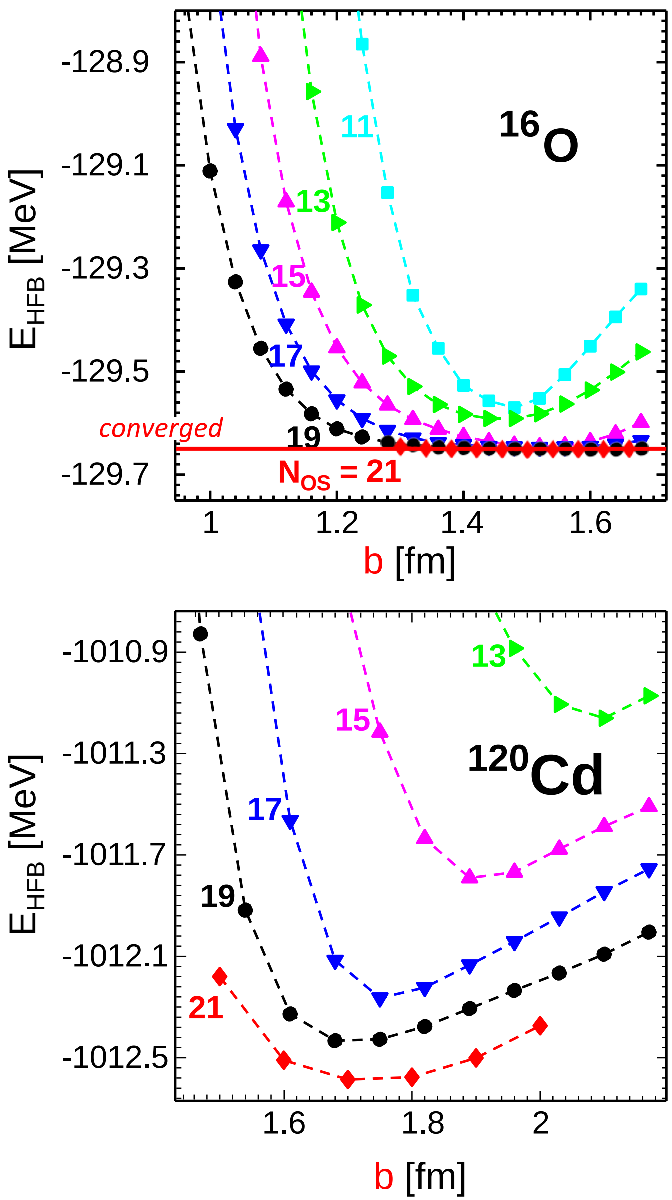

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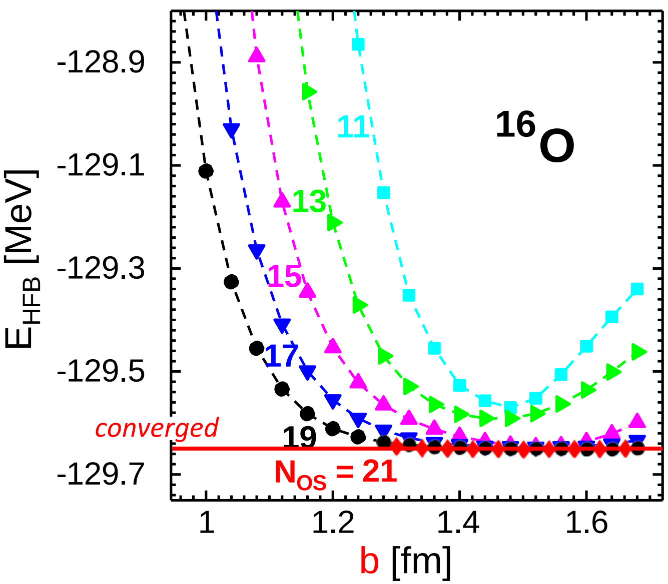

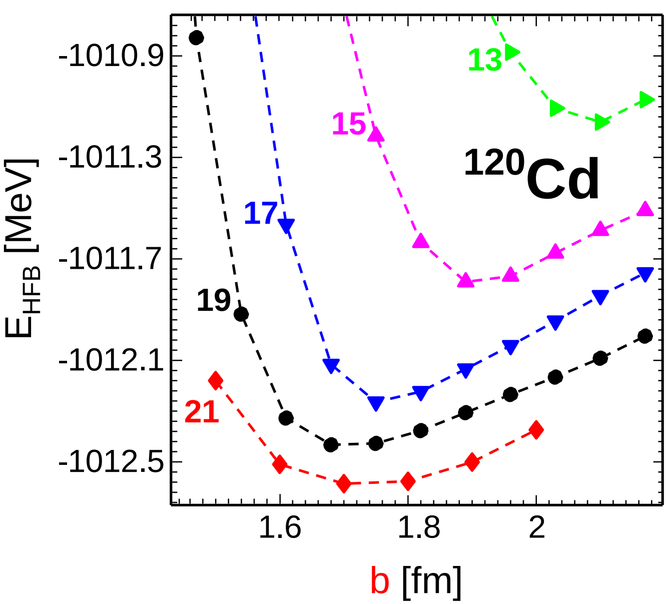

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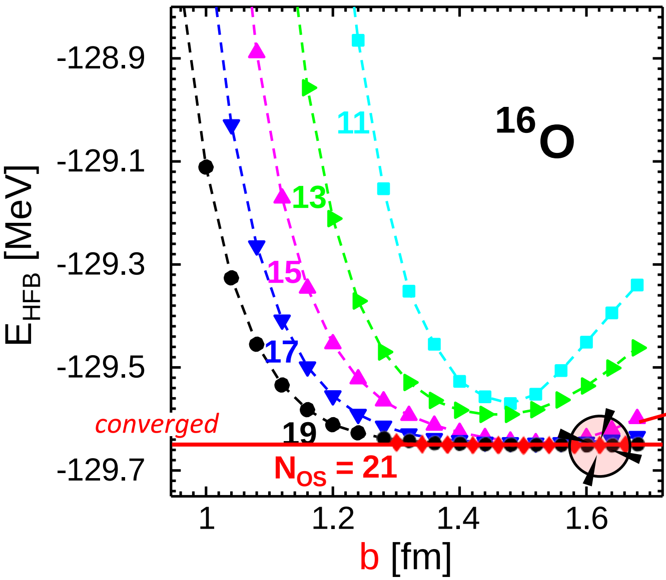
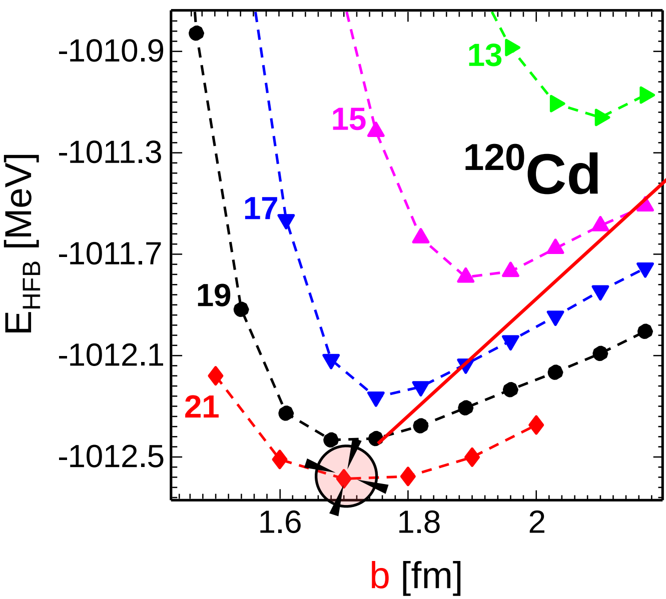
- Recently new IR-extrapolation scheme with firm theoretical background developed

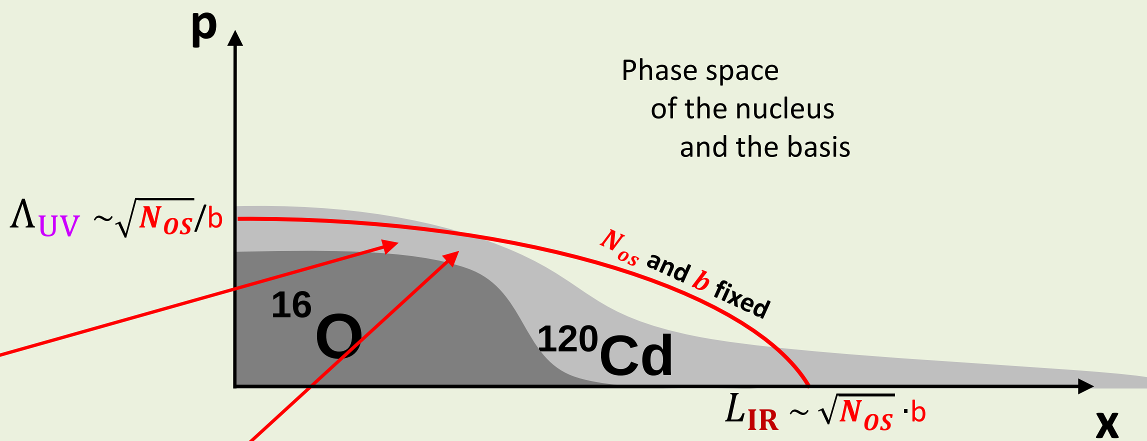
*Furnstahl R.J., Hagen G., Papenbrock T., PRC86, 031301 (**2012**)*
*More S.N. et al., PRC87, 044326 (**2013**)*
*Furnstahl R.J., More S.N., Papenbrock T., PRC89, 044301 (**2014**)*
*Furnstahl R.J. et al, arXiv:1408.0252 (**2014**)*

However, have not yet been systematically tested on whole isotopic chains.

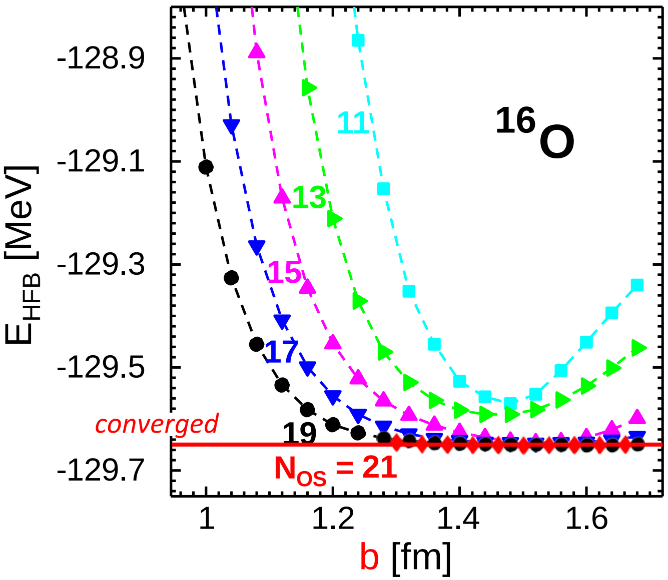


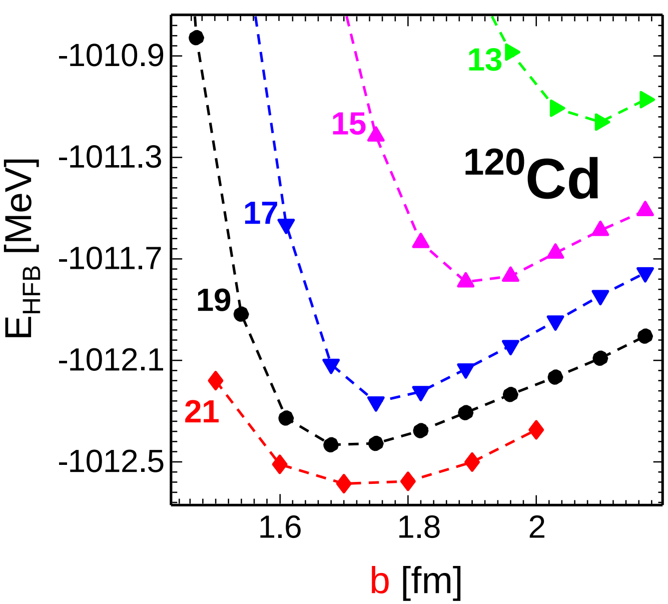


IR-Extrapolation to infinite basis



- Truncating working basis, we effectively impose
  -> **x**: a hard-wall L_{IR} **cutoff**
  -> **p**: analogous sharp Λ_{UV} **cutoff**





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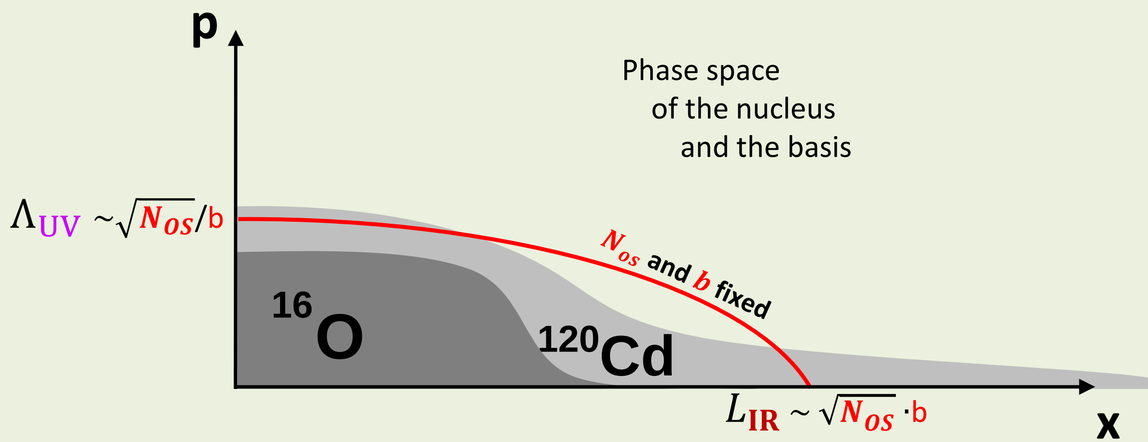

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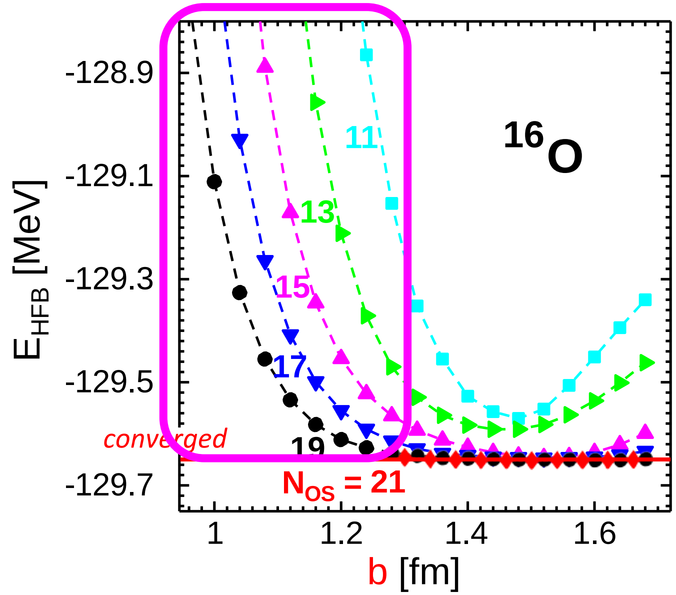
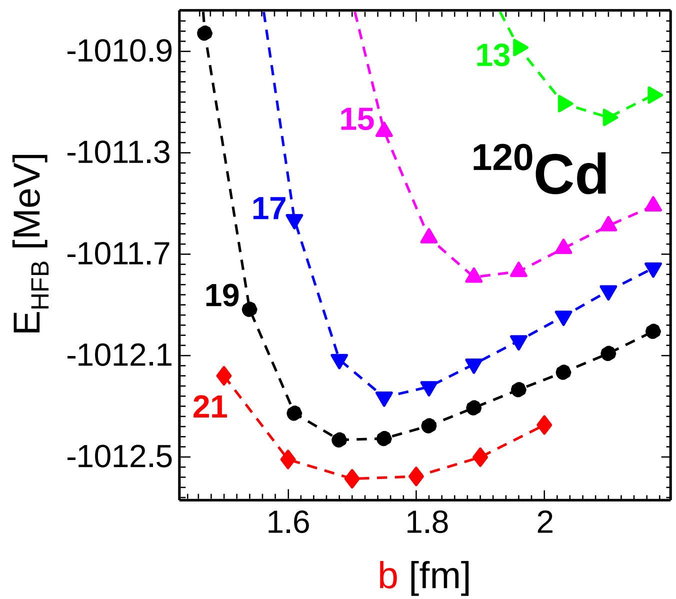
- **Full Convergence** - when nucleus "fits" into SHO basis:

IR convergence:	*Spacial extent of the nucleus*	$r < L_{IR}$
UV convergence:	*Largest mom. scale of interaction*	$\lambda < \Lambda_{UV}$

UV converged for small b-values





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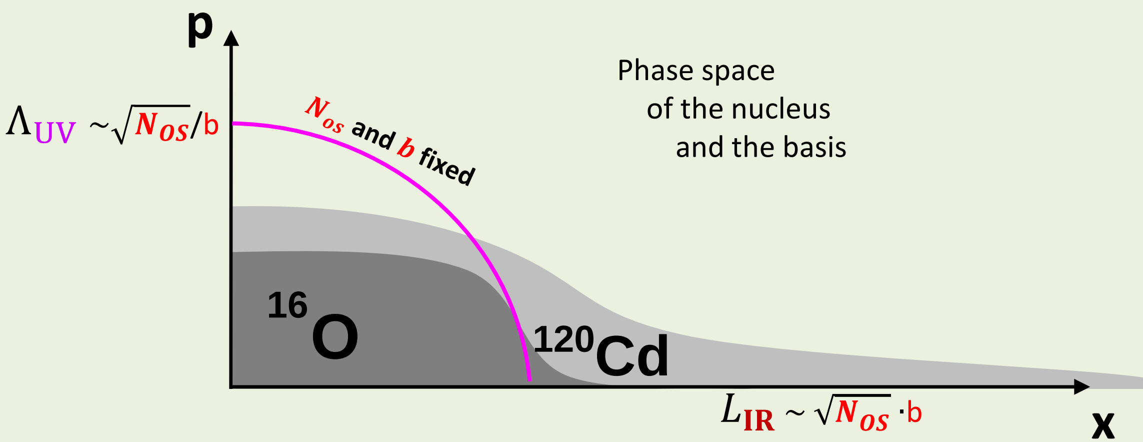

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- **IR-Extrapolation** - binding energy correction in the limit of UV converged results!

✗ **IR convergence:** *Spacial extent of the nucleus* (exponential) $r < L_{IR}$

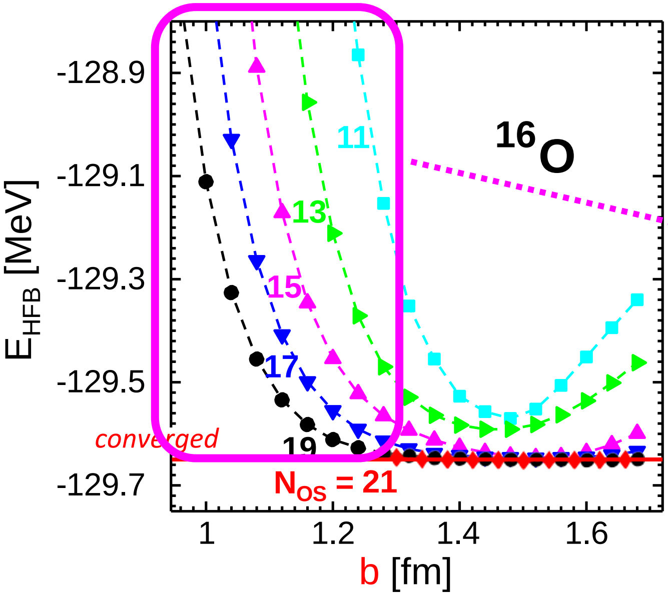
✓ **UV convergence:** *Largest mom. scale of interaction* (Gaussian) $\lambda < \Lambda_{UV}$

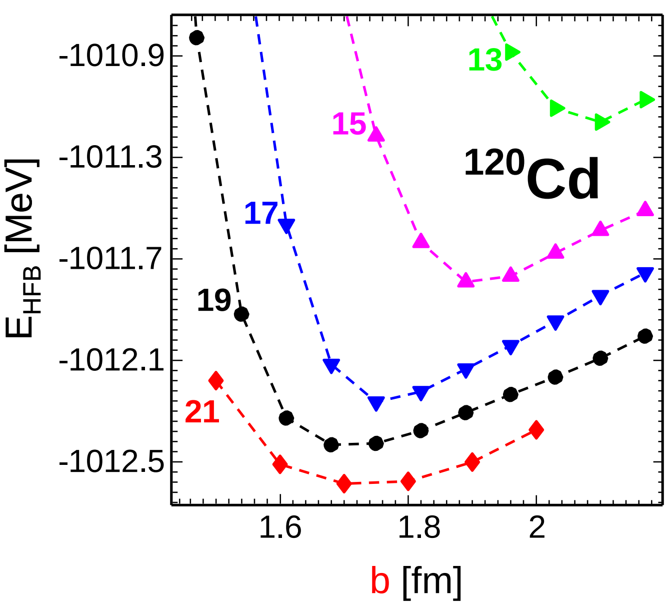
$$E_{HFB}(L_{IR}) = a_0 e^{(-2k_\infty L_{IR})} + E_\infty$$

where a_0 , k_∞ and E_∞ are fit constants, and L_{IR} = *depends on basis and nucleus*

Convergence analysis

UV converged for small b-values





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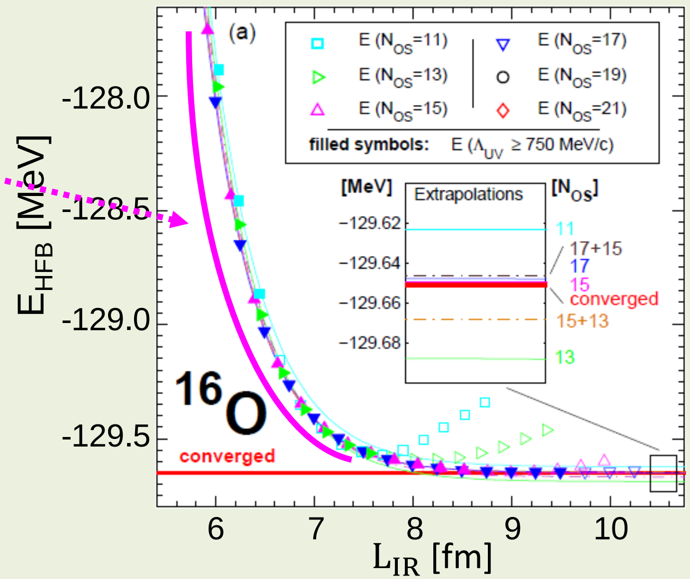

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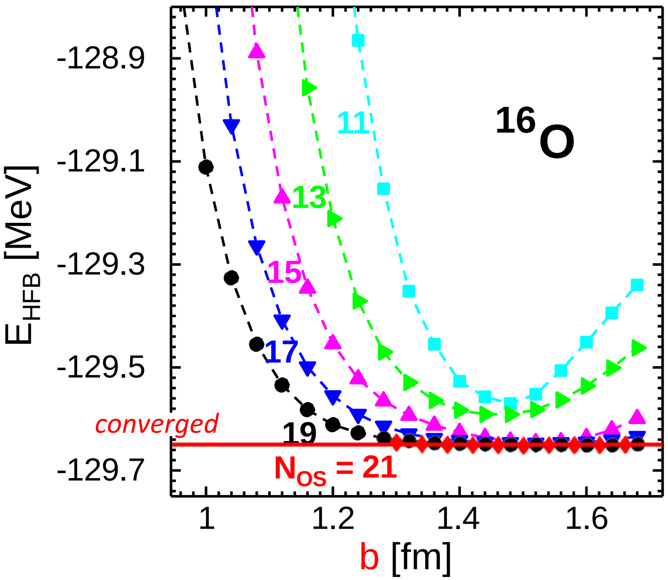

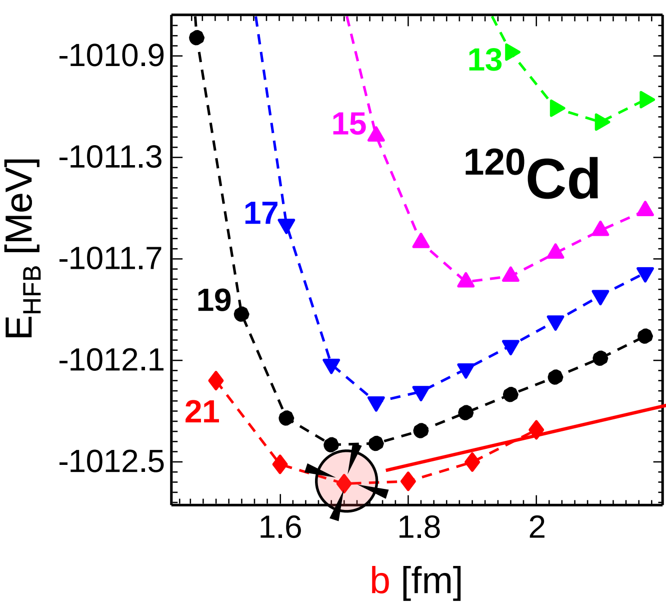

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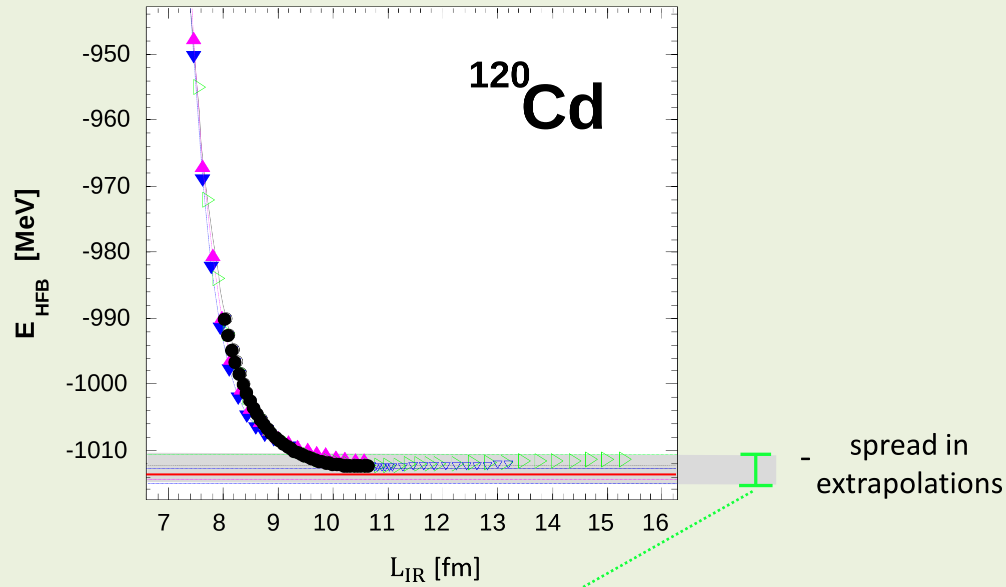
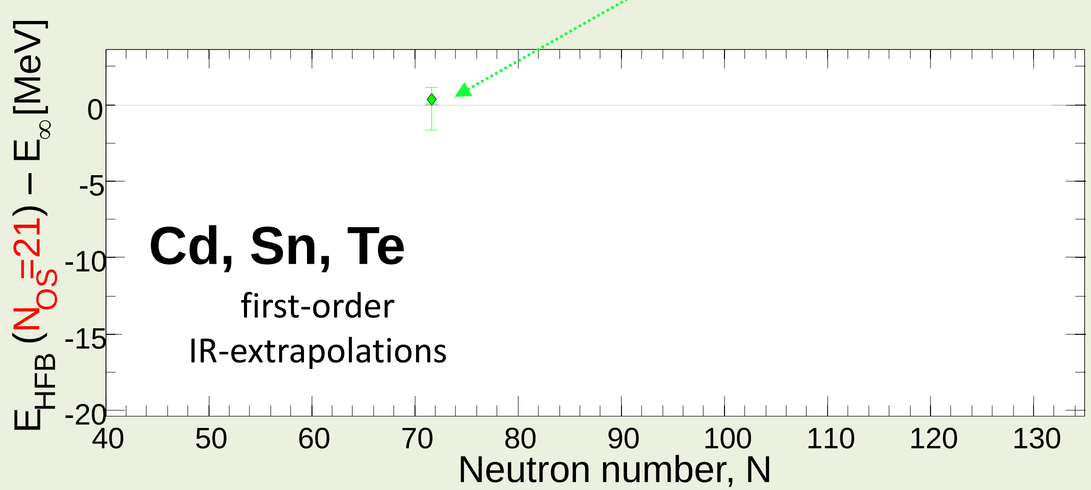
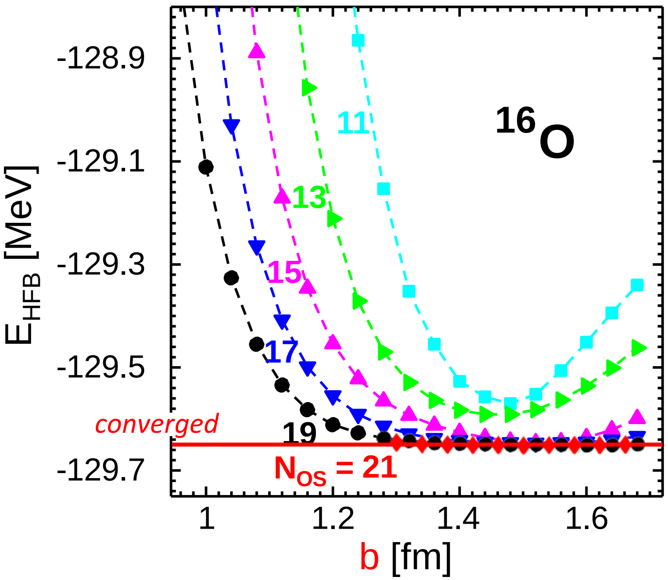
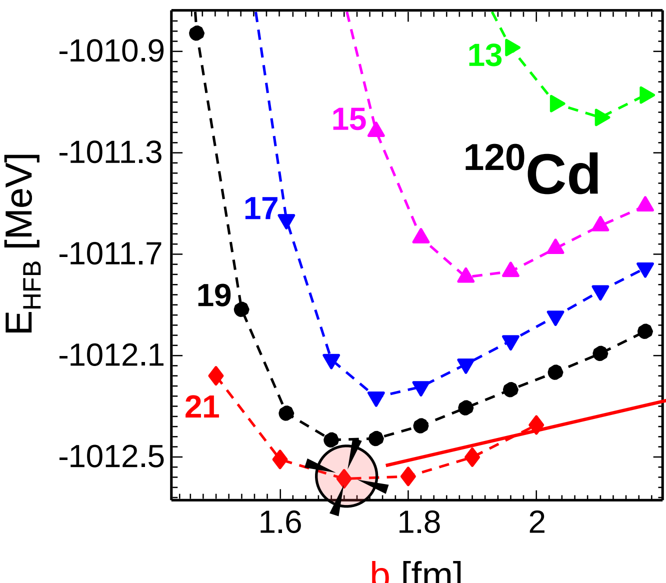




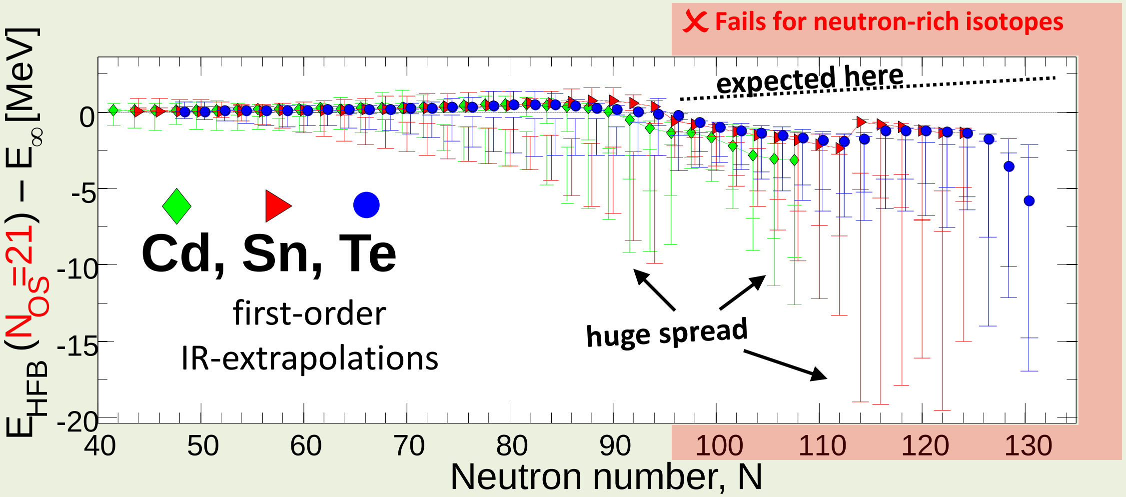




IR-Extrapolation to infinite basis

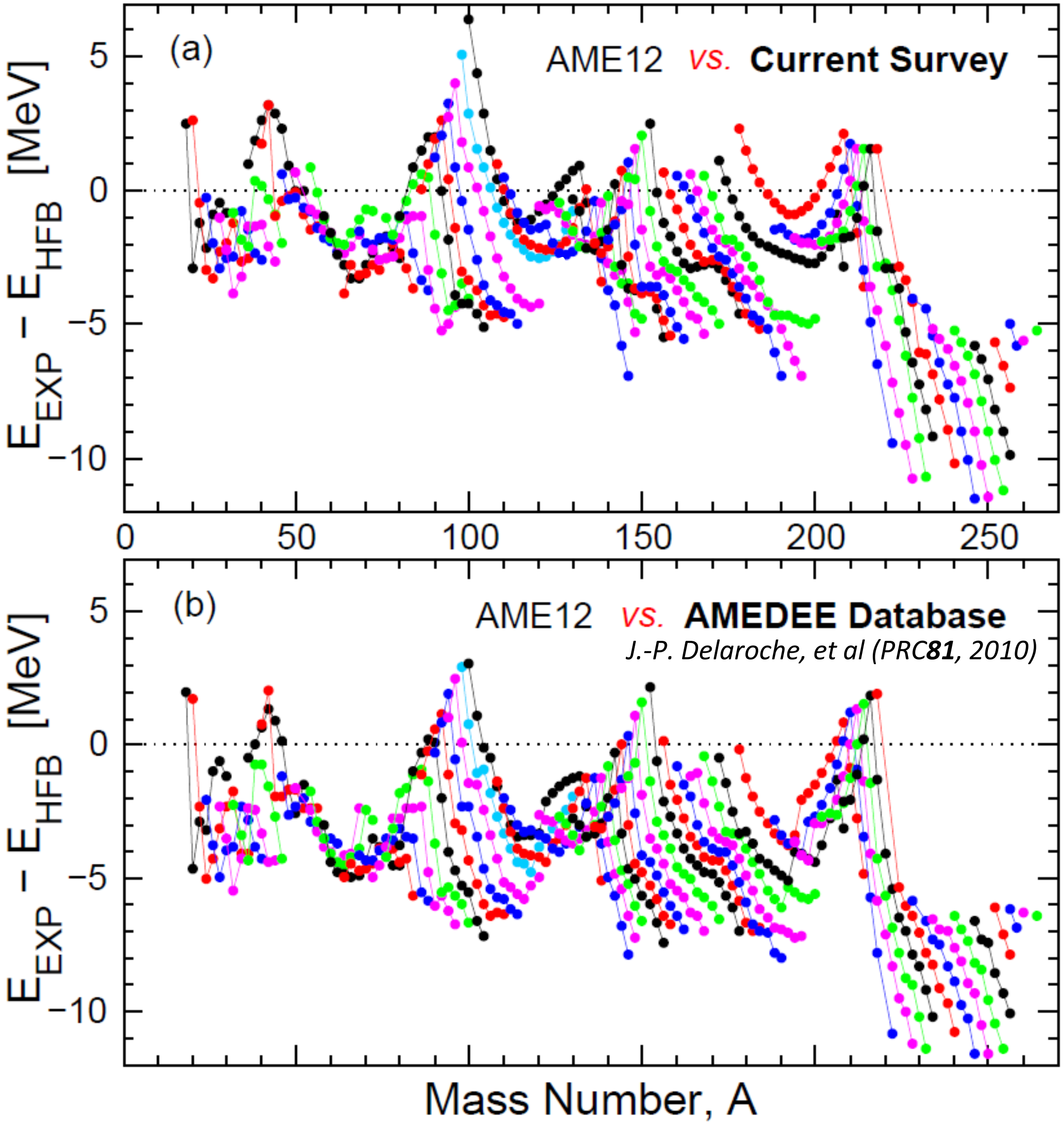
⟹ **Second-order IR-corrections for loosely bound nuclei?**
Preliminary checks unsatisfactory.
Still not adapted for atomic nuclei.

⟹ At present we do not have a reliable and universal extrapolation method for binding energies to the limit of an infinite basis for HFB-based models!



Large-scale HFB calculation
and **Beyond-Mean-Field corrections**

global mass surveys for ***axially deformed Mean Field HFB-D1S*** *calculation for* ***even-even*** *nuclei*



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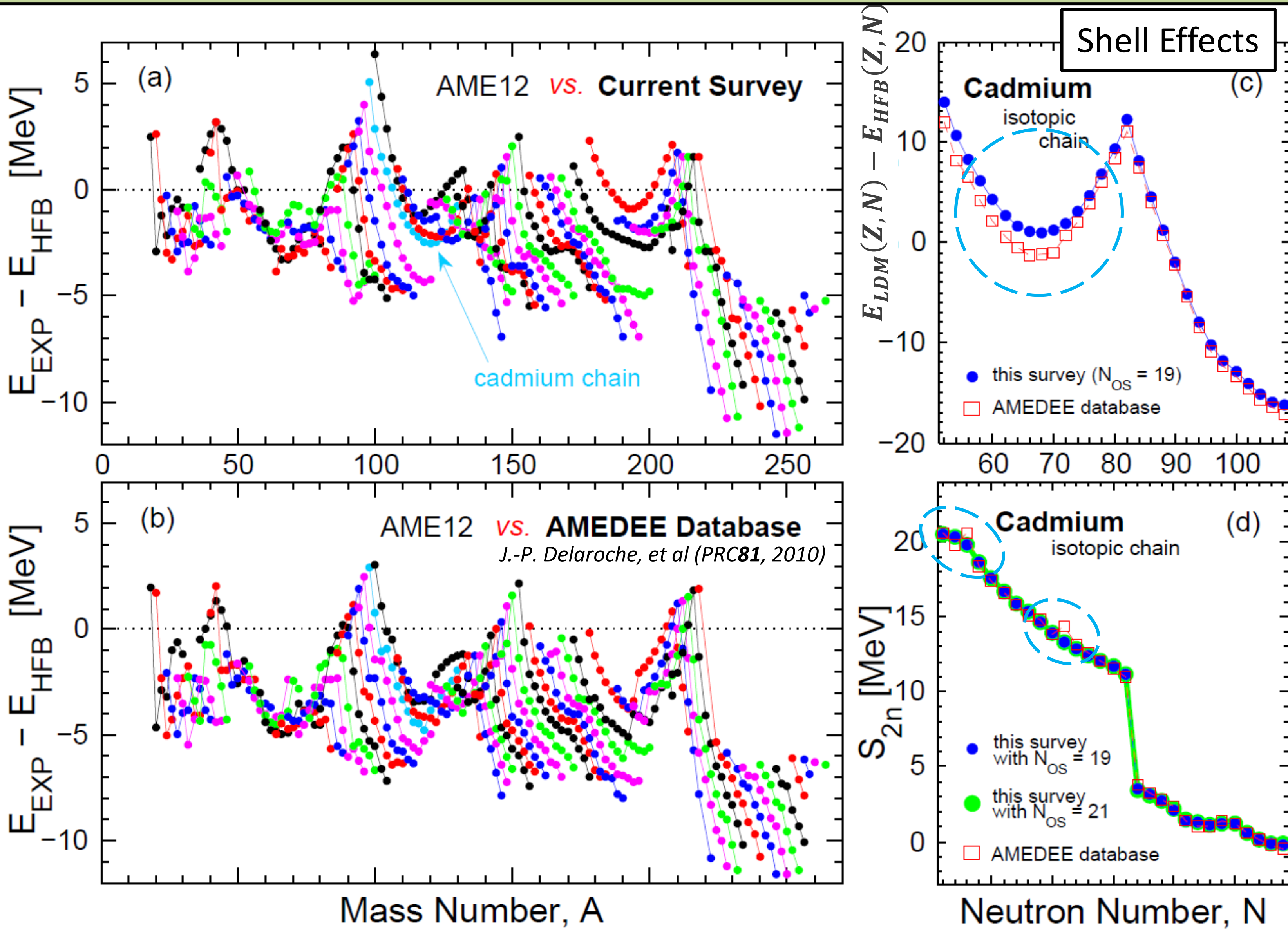

- **Mean Field approach of HFB:**
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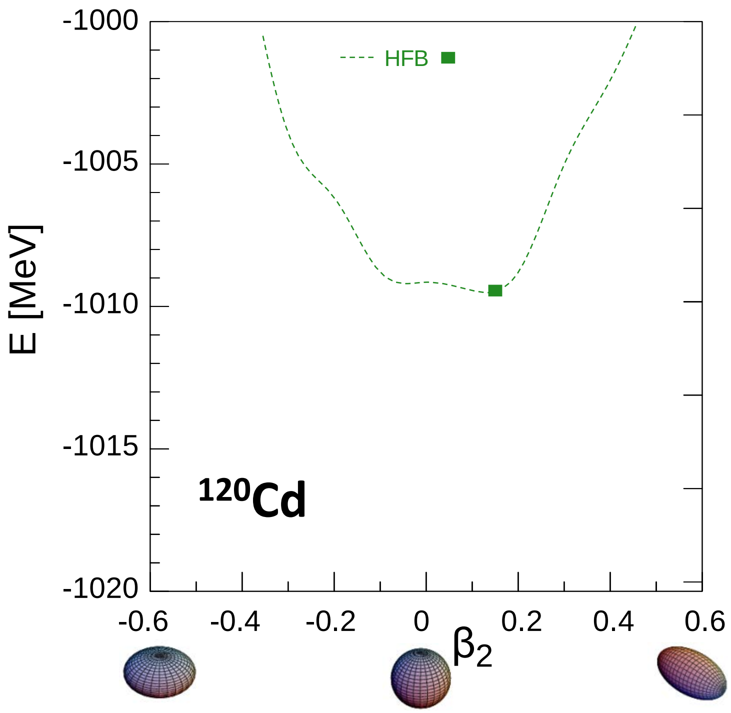

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Digging Beyond the Mean Field

Symmetry restoration by

- **Variation After Particle Number Projection (PN-VAP):**
  $\Delta E_{PN-VAP} \sim 2.3$ MeV

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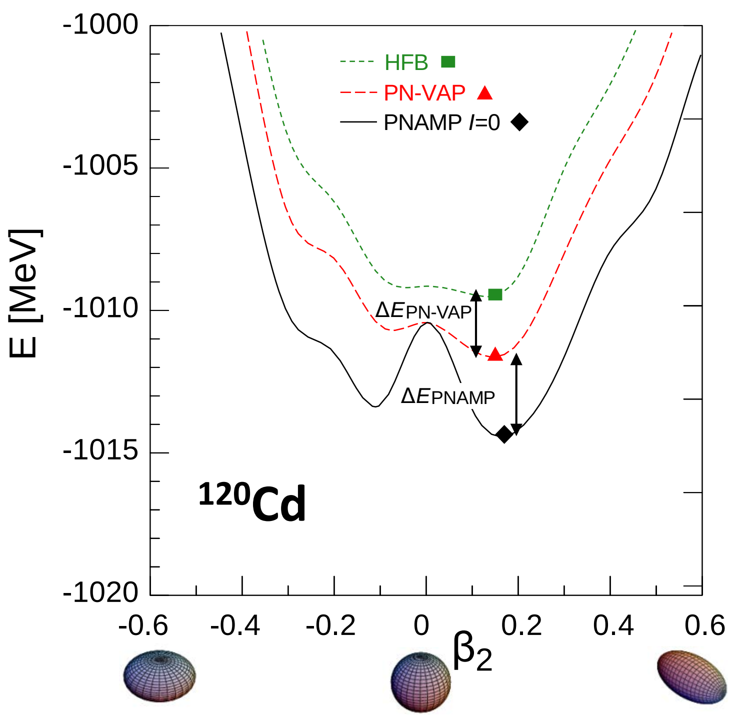

BMF correlations

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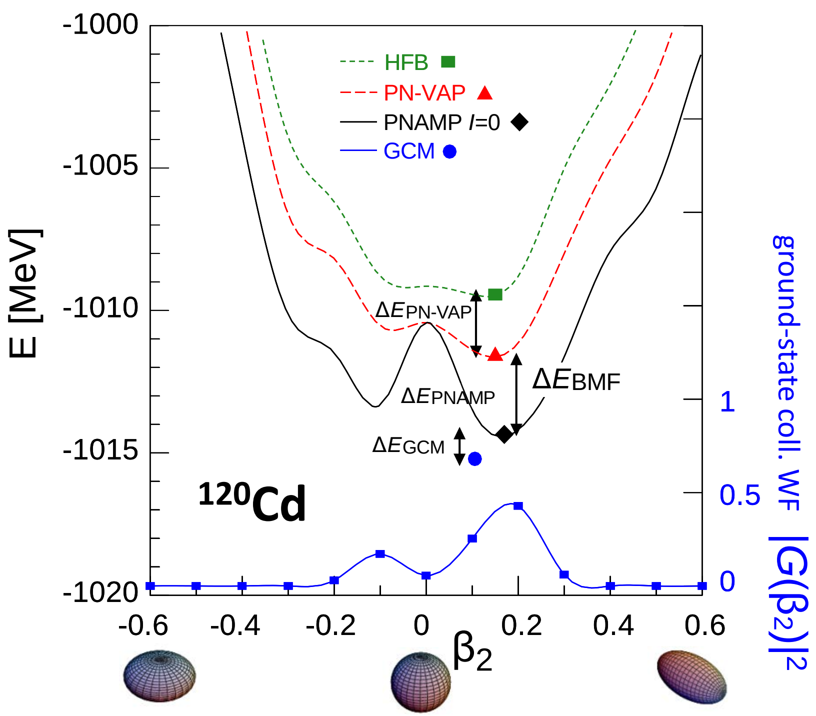

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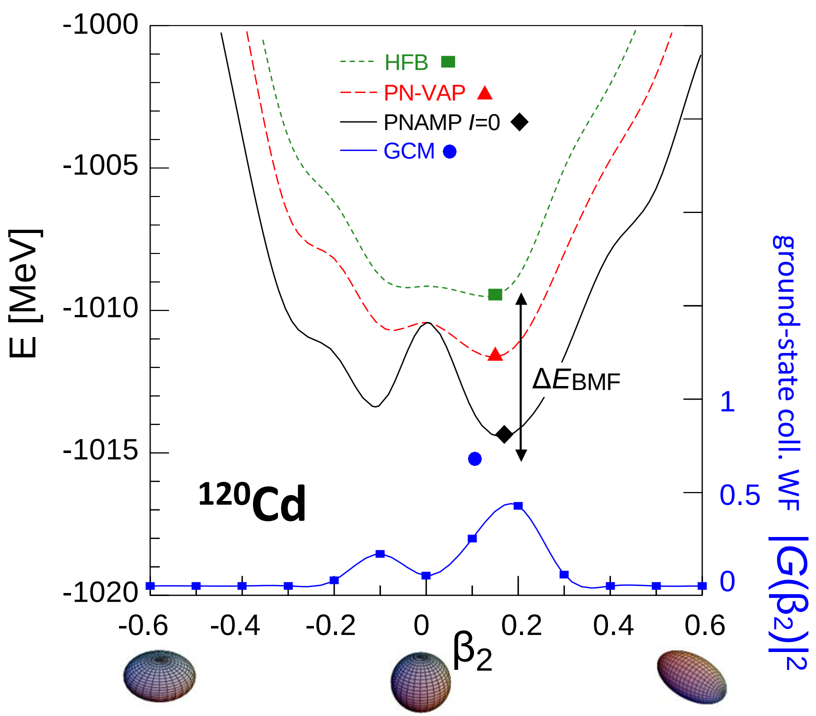

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$$E_{GCM} = E_{HFB}(N_{OS} = 19) - \Delta E_{BMF}$$

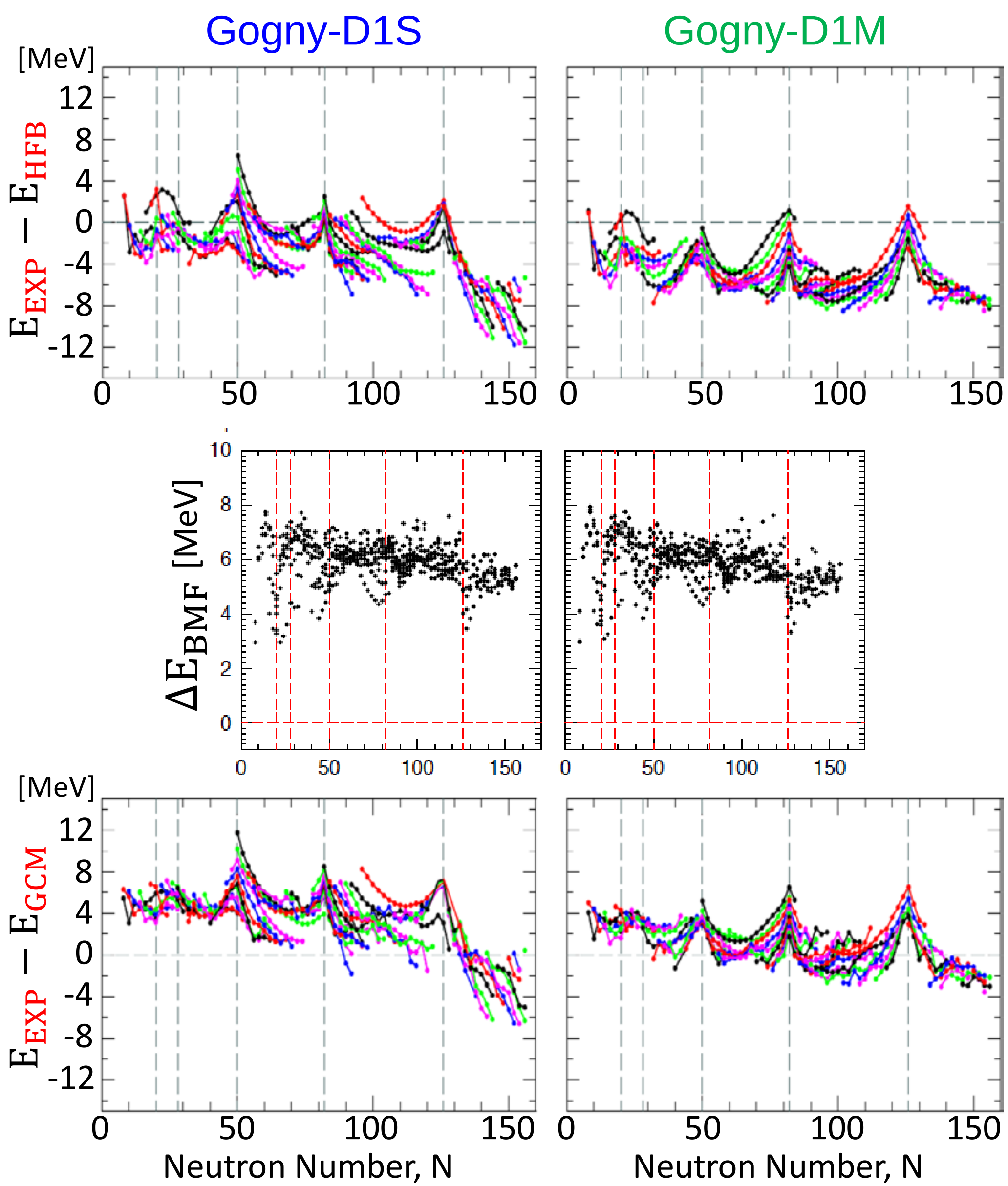
where the BMF correlations are calculated as

$$\Delta E_{BMF} = E_{HFB}(N_{OS} = 11) - E_{BMF}(N_{OS} = 11)$$

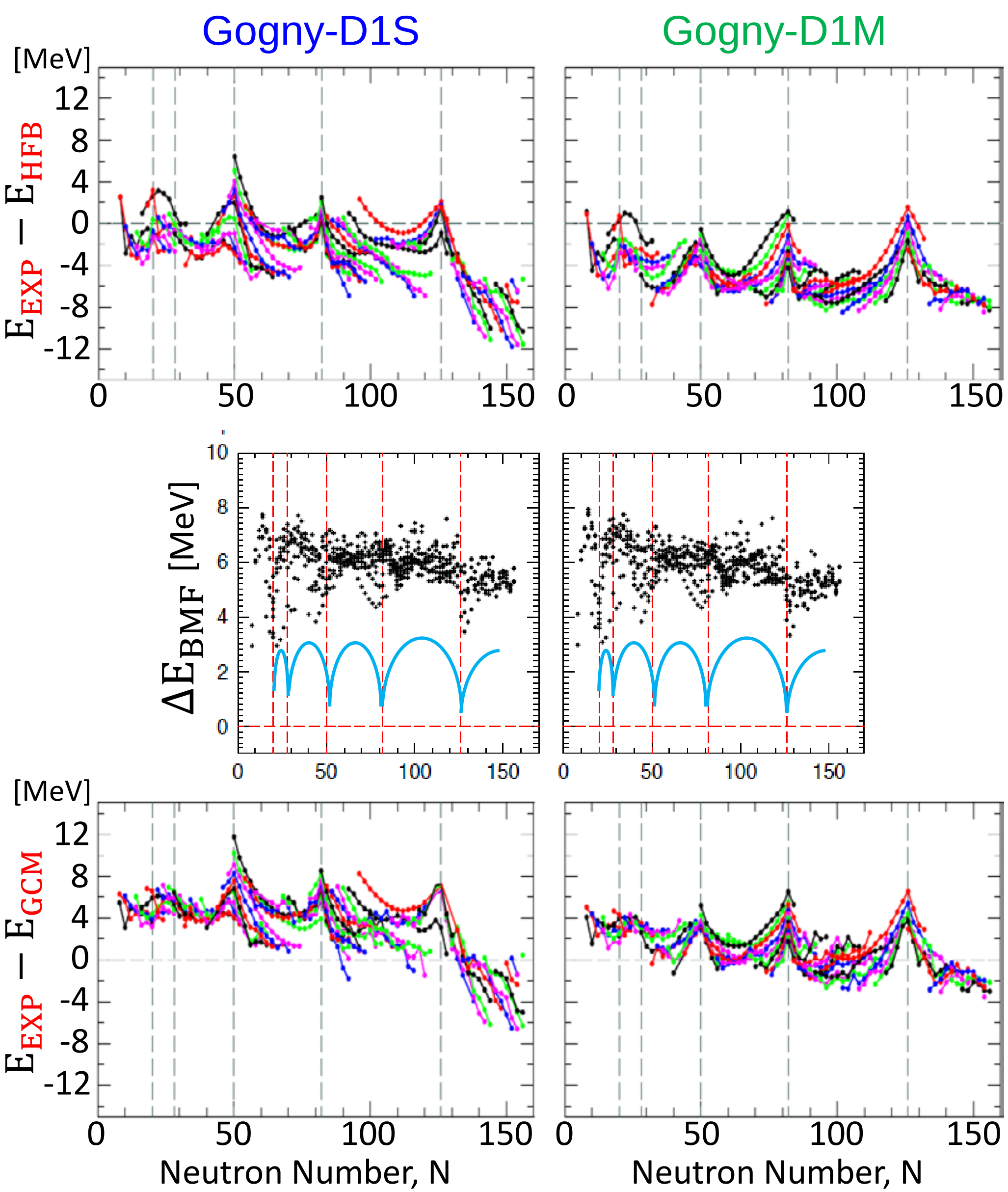
because of heavy computational burden

$t_{BMF}(N_{OS} = 11) \approx 60h$ $\qquad$ $t_{BMF}(N_{OS} = 19) > 1000h$

BMF correlations



- Similar behavior of $\Delta \mathrm{E_{BMF}}$ −corrections for both Gogny functionals D1S and D1M with $\Delta \mathrm{E_{BMF}} \sim 5.8$ MeV



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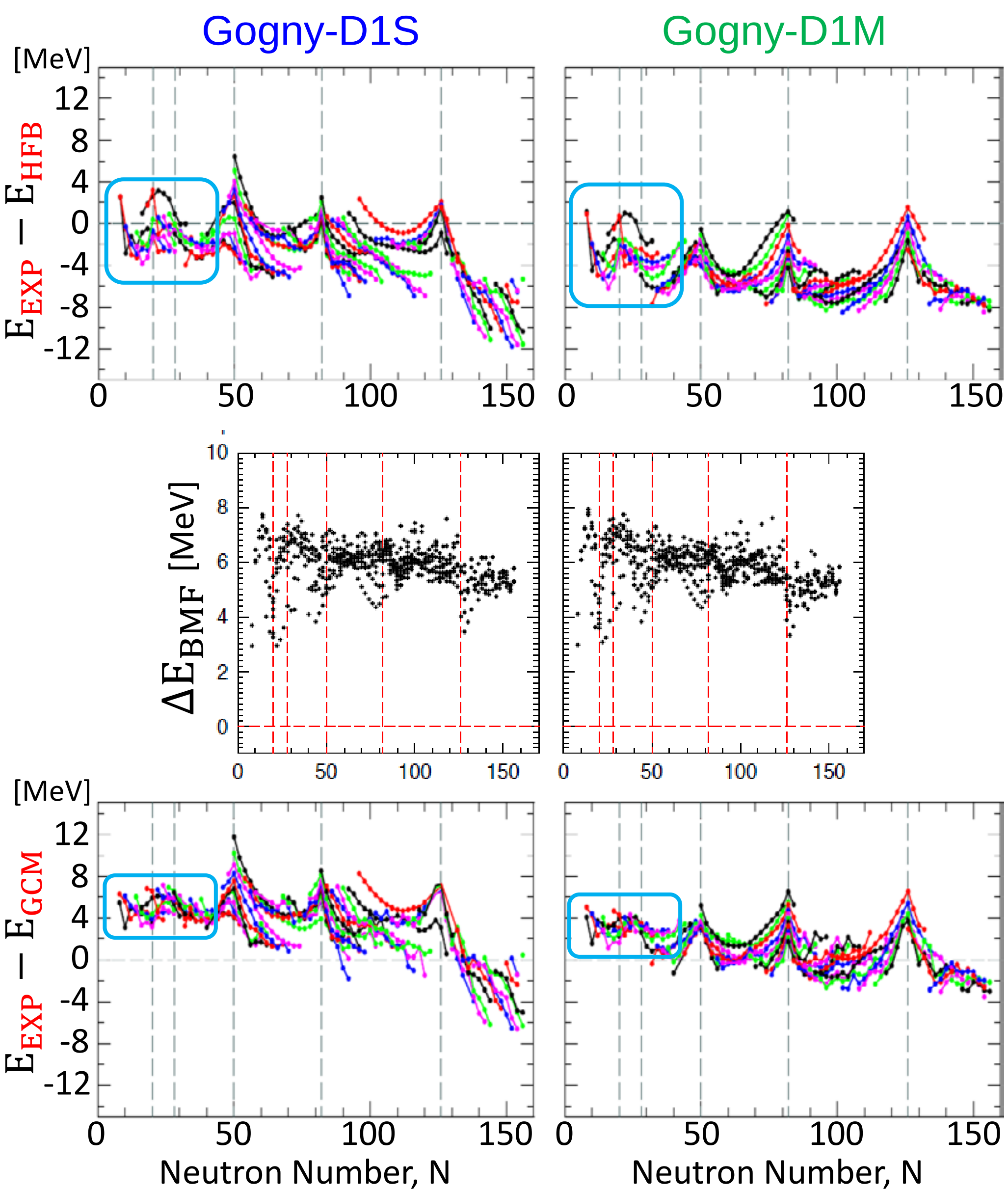

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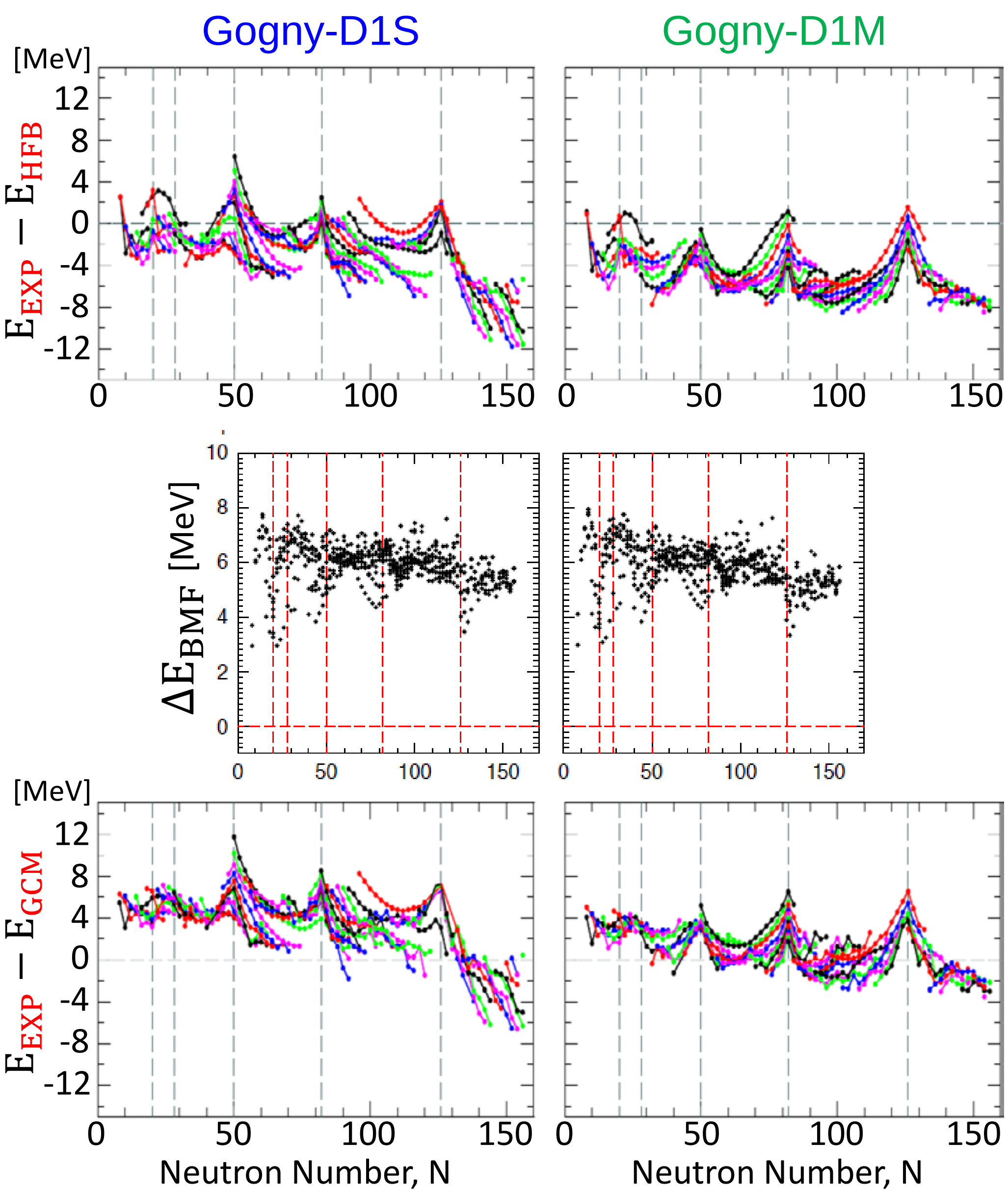

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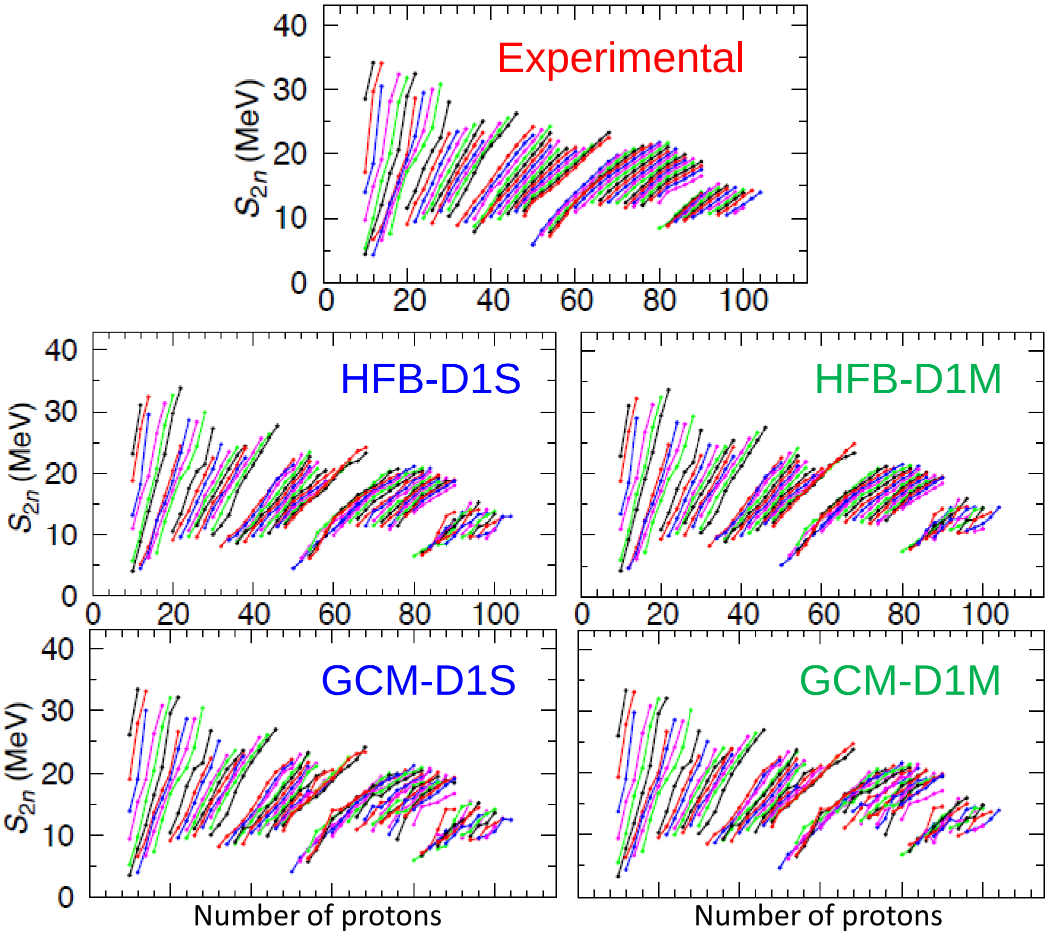
- Spread light nuclei $(N = 10 - 40)$ is significantly reduced when BMF correlations are taken into accout
- Overbinding for both D1S and D1M can be solved by re-fitting the EDF functional
- ... but it is still an open question whether re-fitting EDF functional with these and other BMF effects *self-consistently* can flatten the curves ?

BMF correlations



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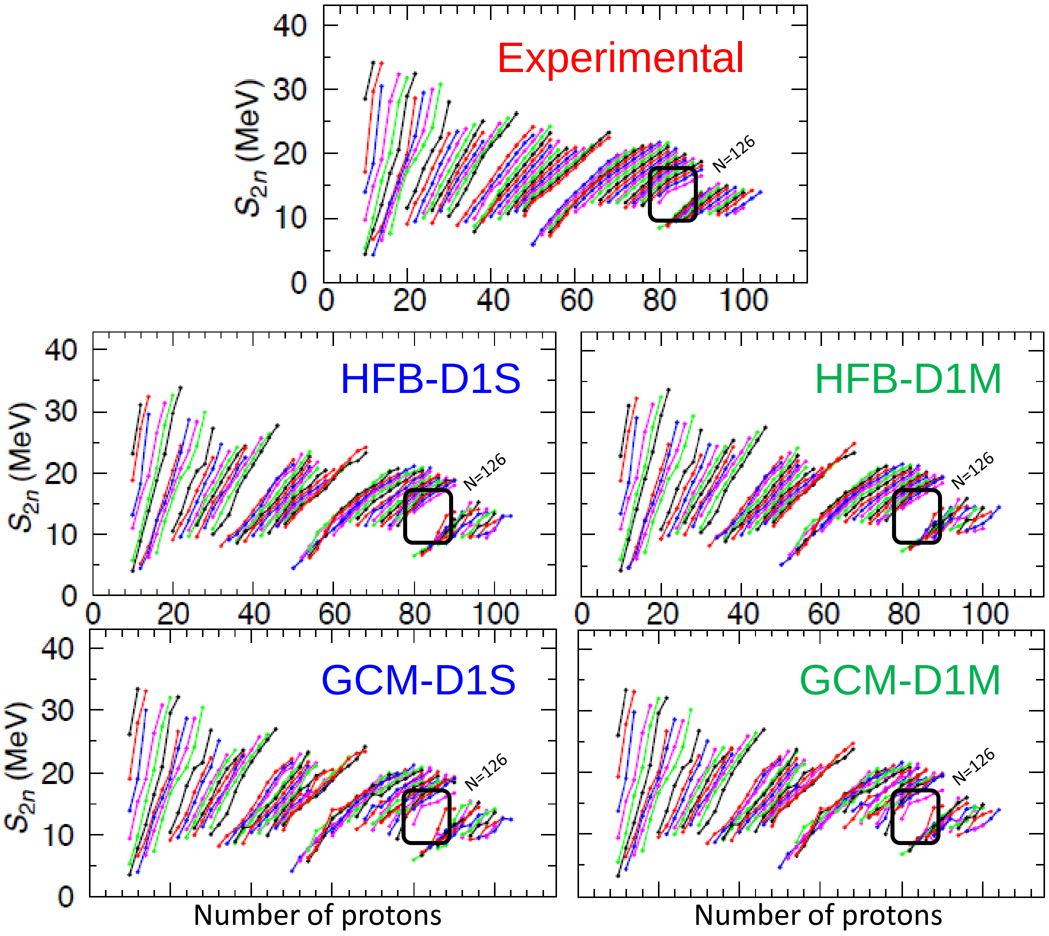

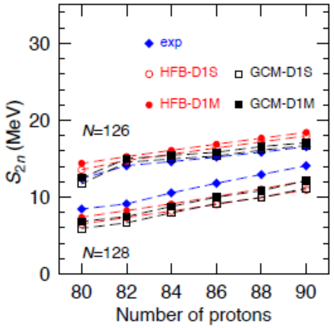

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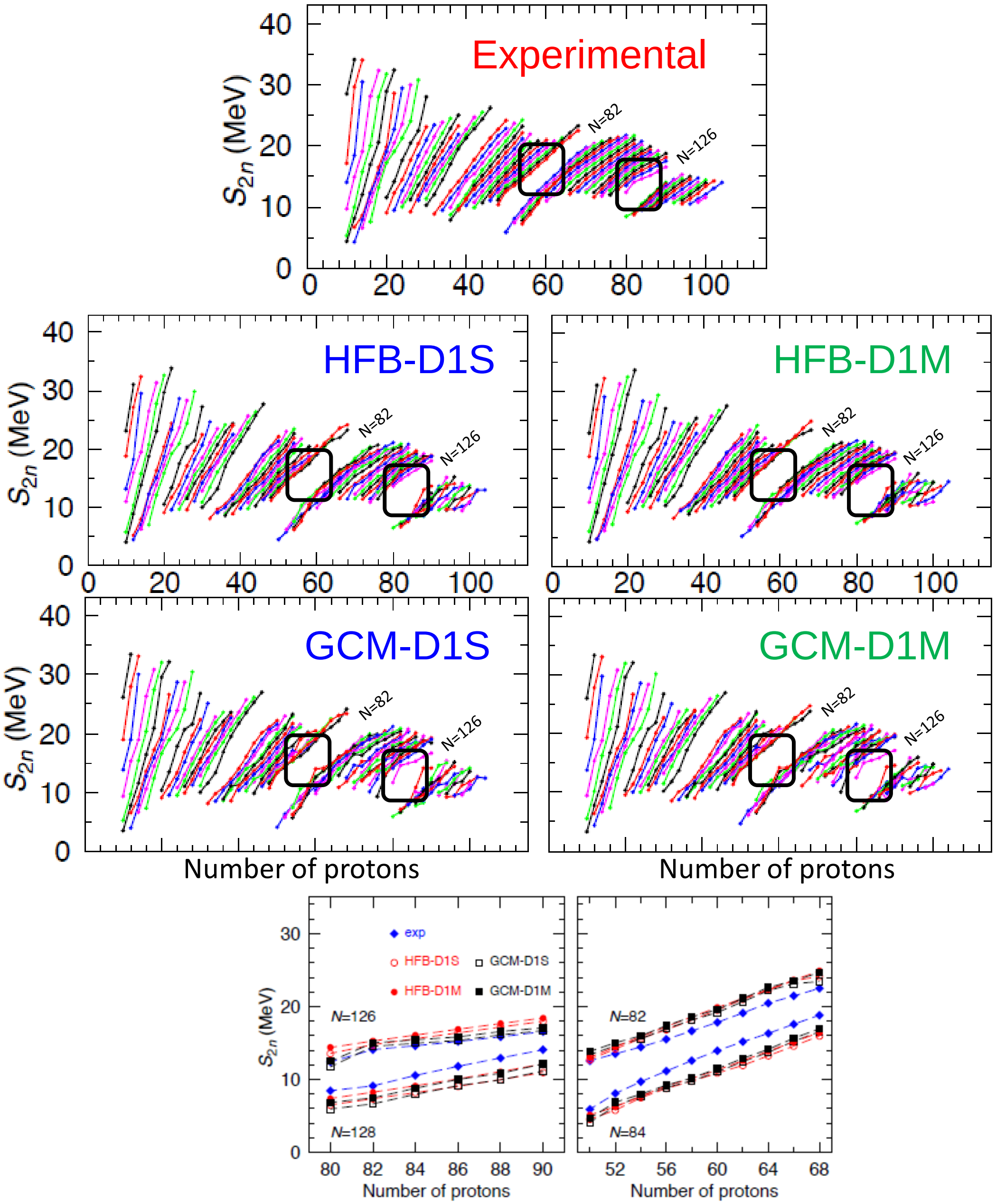

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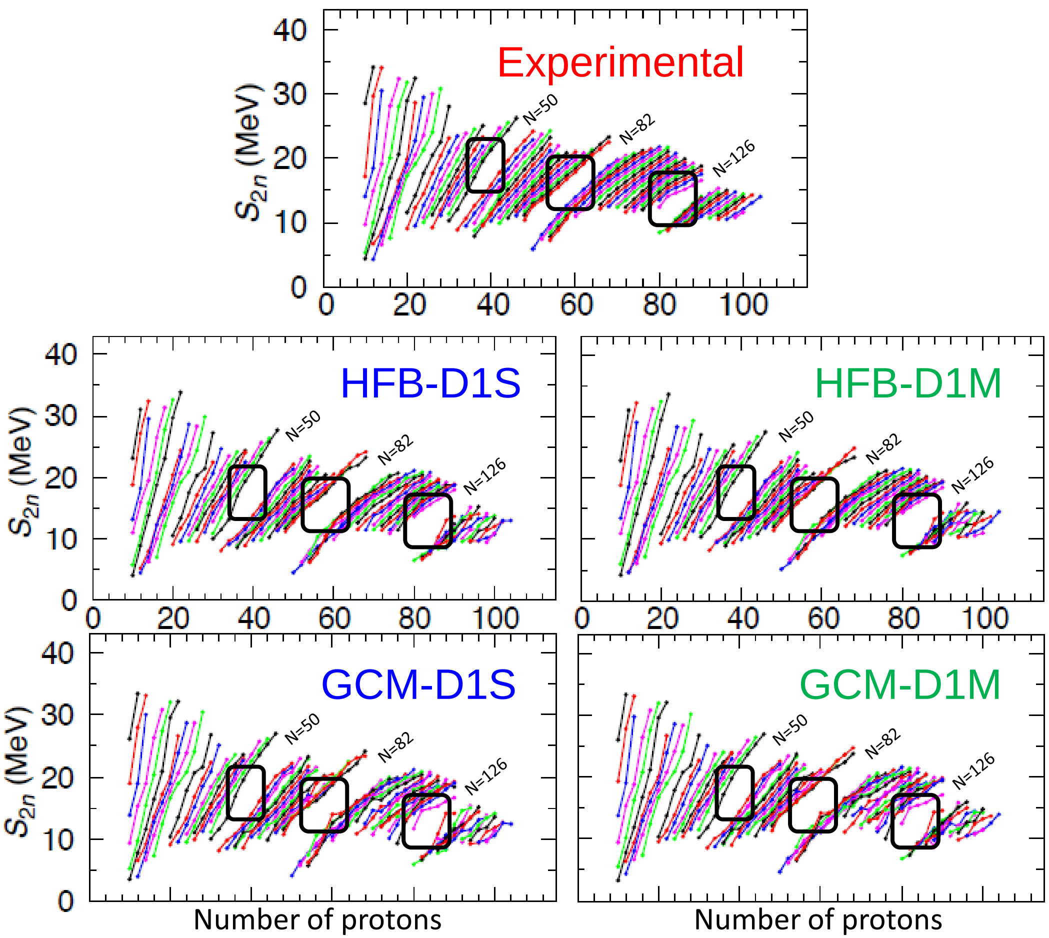

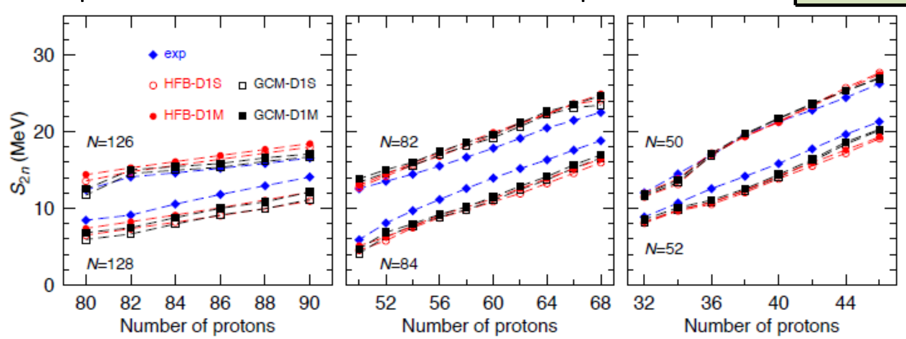

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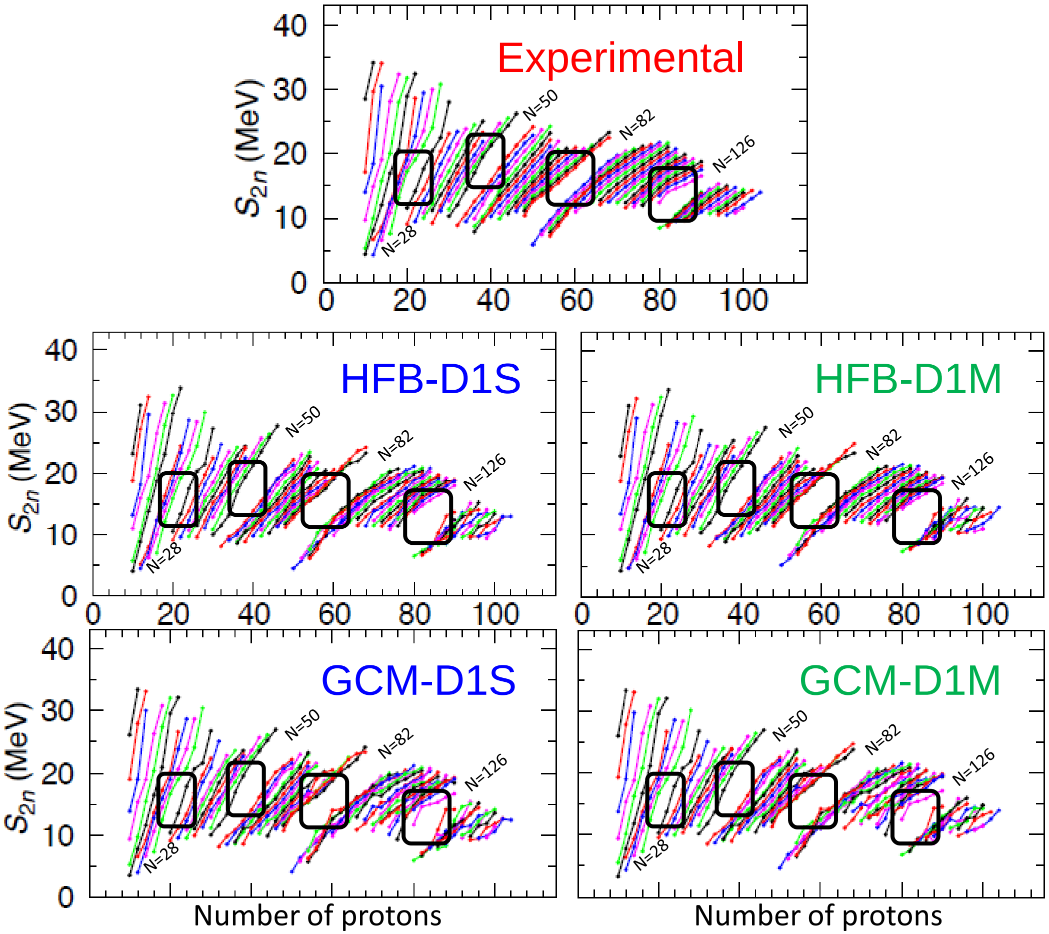

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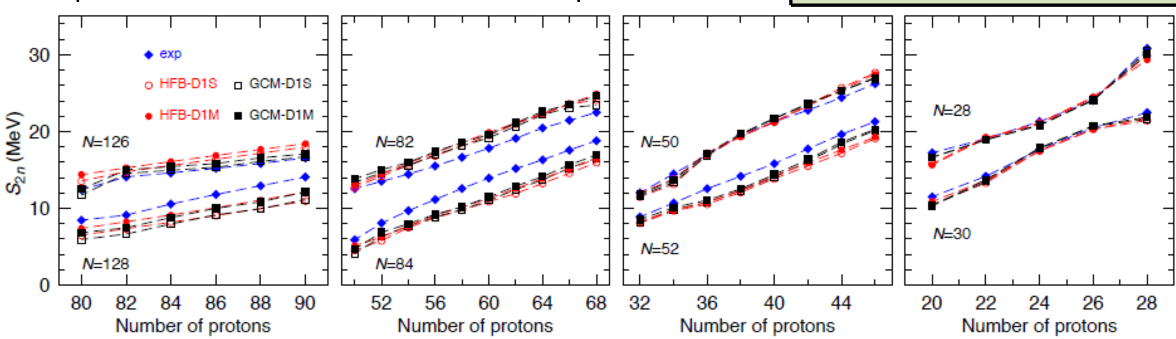

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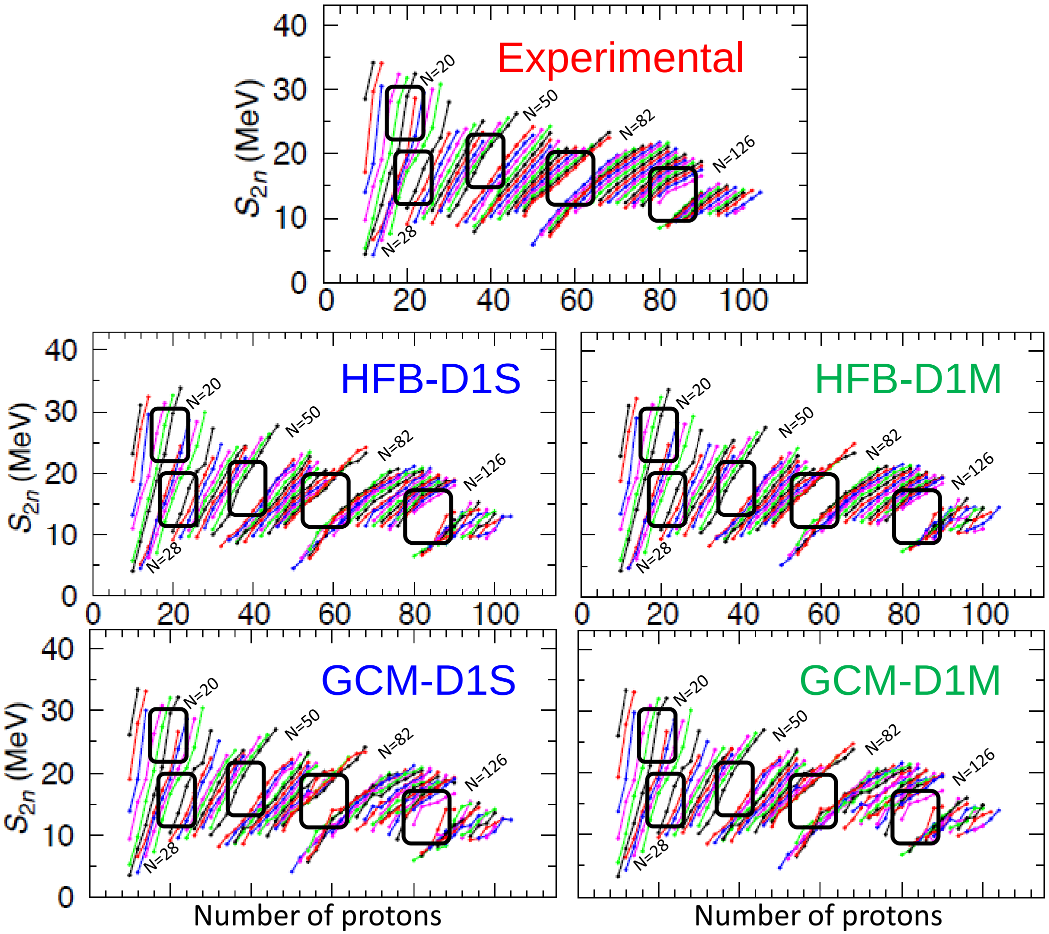

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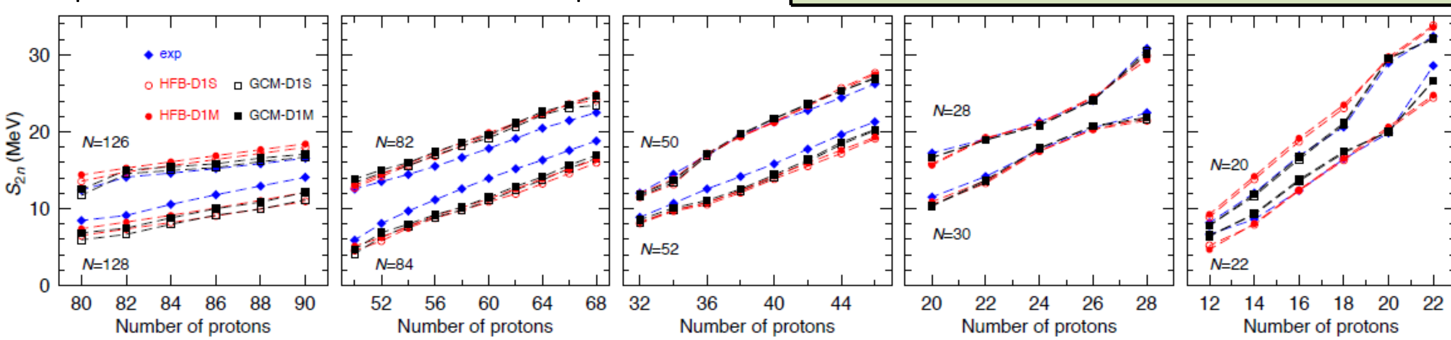
- ... but the reduction is not as strong as in the similar surveys with BMF methods

*Bender M, et al., PRC**78**, 054312, 2008* *[GOA]*

*Delaroche J-P, et al., PRC**81**, 014303, 2010* *[5DCH]*

- Could be related to approximated BMF techniques used there (GOA, 5DCH)



Summary and Outlook

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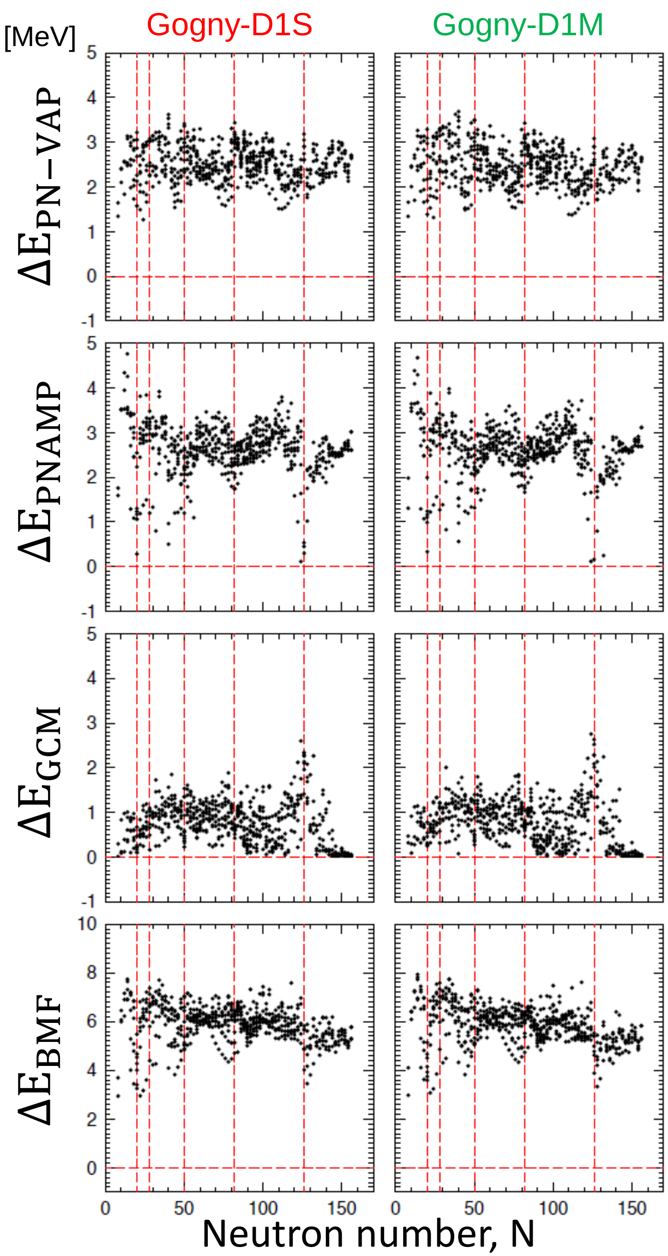
- Despite that this global BMF–calculation with much improved convergence and GCM treatment is still far from precision level of other sophisticated mass formulas, this is the right step towards the microscopic global nuclear structure model that is reliably applicable to neutron-rich r-process nuclei.
- Additional degrees of freedom (*e.g.* triaxiality, particle-vibration coupling, octupole deformations) must be included explicitly to improve description of both spectral and ground state energies.
- Further investigation of odd-nuclei approximation techniques, or implementation of explicit time-reversal breaking is needed.
- Particular attention must be paid to the convergence properties of the harmonic oscillator working basis.
- Finally, a significant improvement is to be made from a new EDF parametrization tuned to include the relevant BMF effects.

$$\tau_{END}$$

Additional Slides



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because

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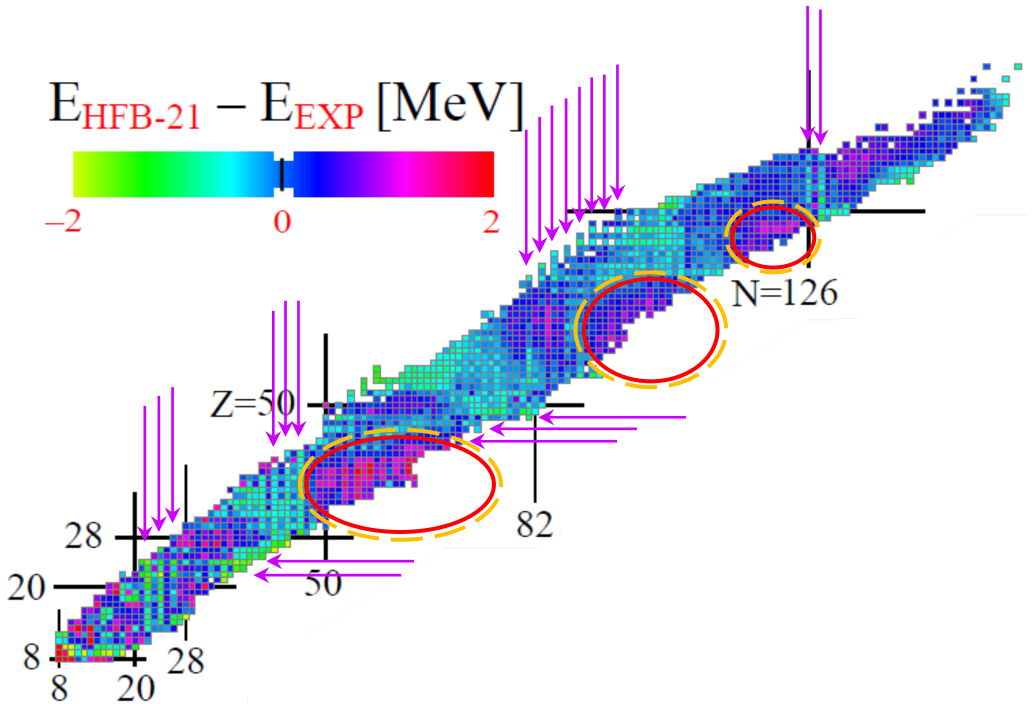
Introduction

- Astrophysical models require as an input thousands of **nuclear masses** beyond experimental reach
- Need accurate predictions from theoretical **global mass models**
- All models have similar rms, but more fundamental **HFB models** *should provide* greater confidence in describing unknown isotopes
- **Still some problems with HFB models:**
  - I) **Lack of convergence** due to truncated model space
  - II) Missing some physics without **Beyond-Mean-Field** correlations
  - III) **Odd-mass nuclei** are not treated on the same footing



Outlook

- Construct a **complete mass table** by including odd-mass nuclei
- **Explore more degrees of freedom**
  (triaxiality, particle-vibration coupling, octupole deformations, *etc.*)
- **New energy density functional parametrization**
  adjusted to the Beyond-Mean-Field effects