Convergence and correlations in nuclear masses calculated with energy density functional methods

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530. WE-Heraeus-Seminar Nuclear Masses and Nucleosynthesis

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Outline

1. Introduction

2. Convergence and numerical noise

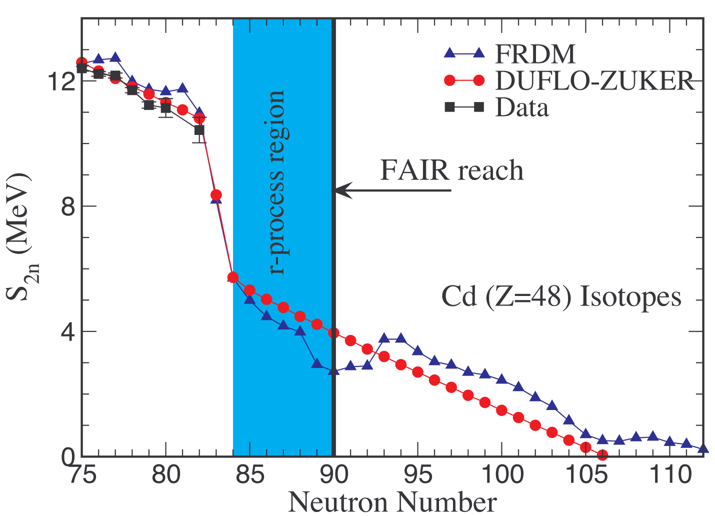
3. Odd-nuclei within the perturbative nucleon addition framework

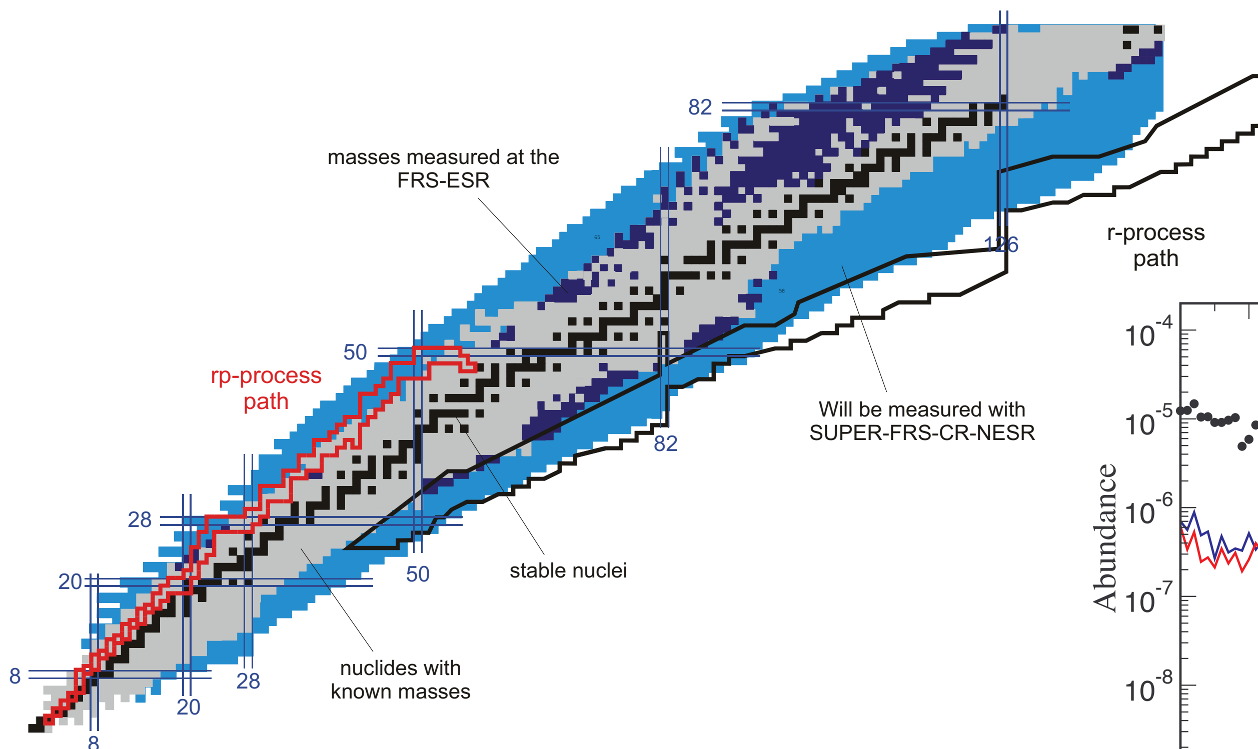
4. Beyond mean field effects and correlations

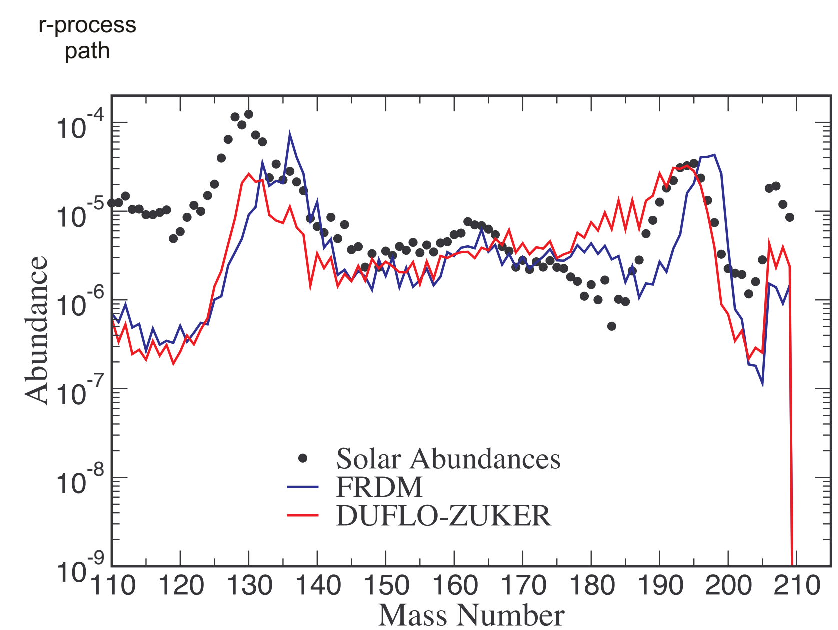
5. Summary and outlook

Motivation

- Nuclear masses are one of the most relevant input for nucleosynthesis calculations, in particular for the r-process.
- Masses (separation energies) affect significantly (*n*,γ) capture rates, (γ,*n*) photodissociation reactions and *Q*-values for β-decay.
- Only few nuclei are/will be experimentally explored in the relevant region for r-process nucleosynthesis ⇒ <u>we require theoretical predictions.</u>







Courtesy: J. Mendoza-Temis

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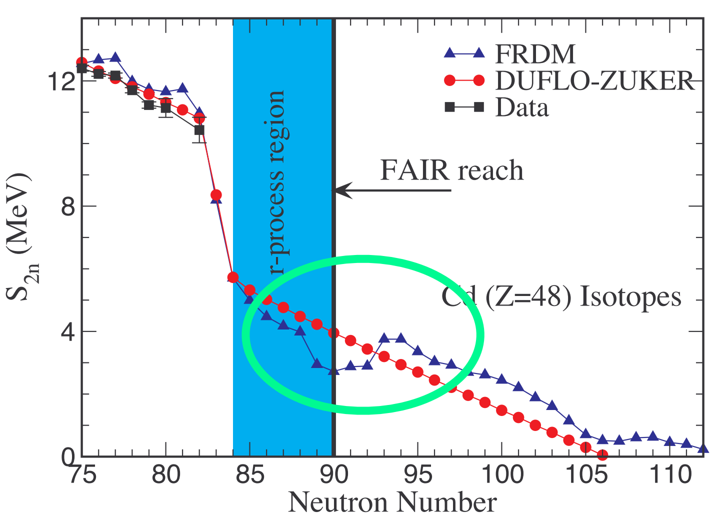

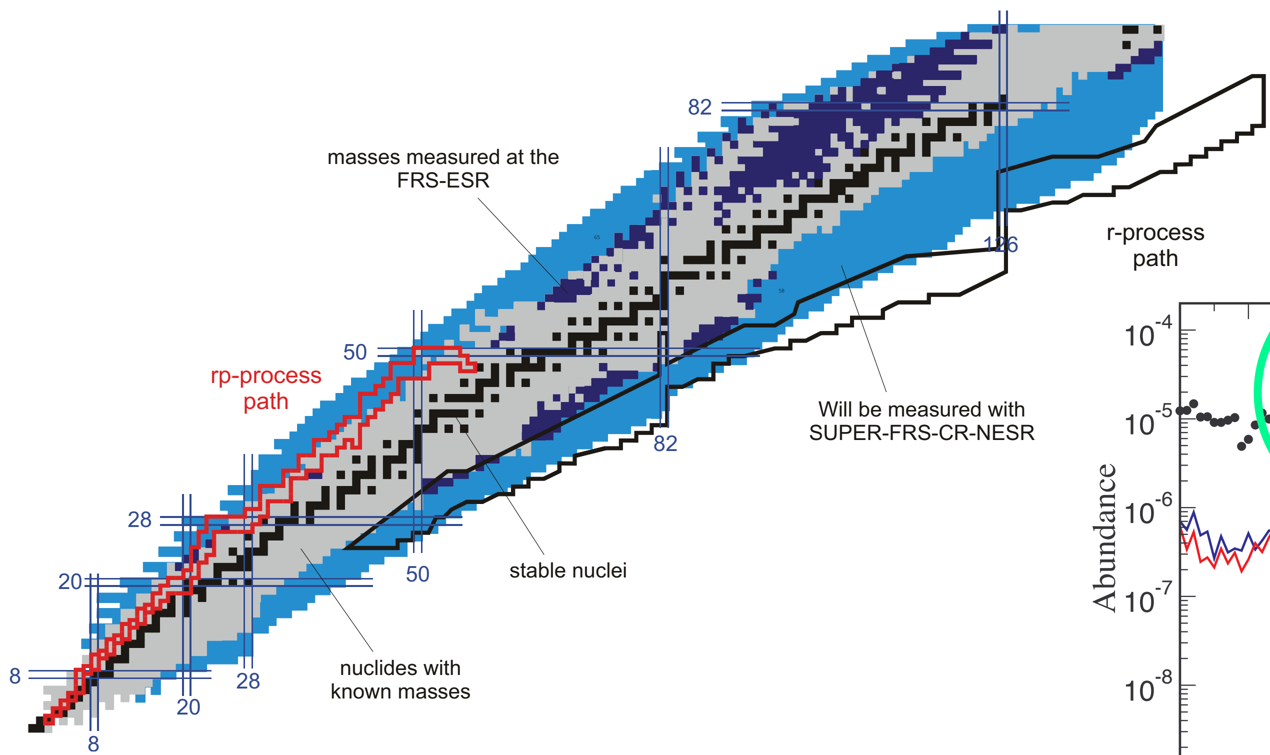

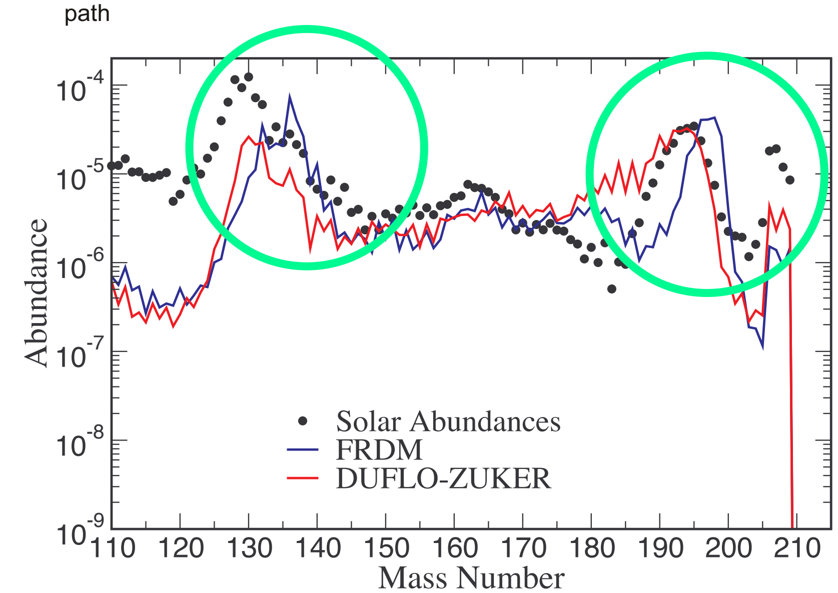

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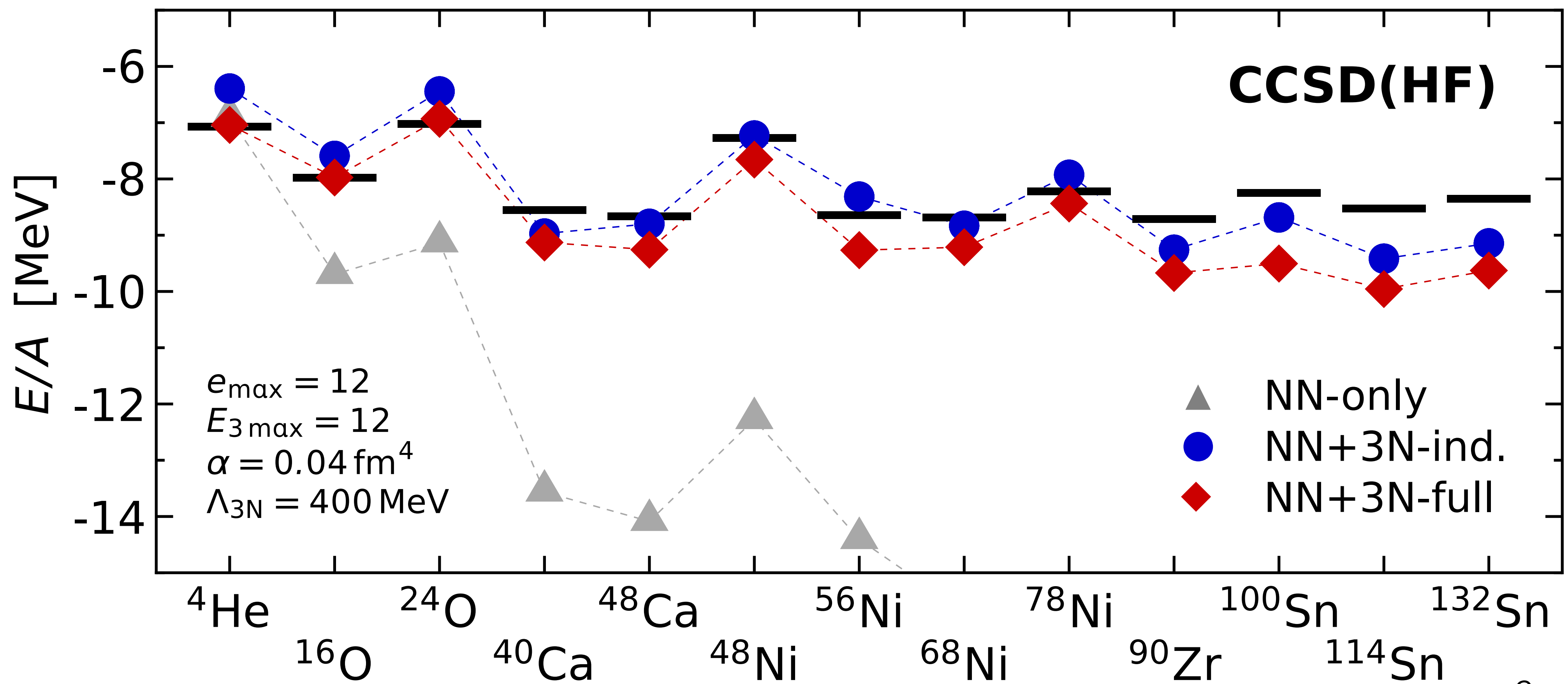
State-of-the-art *ab initio* calculations



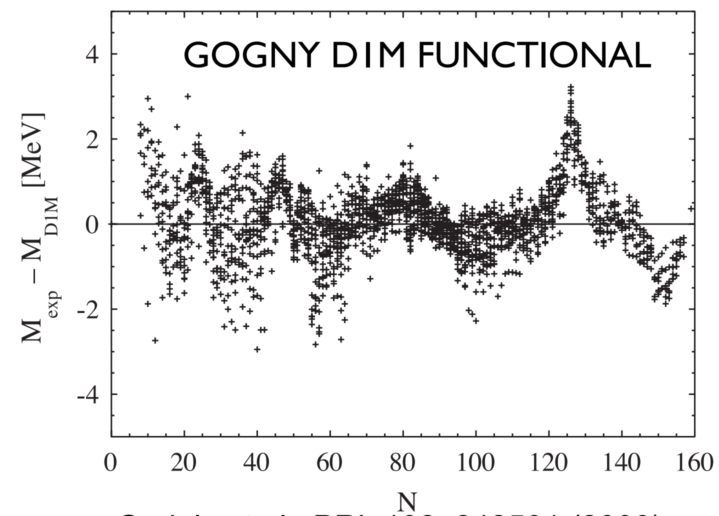
Courtesy: R. Roth

- First calculations for heavier -closed shell- nuclei with chiral NN+3N hamiltonians
- Systematics is well reproduced at this level.
- Improvements are in progress (3N at N^3LO, adjust the 3N, 4N terms, ...)

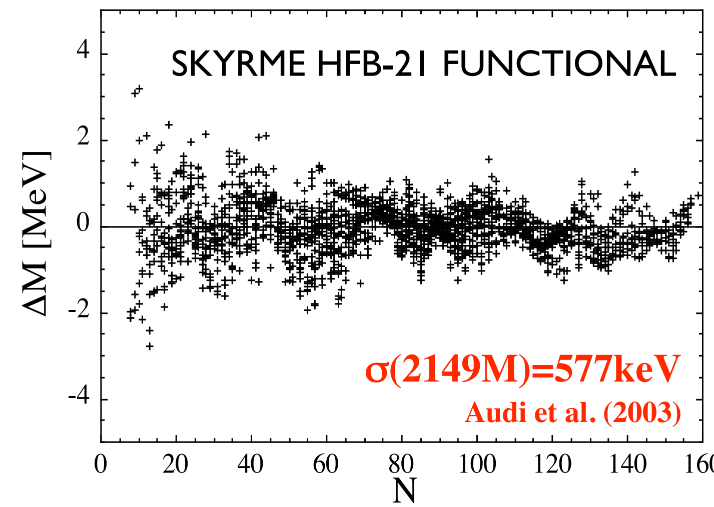
Microscopic mass models

TECHNISCHE UNIVERSITÄT DARMSTADT

- Self-consistent mean field approximations provide a very good description of known data.



Goriely et al., PRL 102, 242501 (2009)



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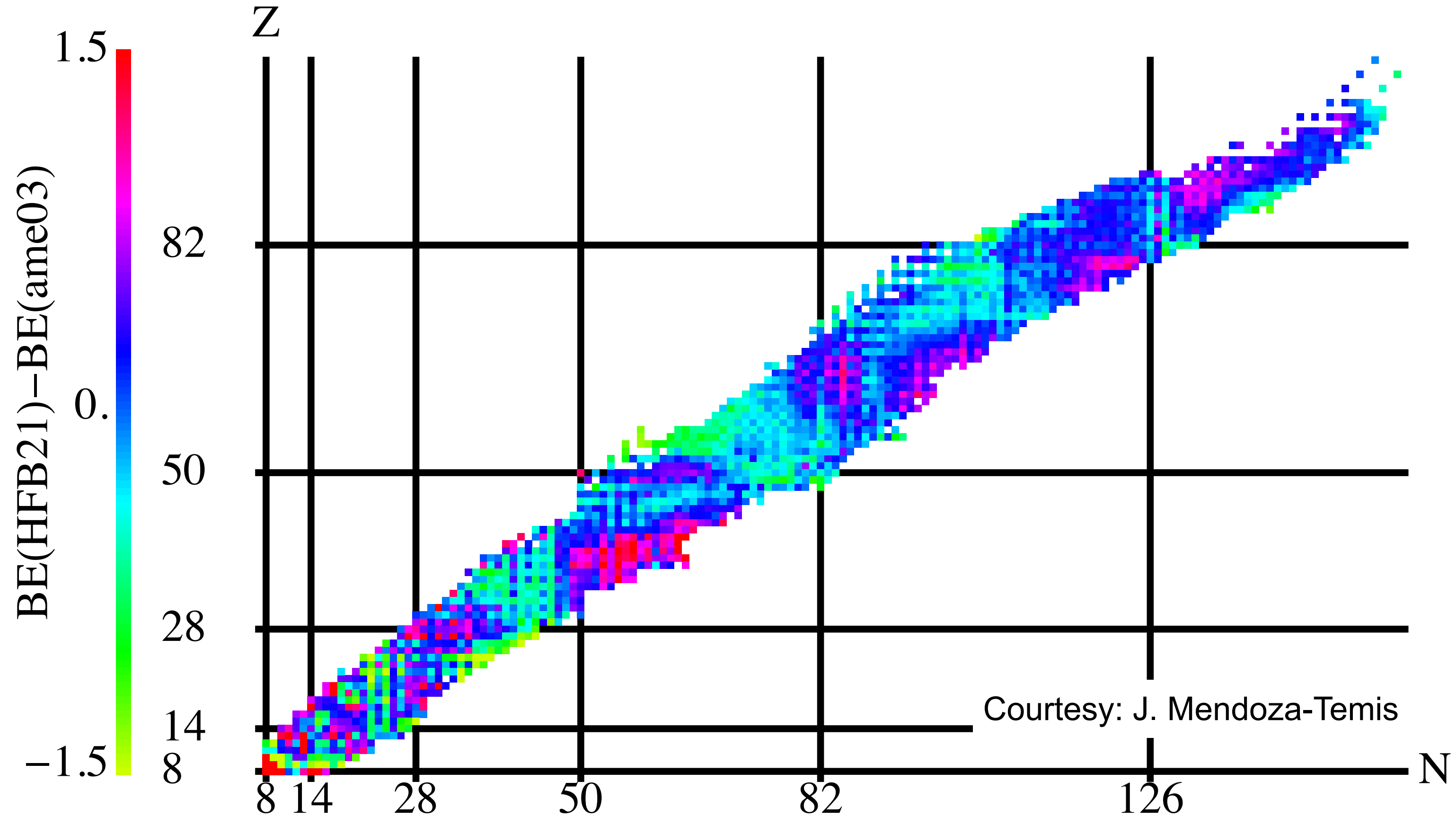
- There are still some problems in transitional regions and local uncertainties:
  - Numerical noise.
  - Some physics missing: Restoration of broken symmetries and configuration mixing.
  - Nuclei with odd number of protons/neutrons are not treated in equal footing as the even-even ones



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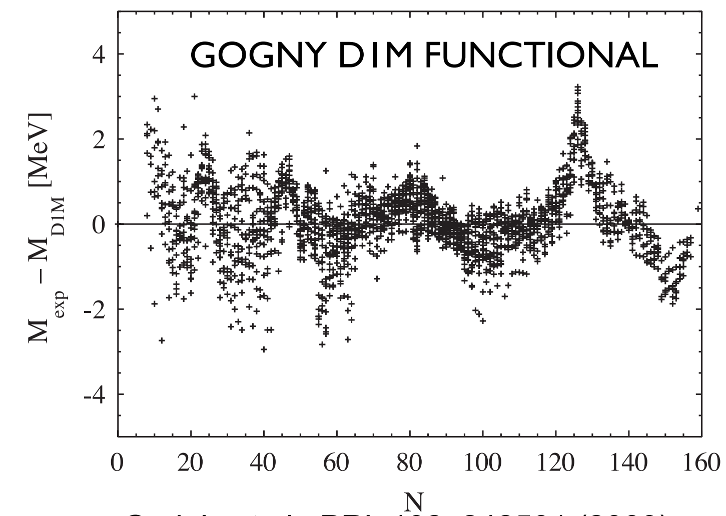

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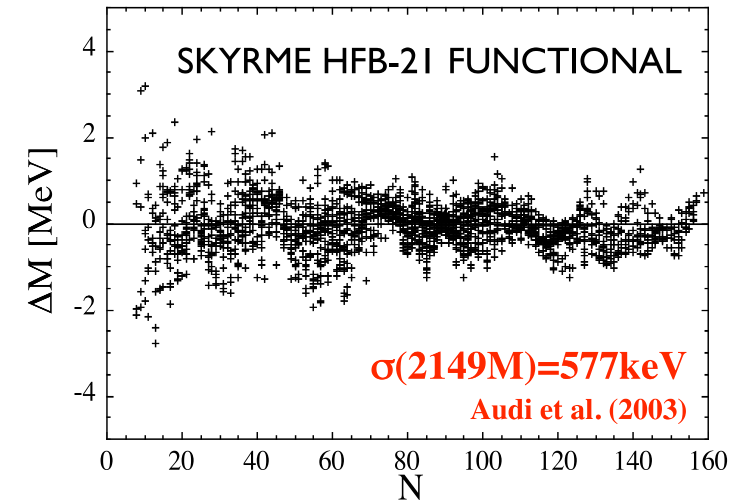

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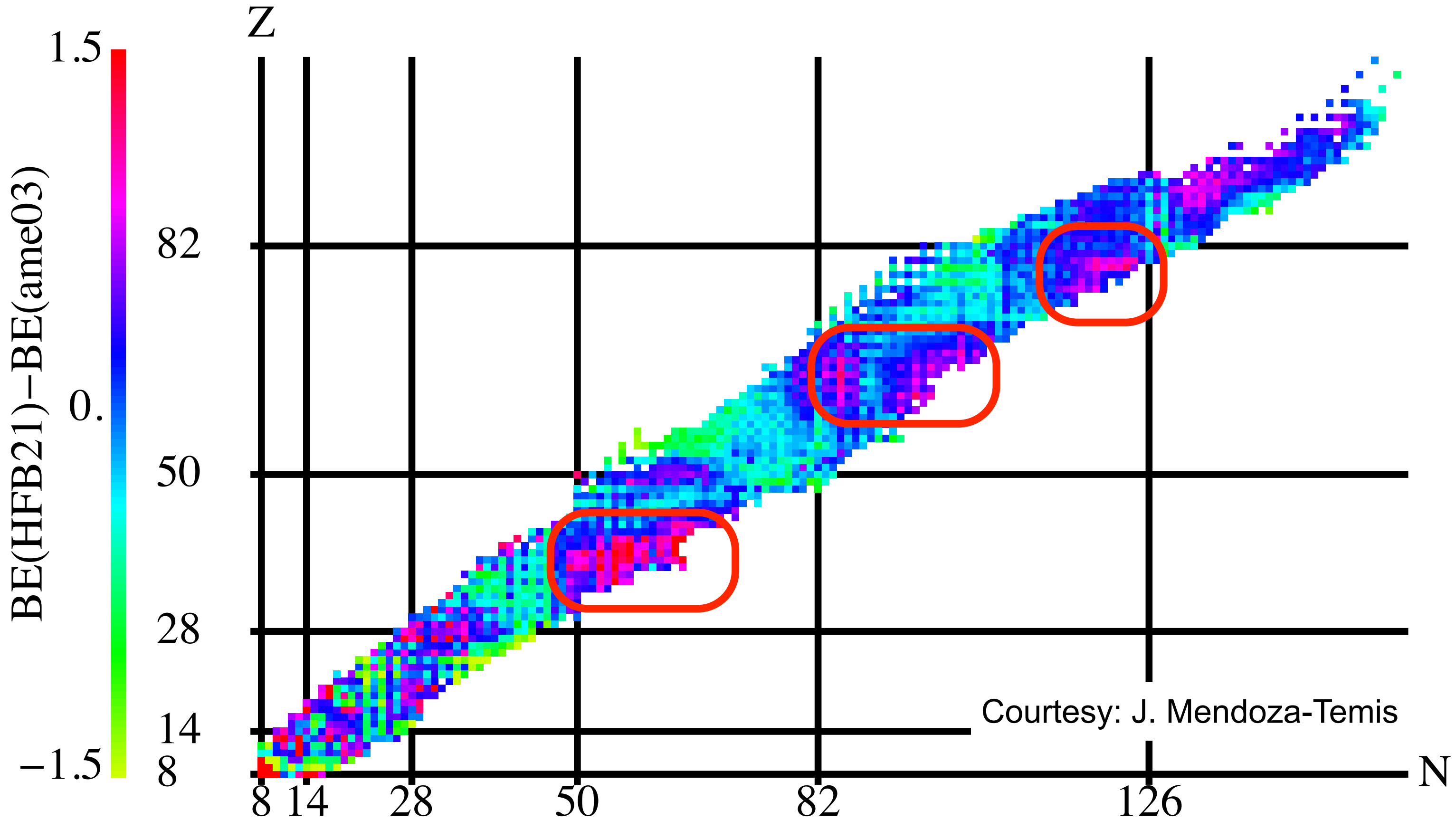

- **Effective nucleon-nucleon interaction:**

Gogny force (D1S-D1M) that is able to describe properly many phenomena along the whole nuclear chart.

$$V(1,2) = \sum_{i=1}^{2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2}\left(W_i + B_i P^{\sigma} - H_i P^{\tau} - M_i P^{\sigma} P^{\tau}\right)$$
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Self-consistent (beyond) mean field description

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spin-orbit term

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Coulomb term

- **Methods of solving the many-body problem: Variational approaches**

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spin-orbit term; density-dependent term

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- **Methods of solving the many-body problem: Variational approaches**

➡**Parameters of the effective interaction are fitted to reproduce experimental data solving the many-body problem at certain level of approximation (mean field normally).**

Hartree-Fock-Bogoliubov (HFB)

Variational space: $\{|\Phi(\vec{q})\rangle\}$ set of **product-type** wave functions which fulfill:

- Quasiparticle vacua: $$\alpha_k(\vec{q})|\Phi(\vec{q})\rangle = 0$$

- Most general linear combination of the arbitrary single particle basis: $$\alpha_k^\dagger(\vec{q}) = \sum_l U_{lk}(\vec{q})c_l^\dagger + V_{lk}(\vec{q})c_l$$

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3. No configuration mixing!!

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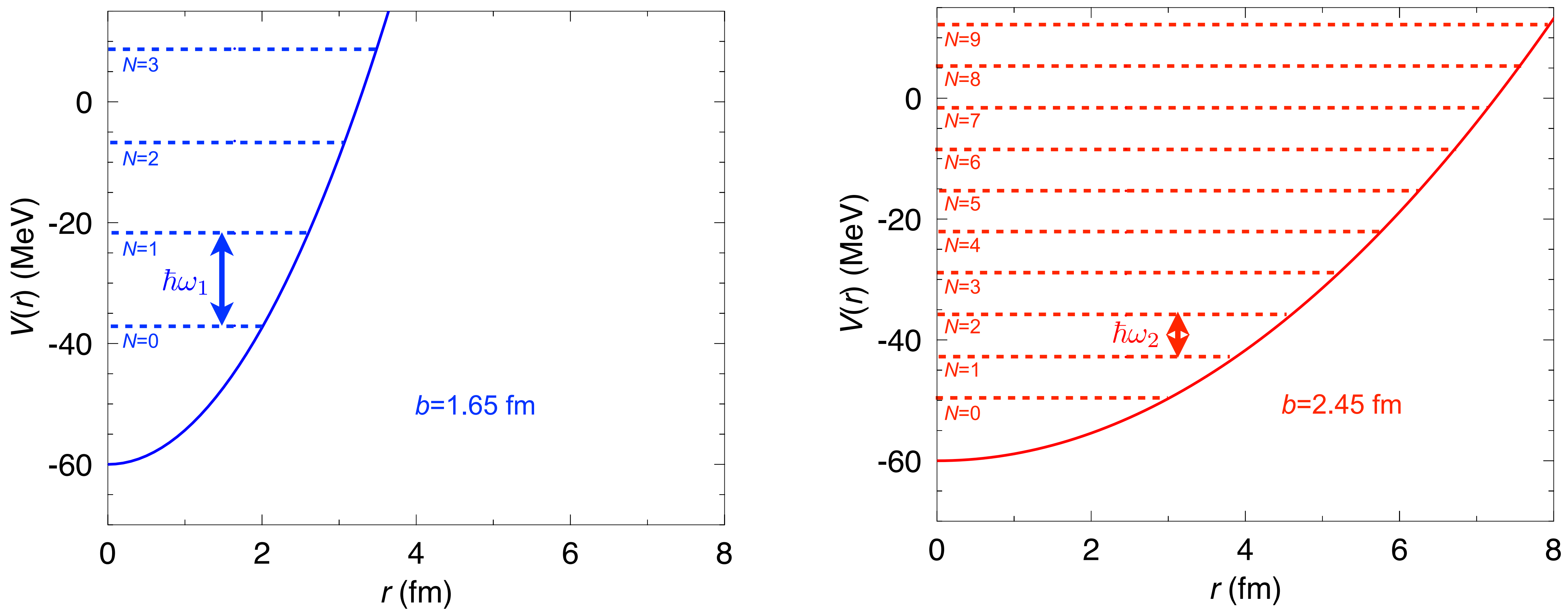
- **Results must not depend on the choice of the arbitrary single particle basis if it is complete.**



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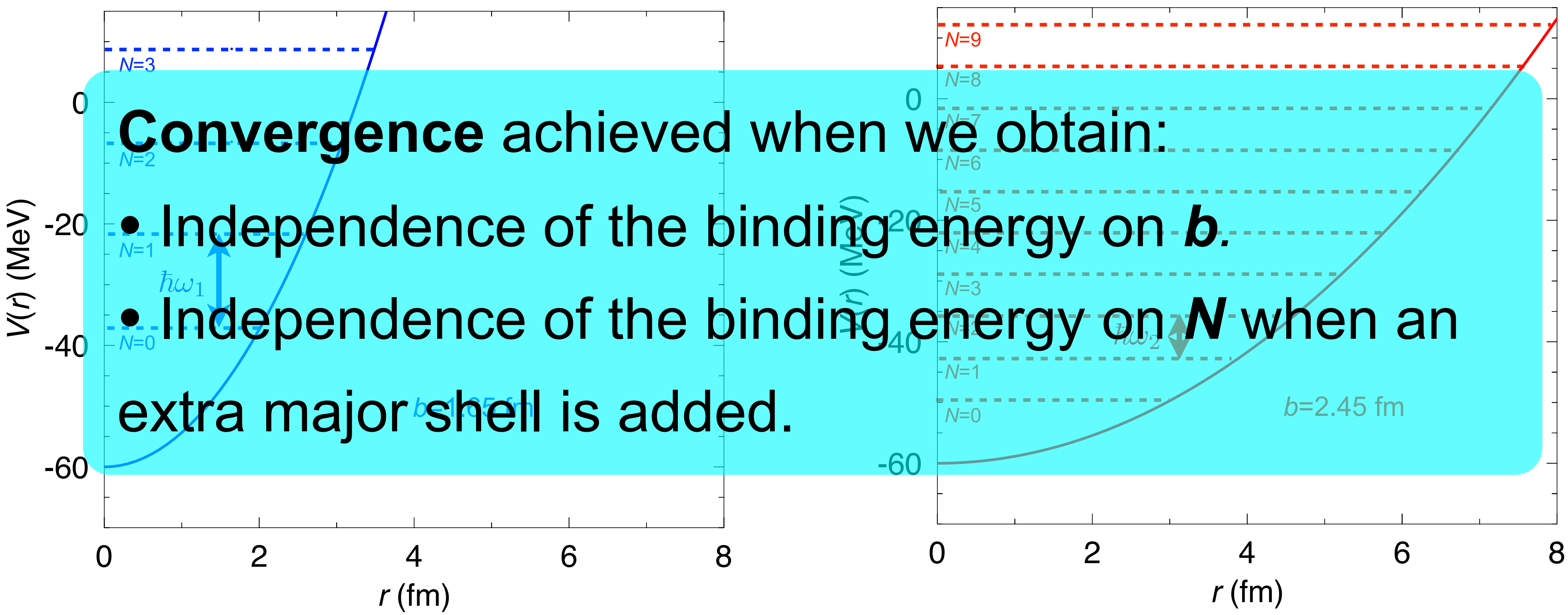


Convergence achieved when we obtain:

- Independence of the binding energy on ***b***.
- Independence of the binding energy on ***N*** when an extra major shell is added.

Examples in *ab-initio* calculations

P. Maris et *al.*, Phys. Rev C 79 (2009)

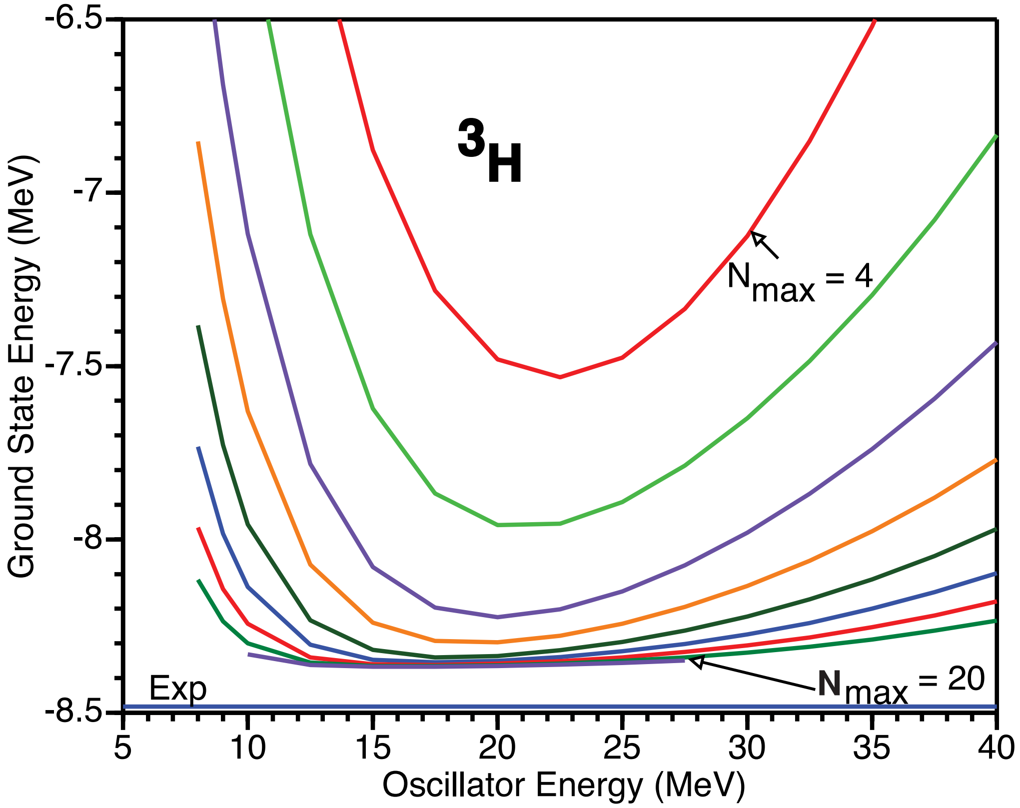


FIG. 10. (Color online) Calculated ground-state energy of ^{3}H as a function of the oscillator energy, $\hbar\Omega$, for selected values of N_{max}. The curve closest to experiment corresponds to the value $N_{max} = 20$ and successively higher curves are obtained with N_{max} decreased by two units for each curve.

R. Roth, Phys. Rev C 79 (2009)

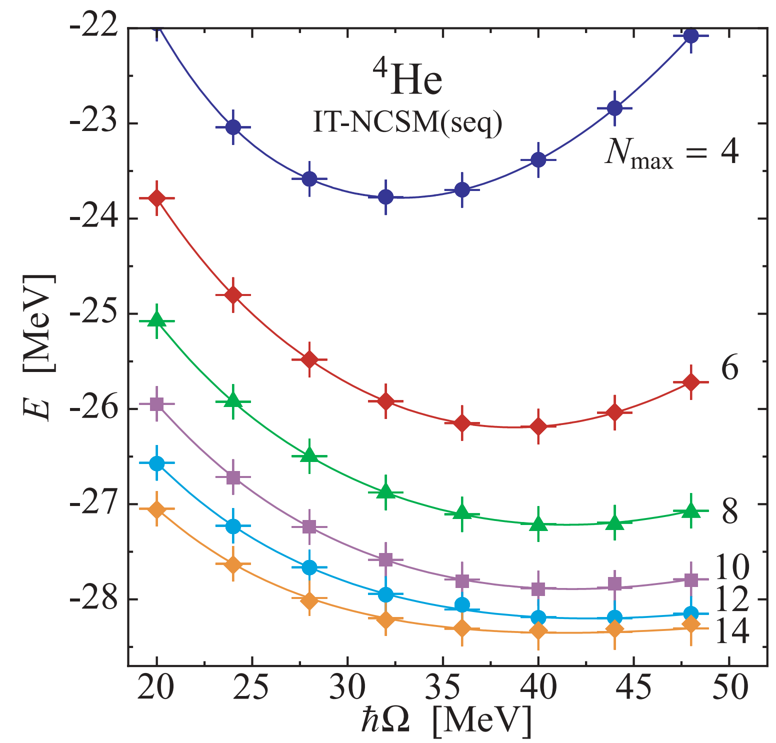
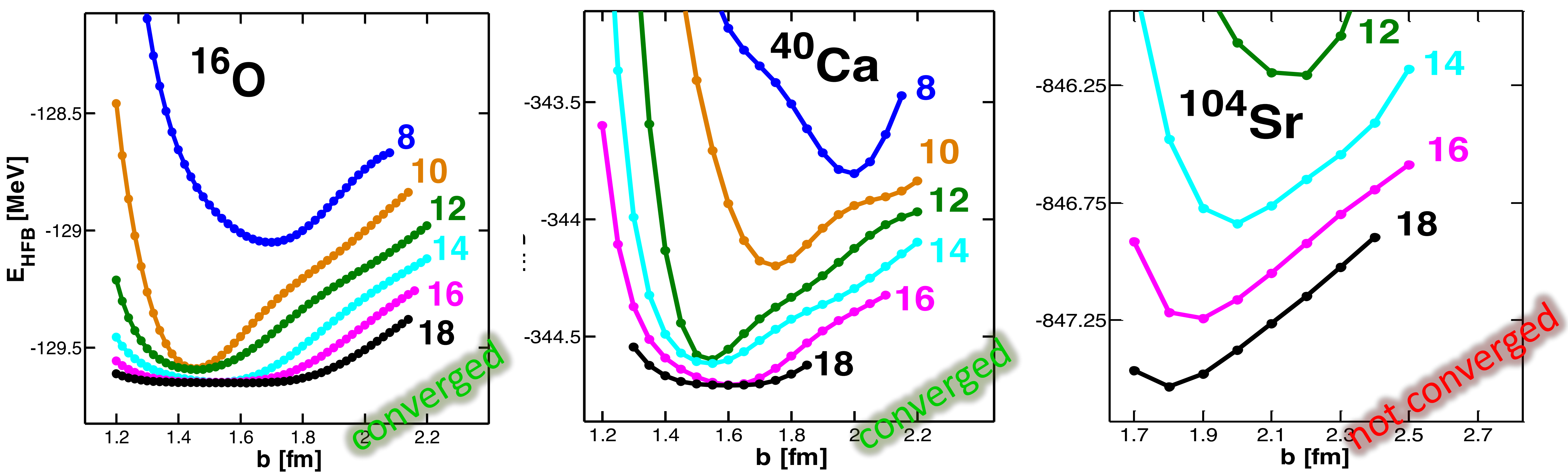


FIG. 7. (Color online) Ground-state energies of ^{4}He obtained for the V_{UCOM} interaction as function of the oscillator frequency $\hbar\Omega$ for different $N_{max}\hbar\Omega$ model spaces. Results of IT-NCSM(seq) calculations (solid symbols) are compared with full NCSM calculations (crosses).

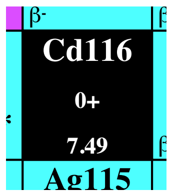
Examples in EDF calculations

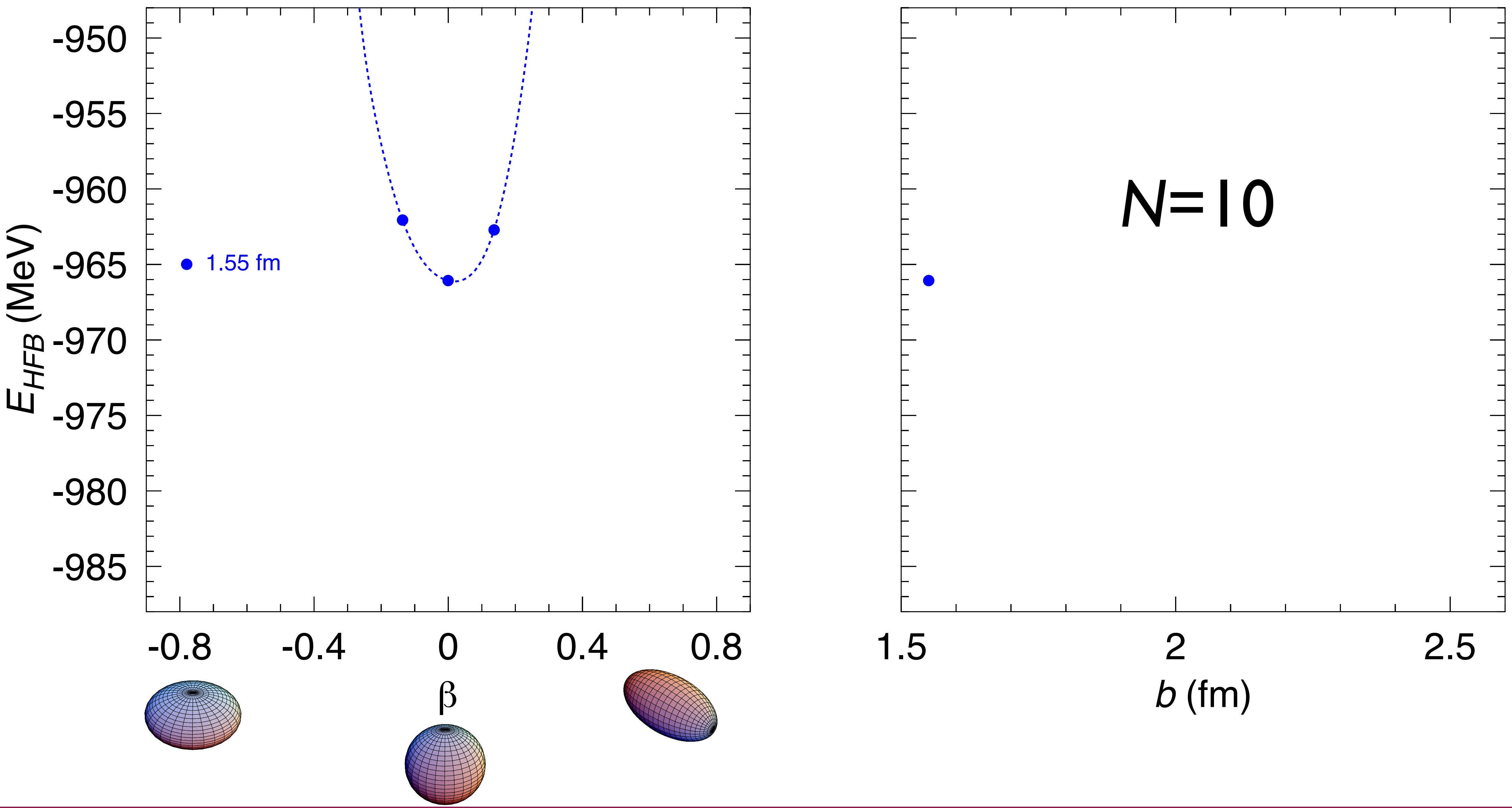
A. Arzhanov, Master Thesis



- ^{16}O and ^{40}Ca show independence on b and N → converged.
- ^{104}Sr is not fully converged → asymptotic behavior of HO is gaussian while realistic densities fall off exponentially.

Effects of deformation on the convergence

Example: 



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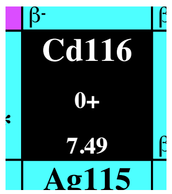
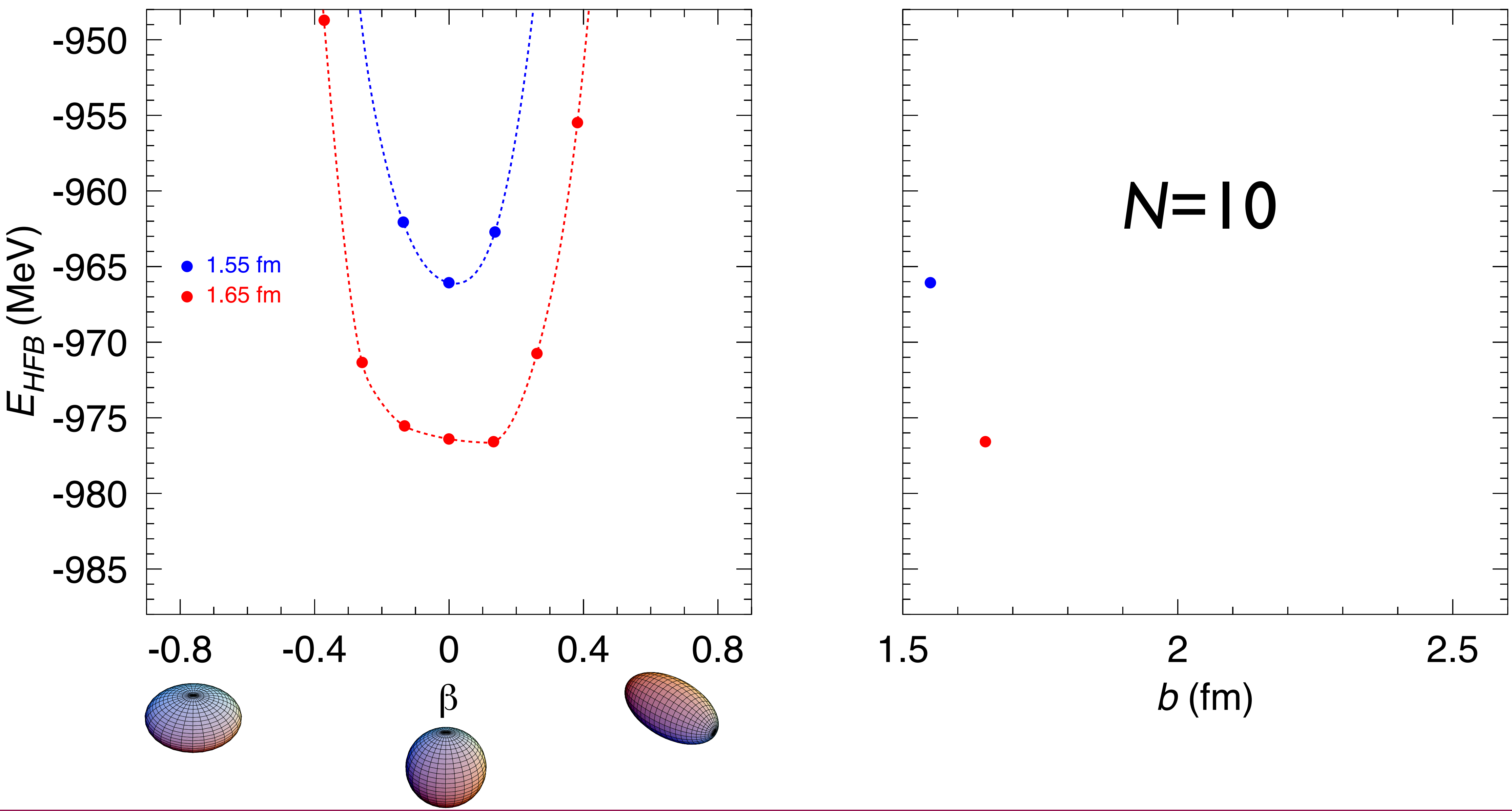
Example: 



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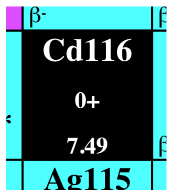
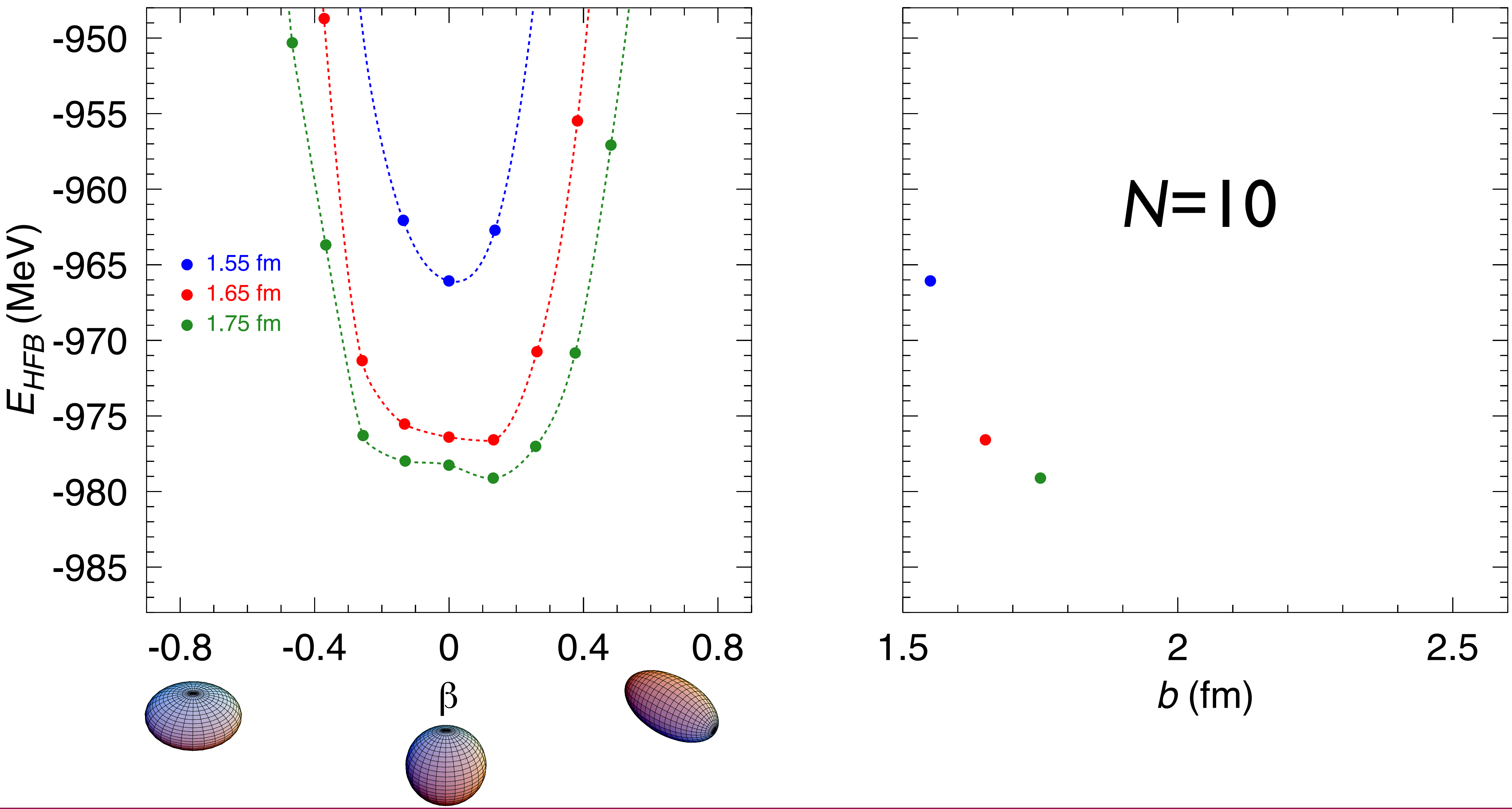
Example: 



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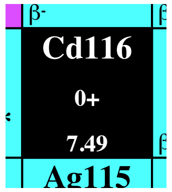
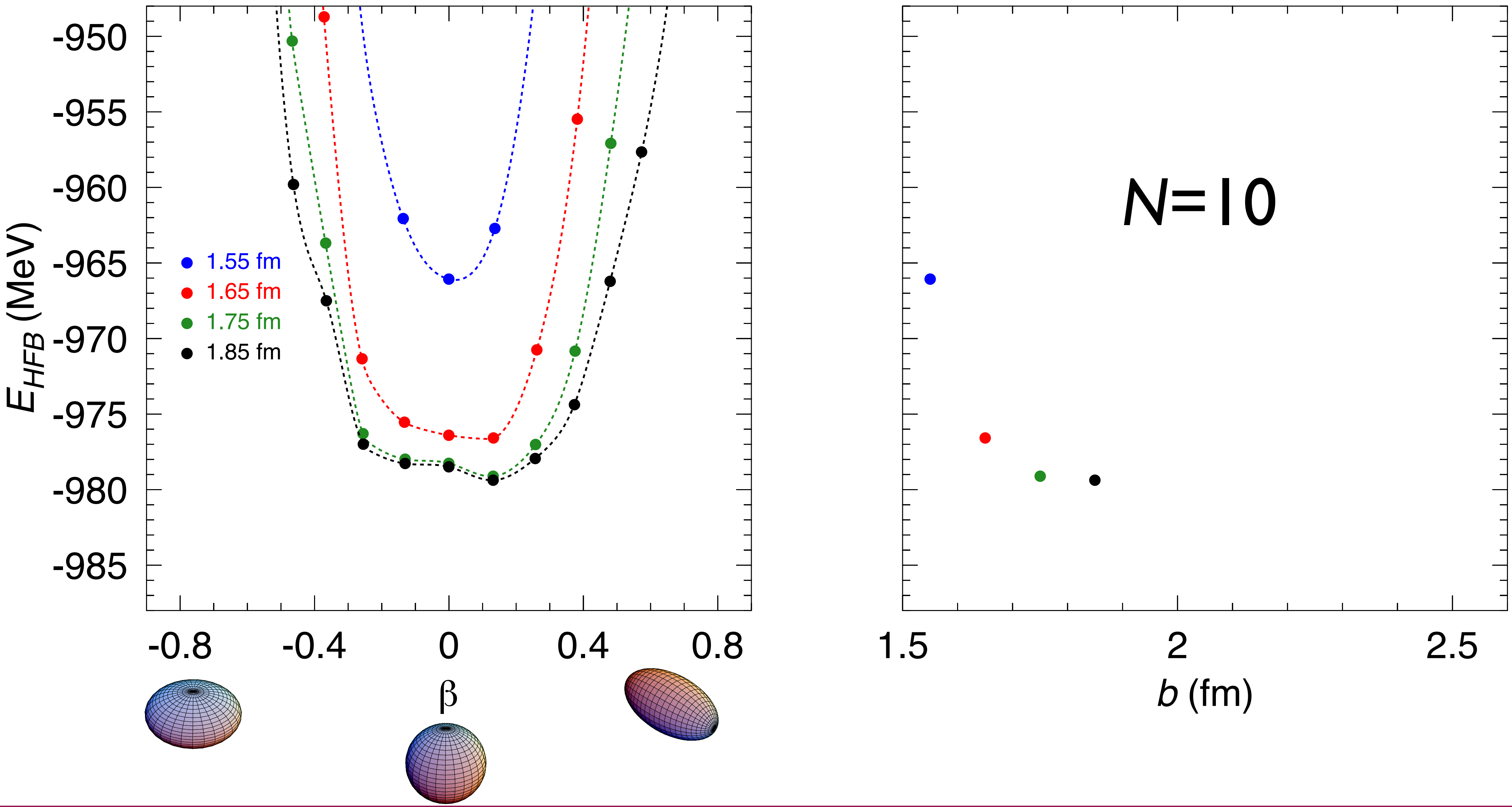
Example: 



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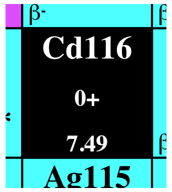
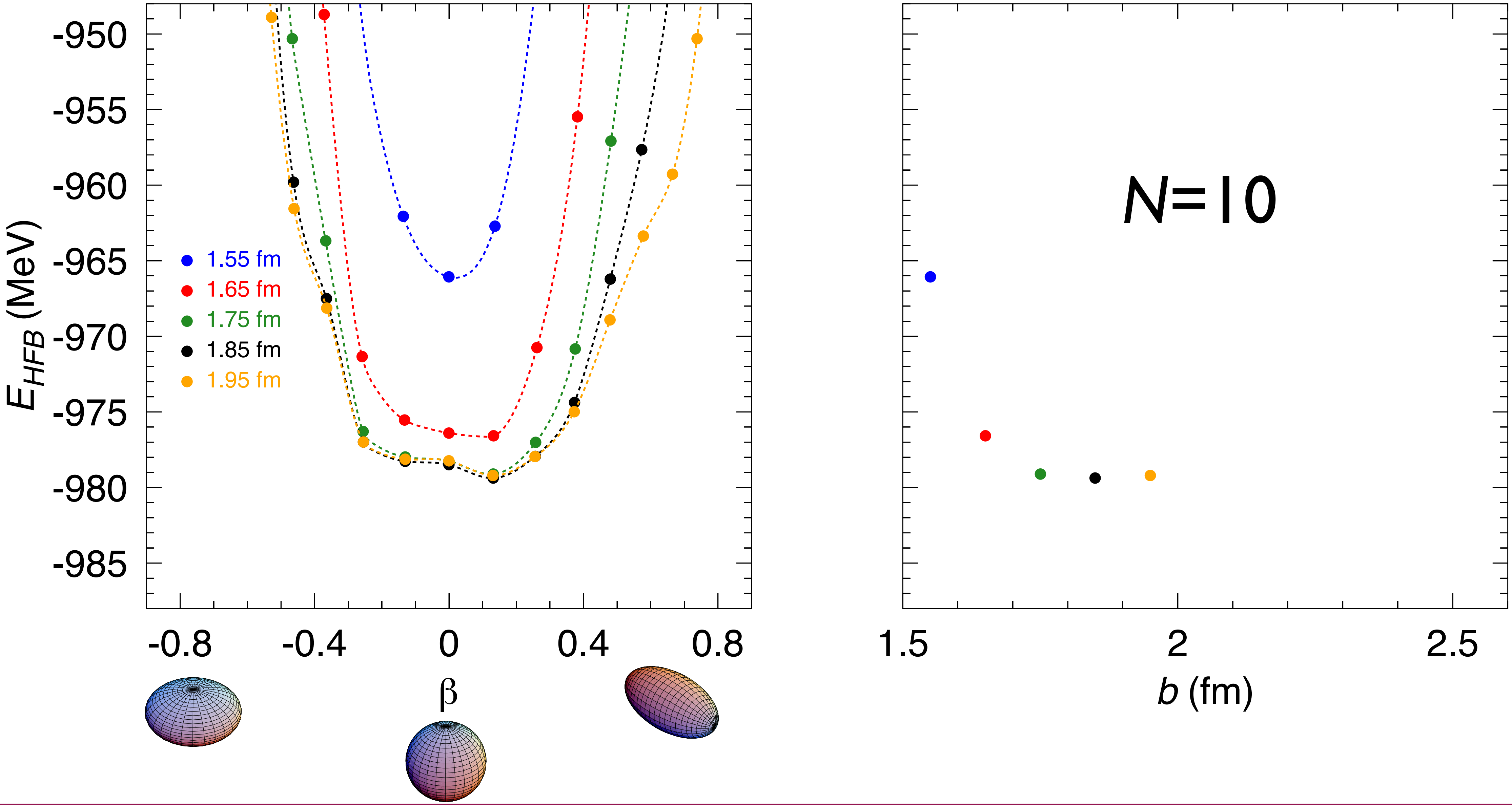
Example: 



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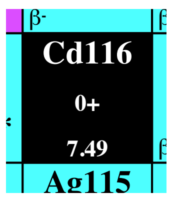
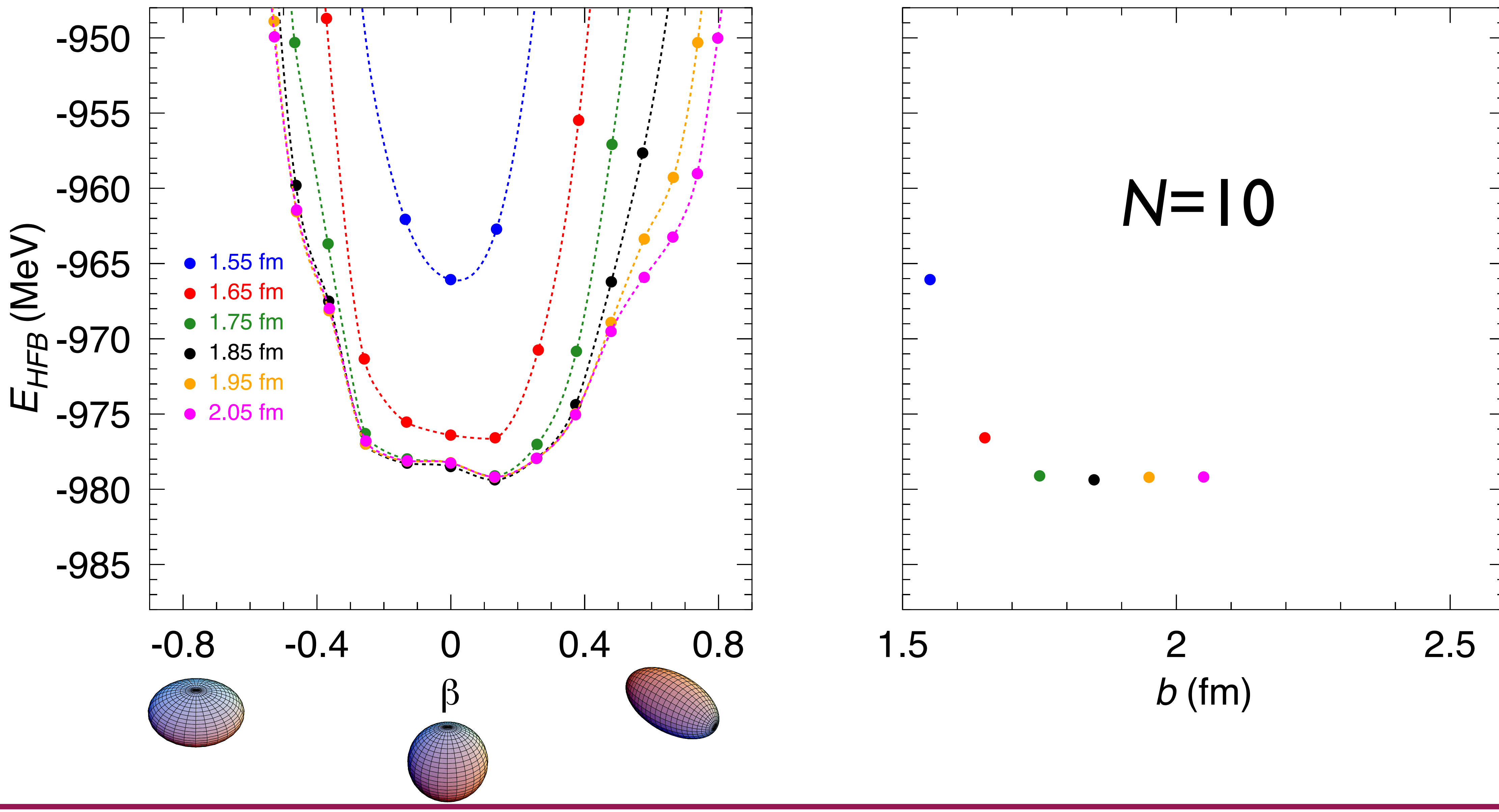
Example: 



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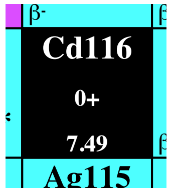

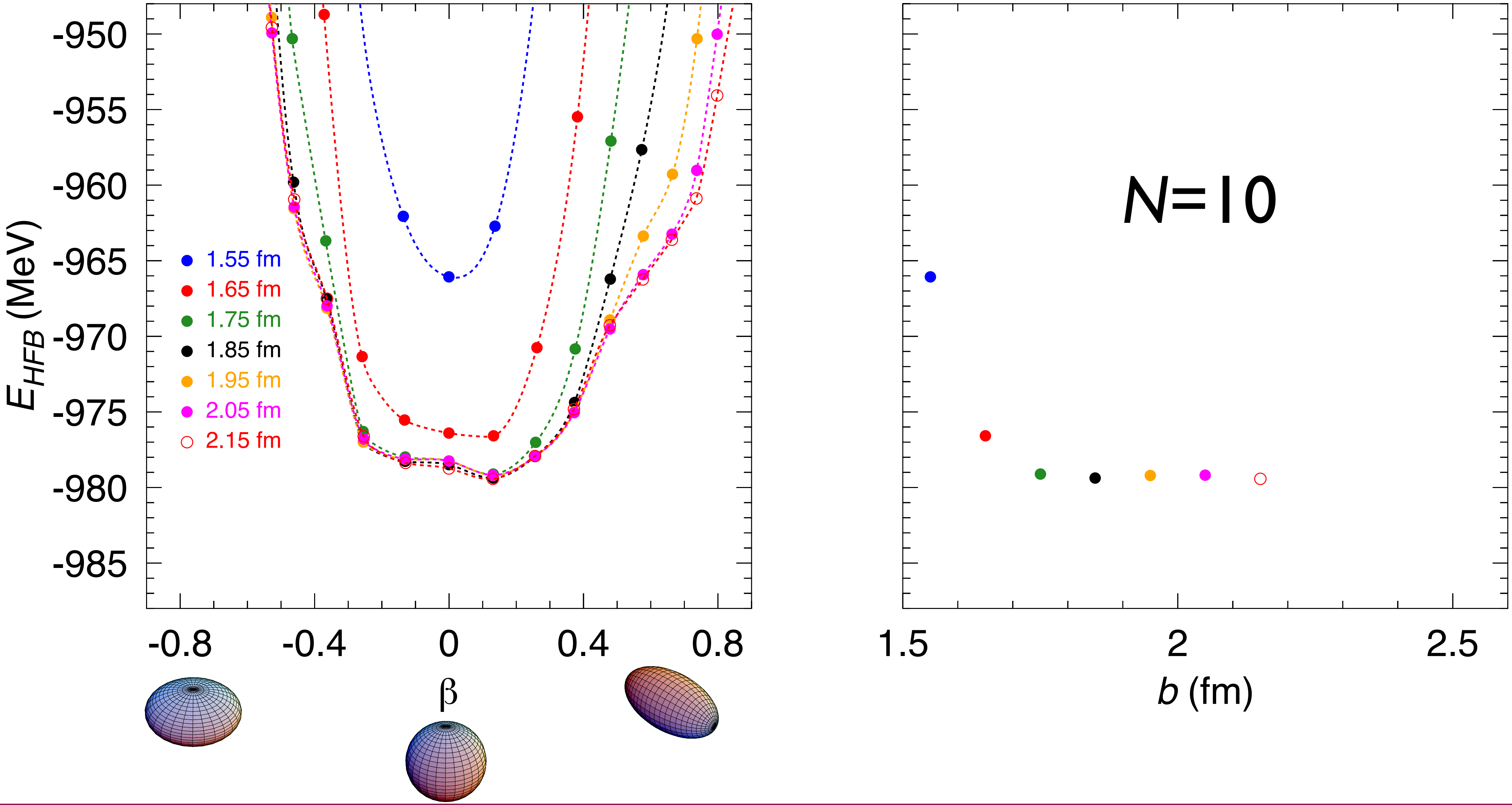

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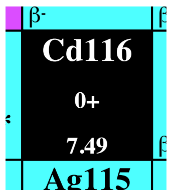
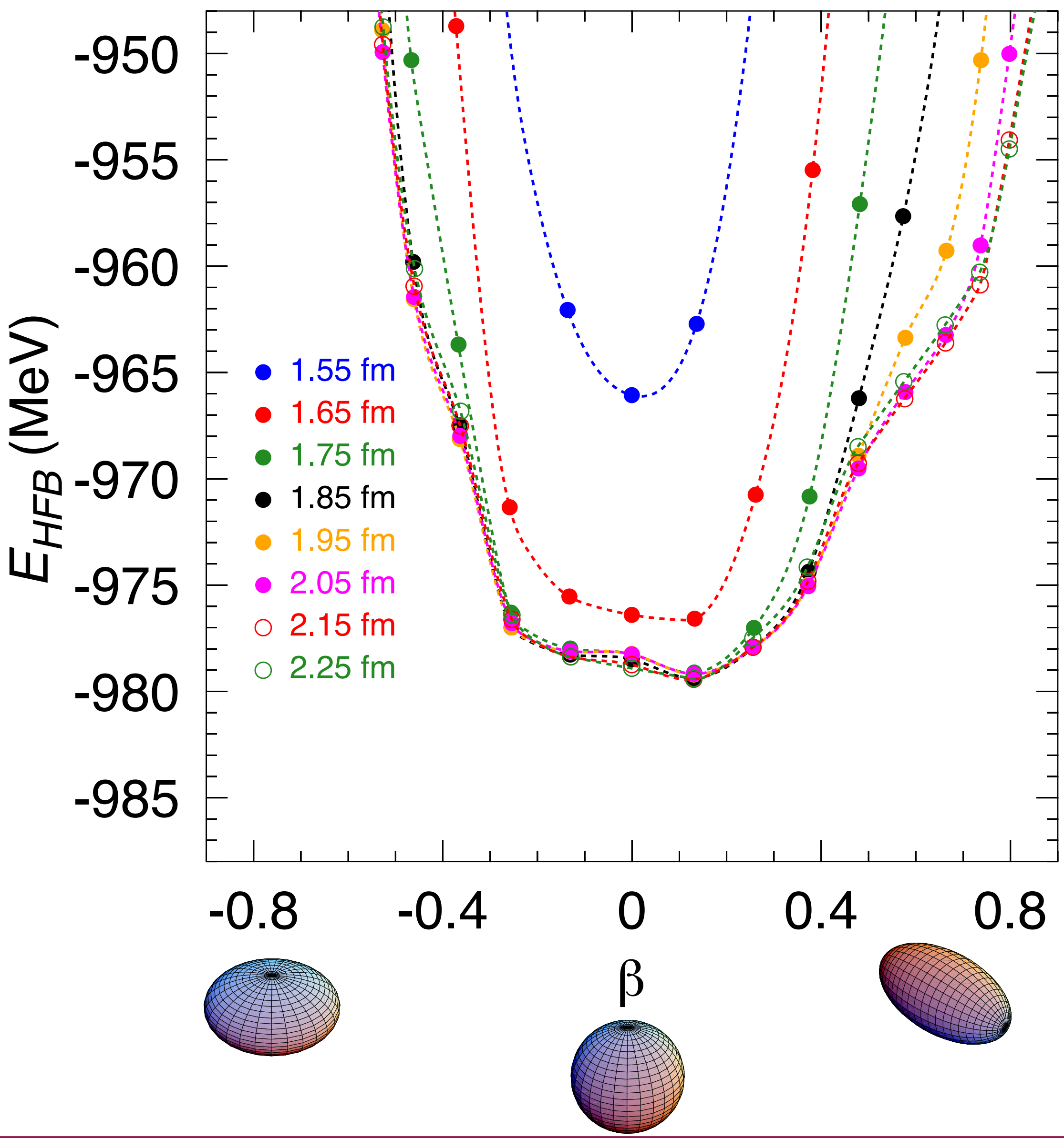
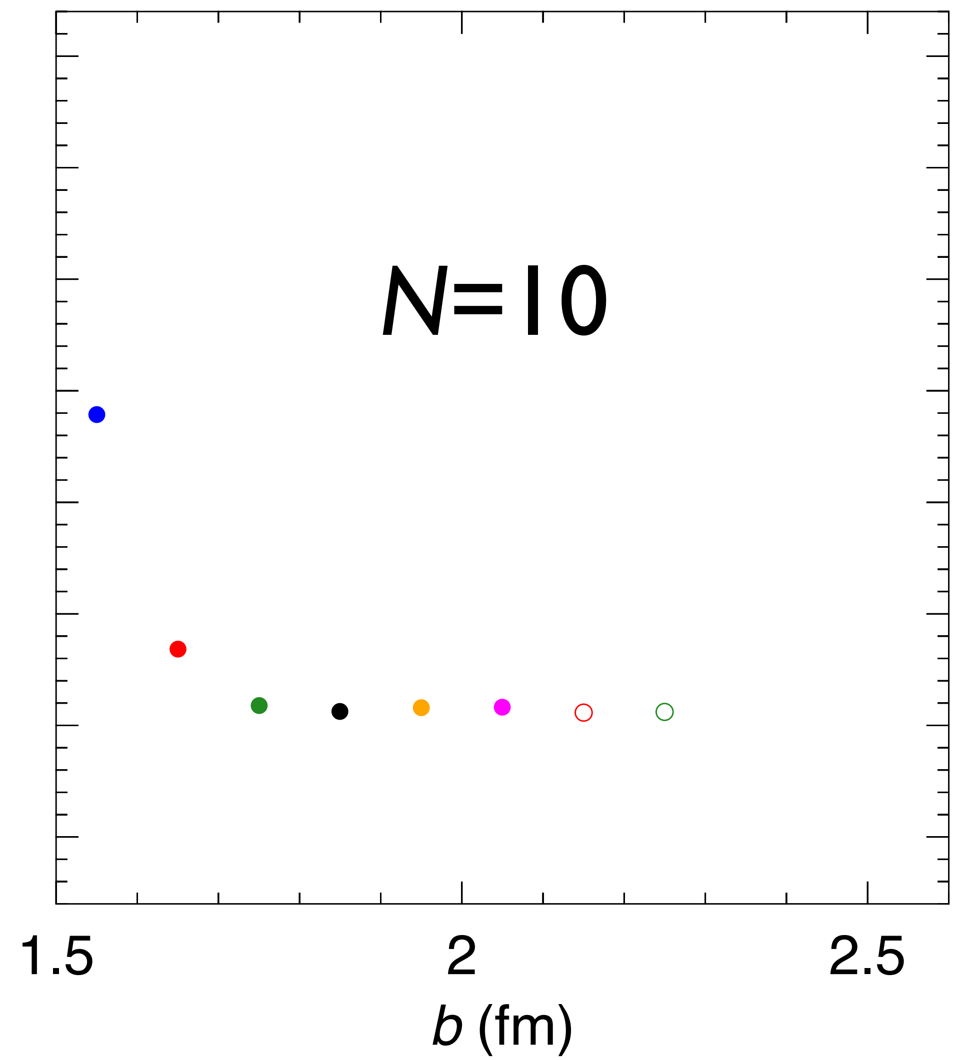
Example: 





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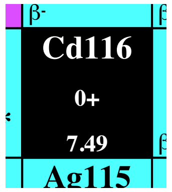

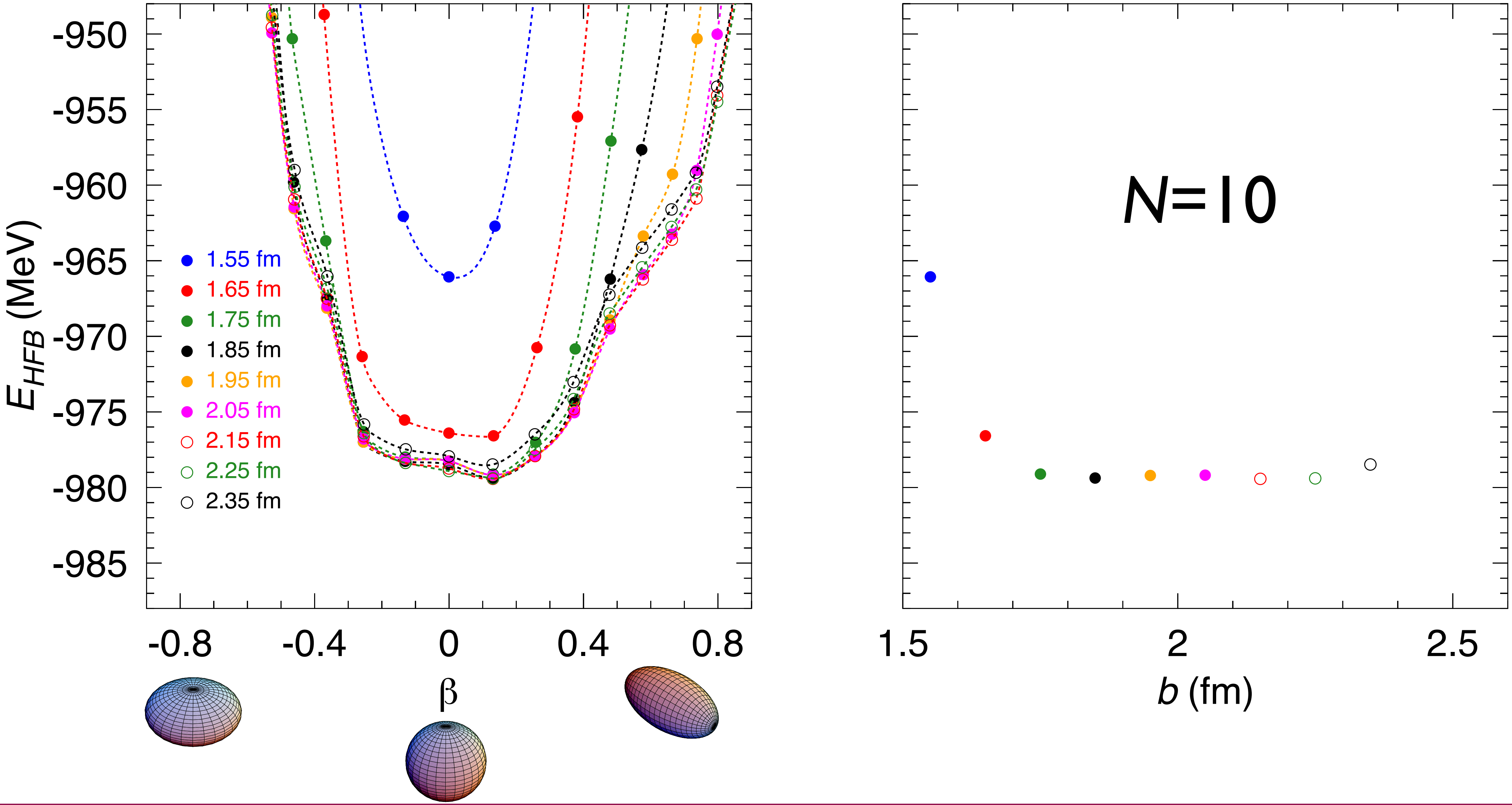

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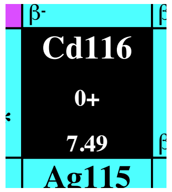

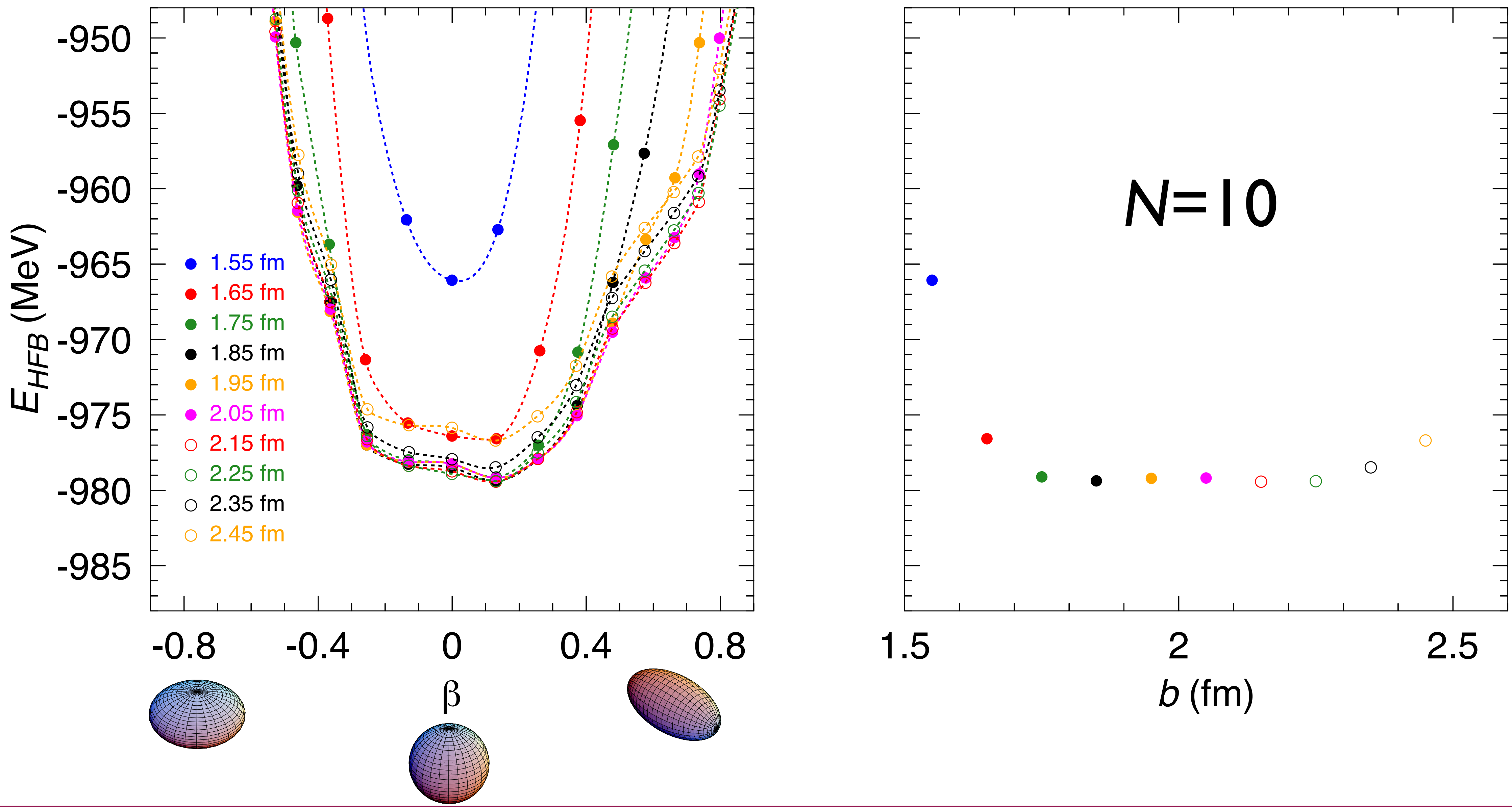

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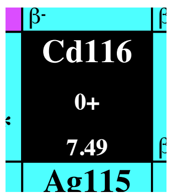
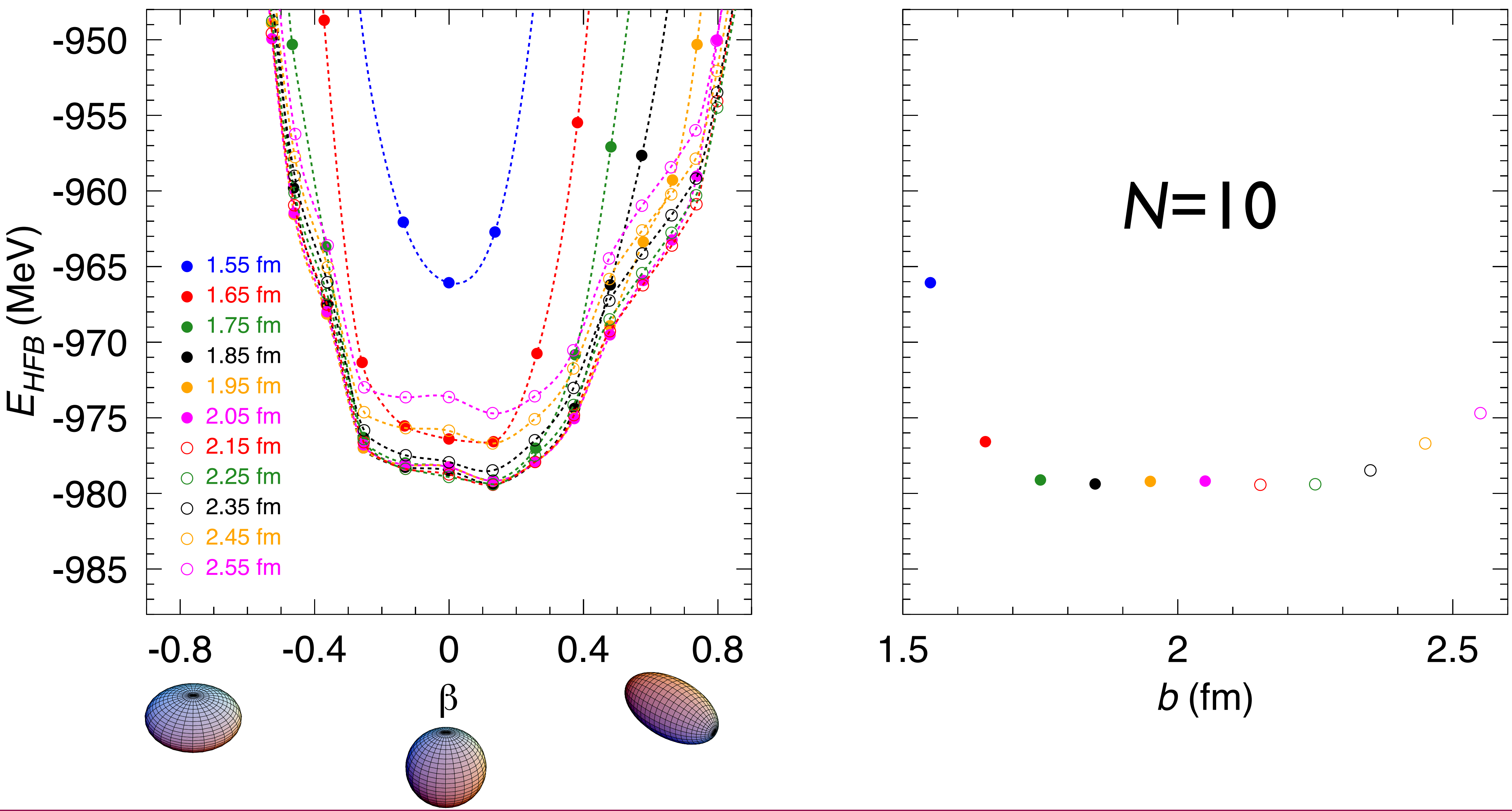
Example: 



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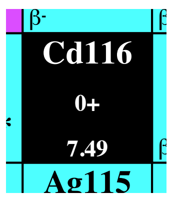
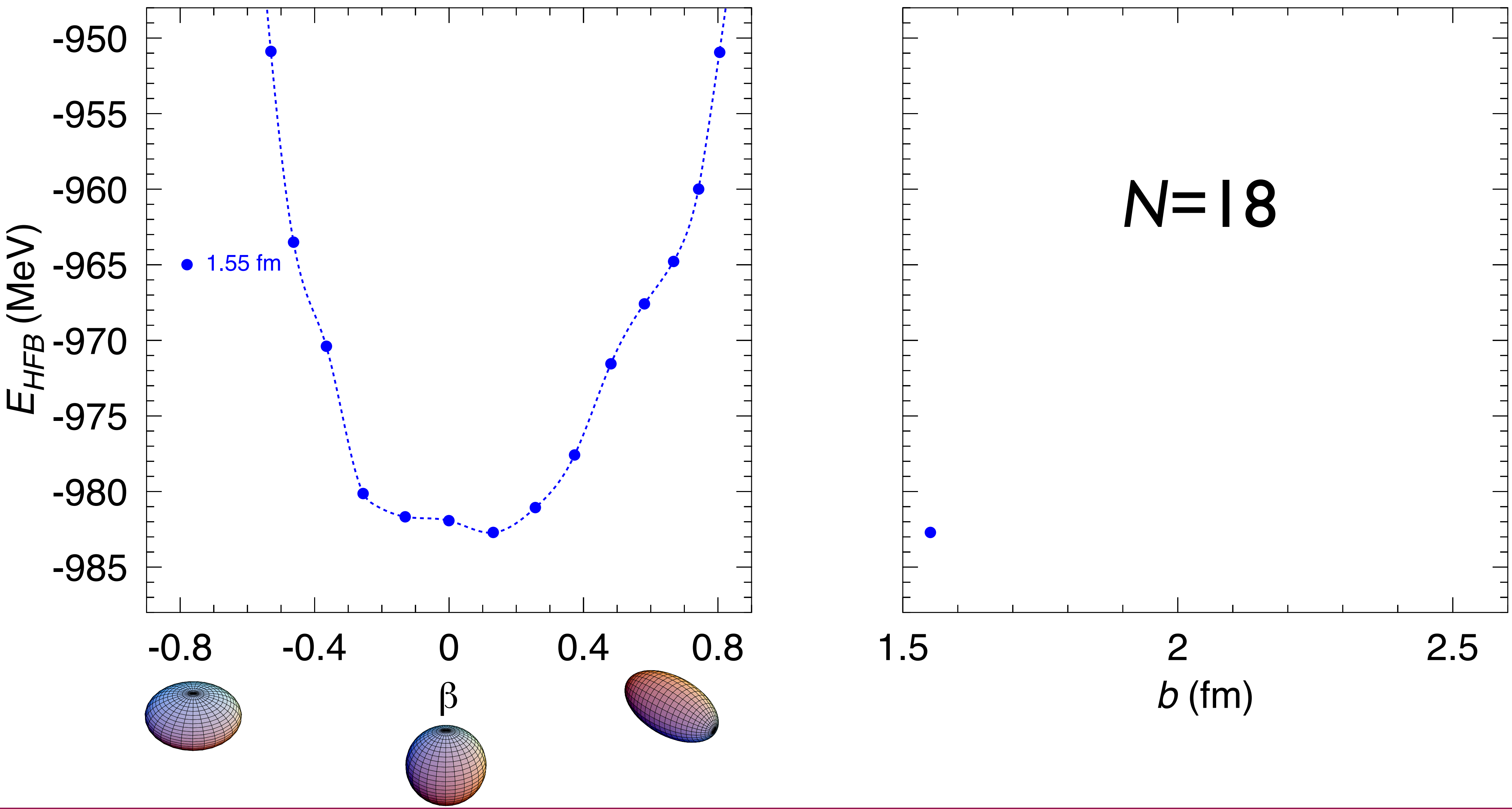
Example: 



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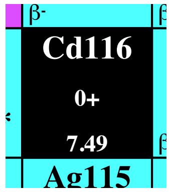
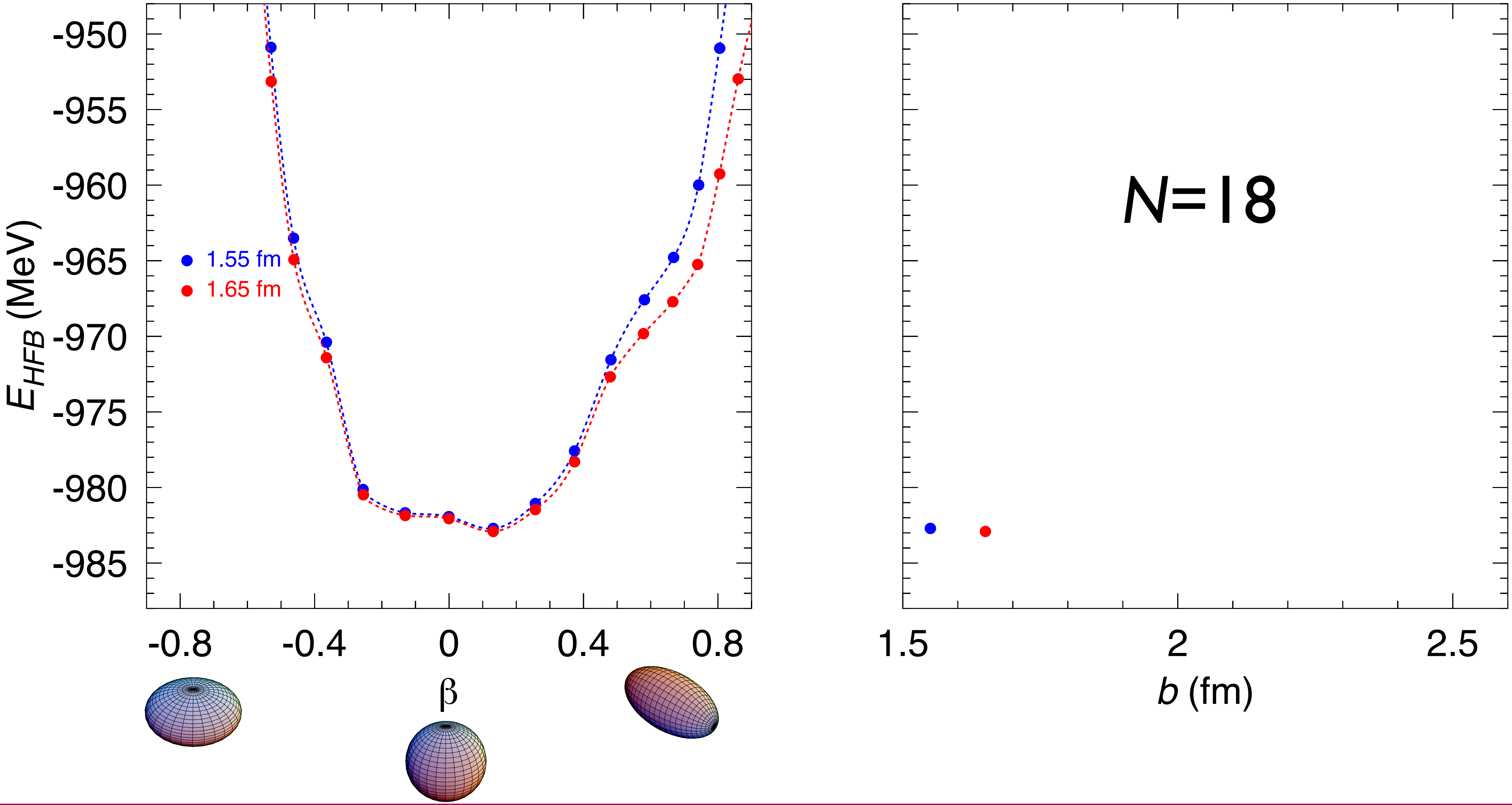
Example: 



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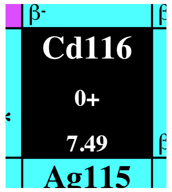
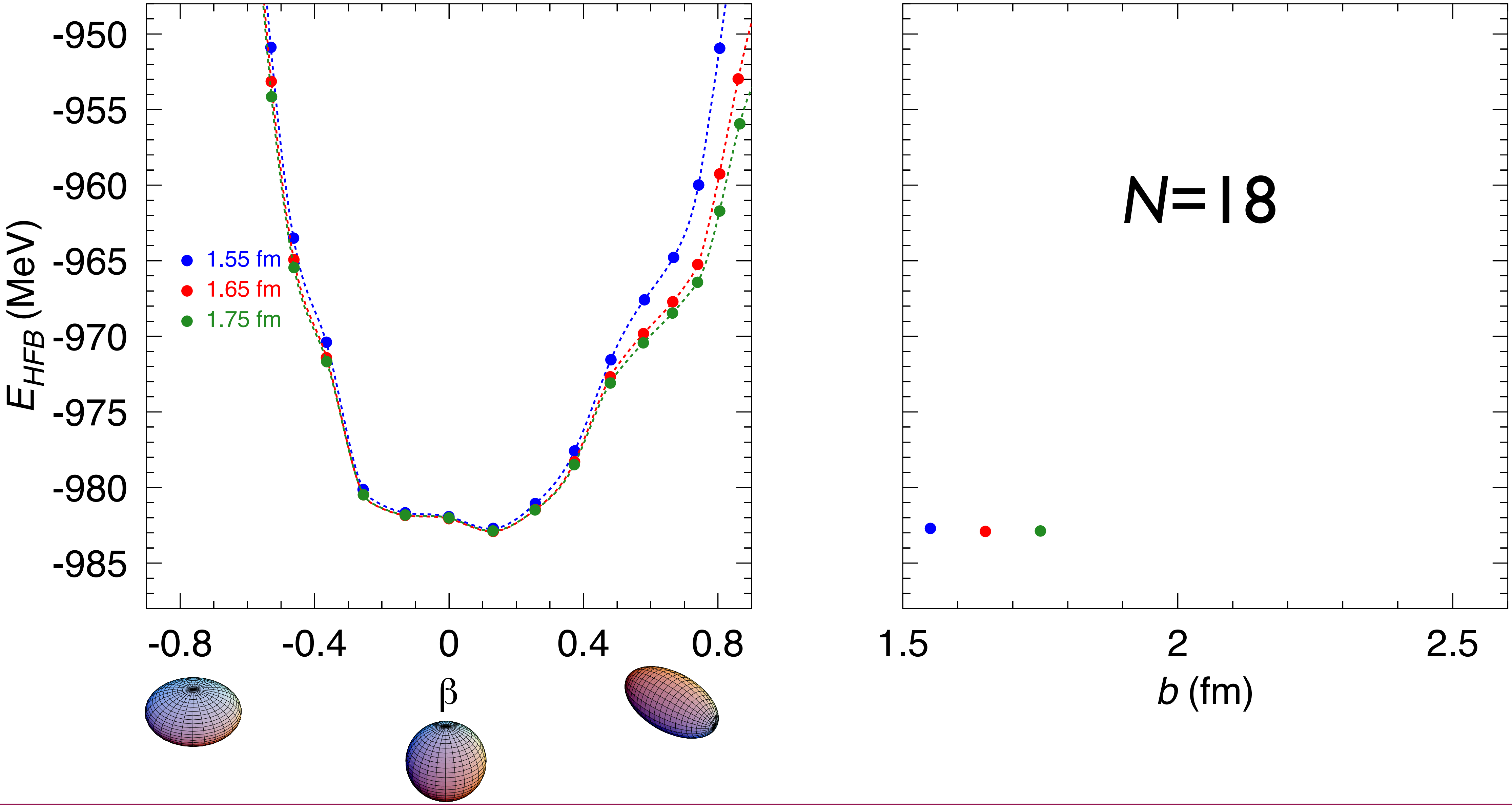
Example: 



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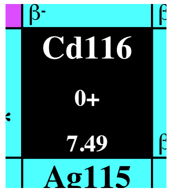
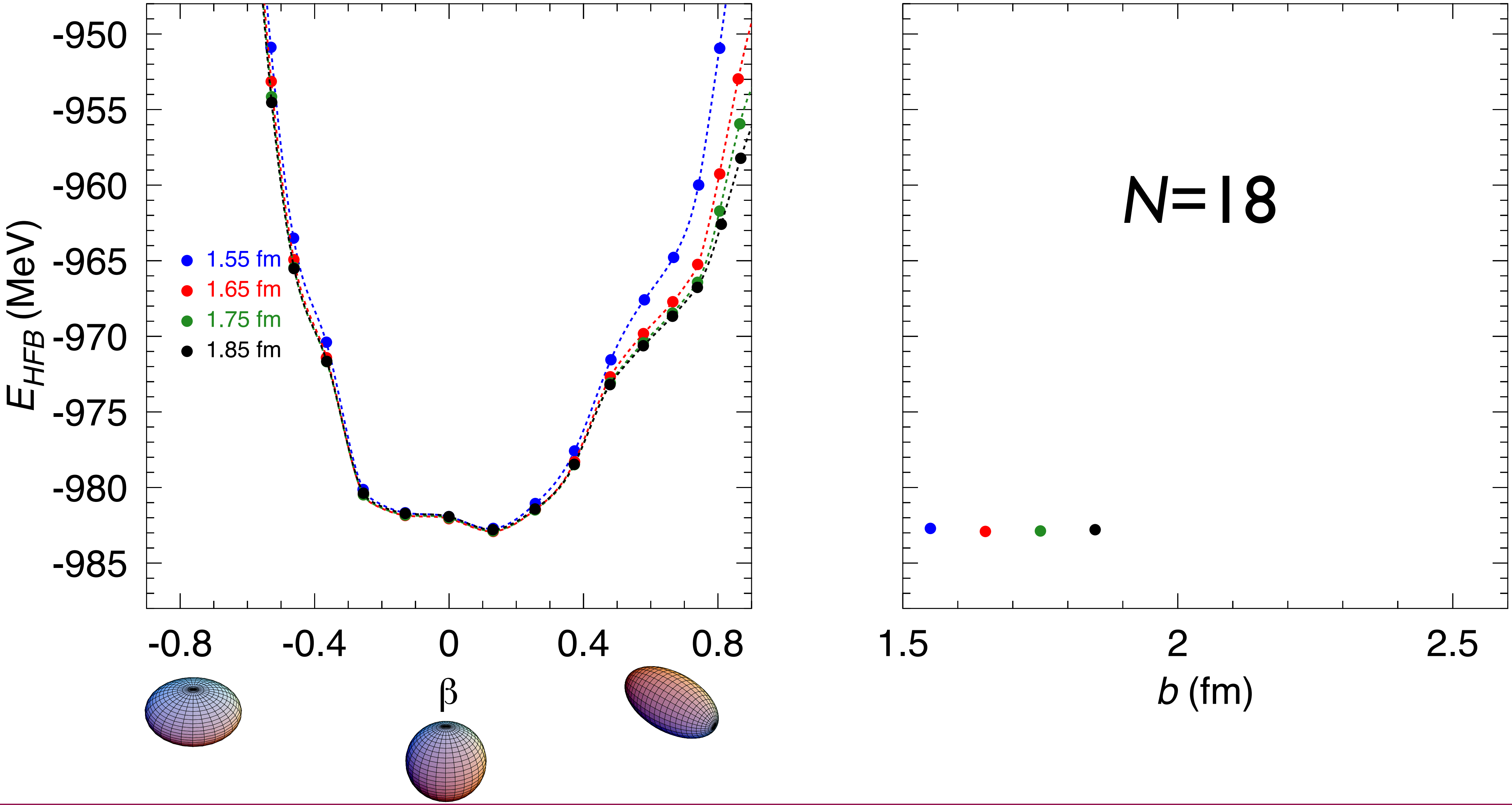
Example: 



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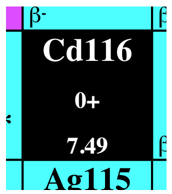
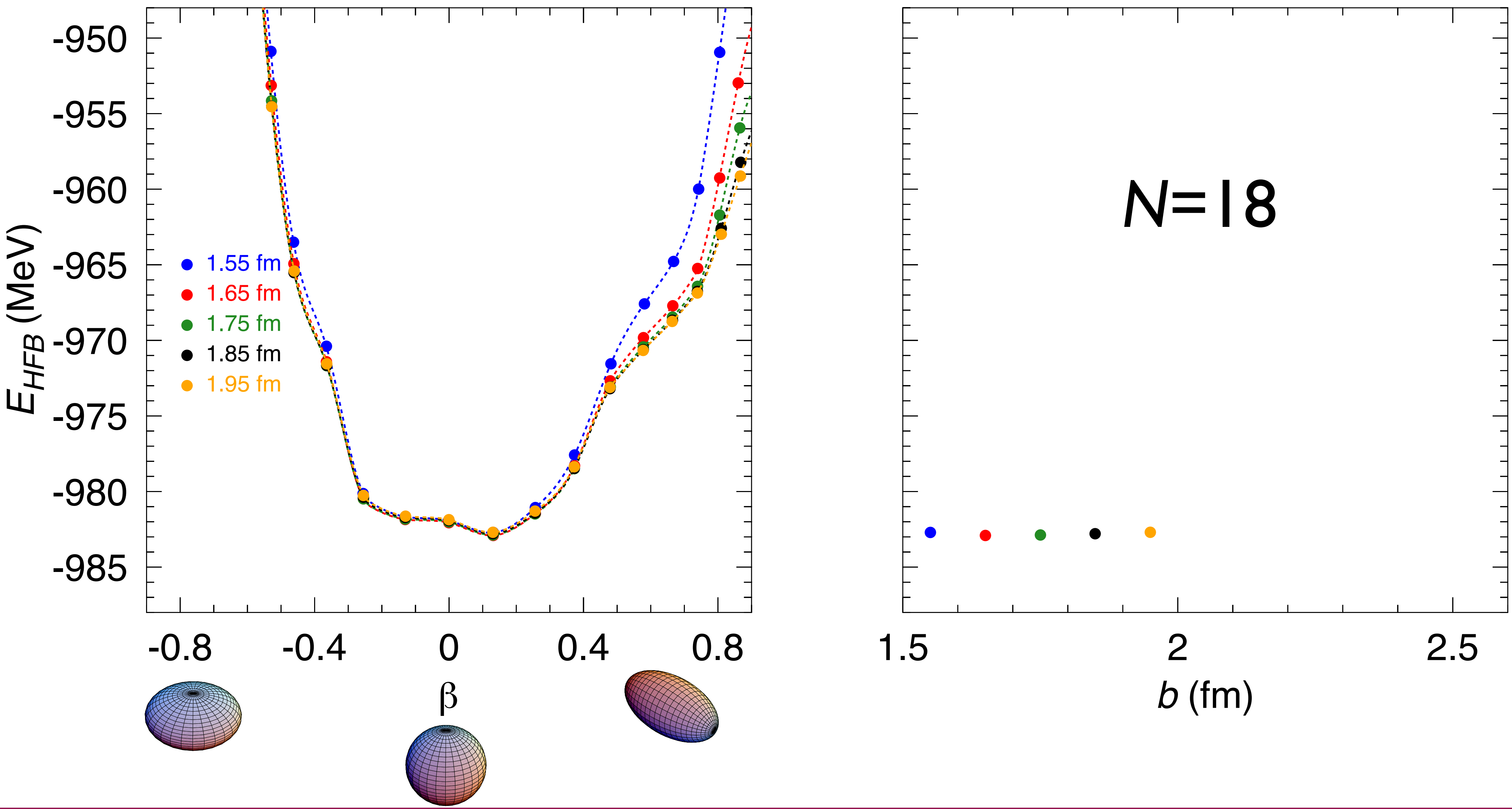
Example: 



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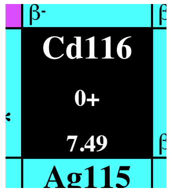

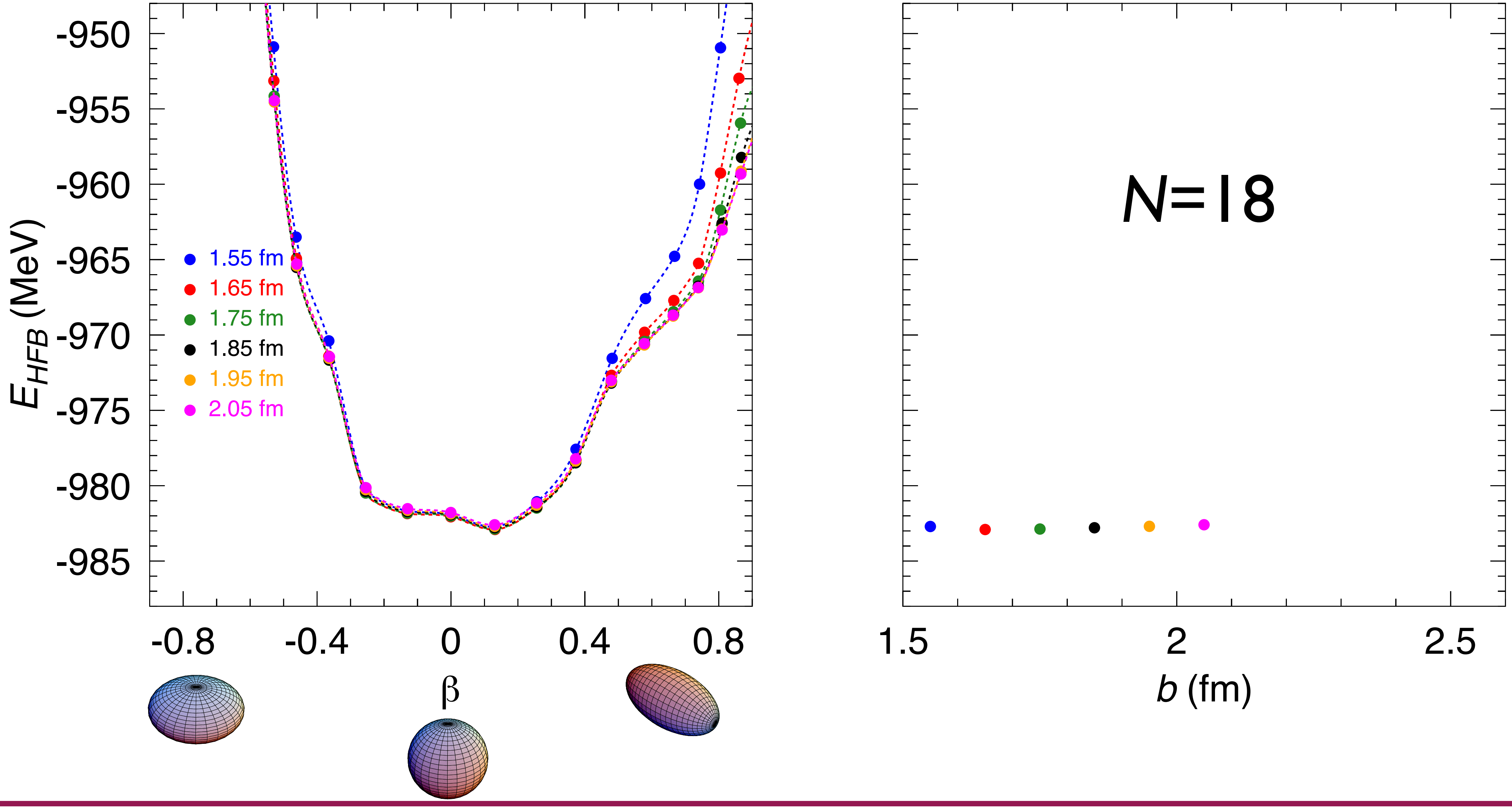

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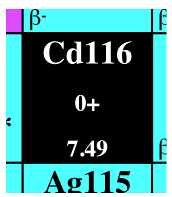
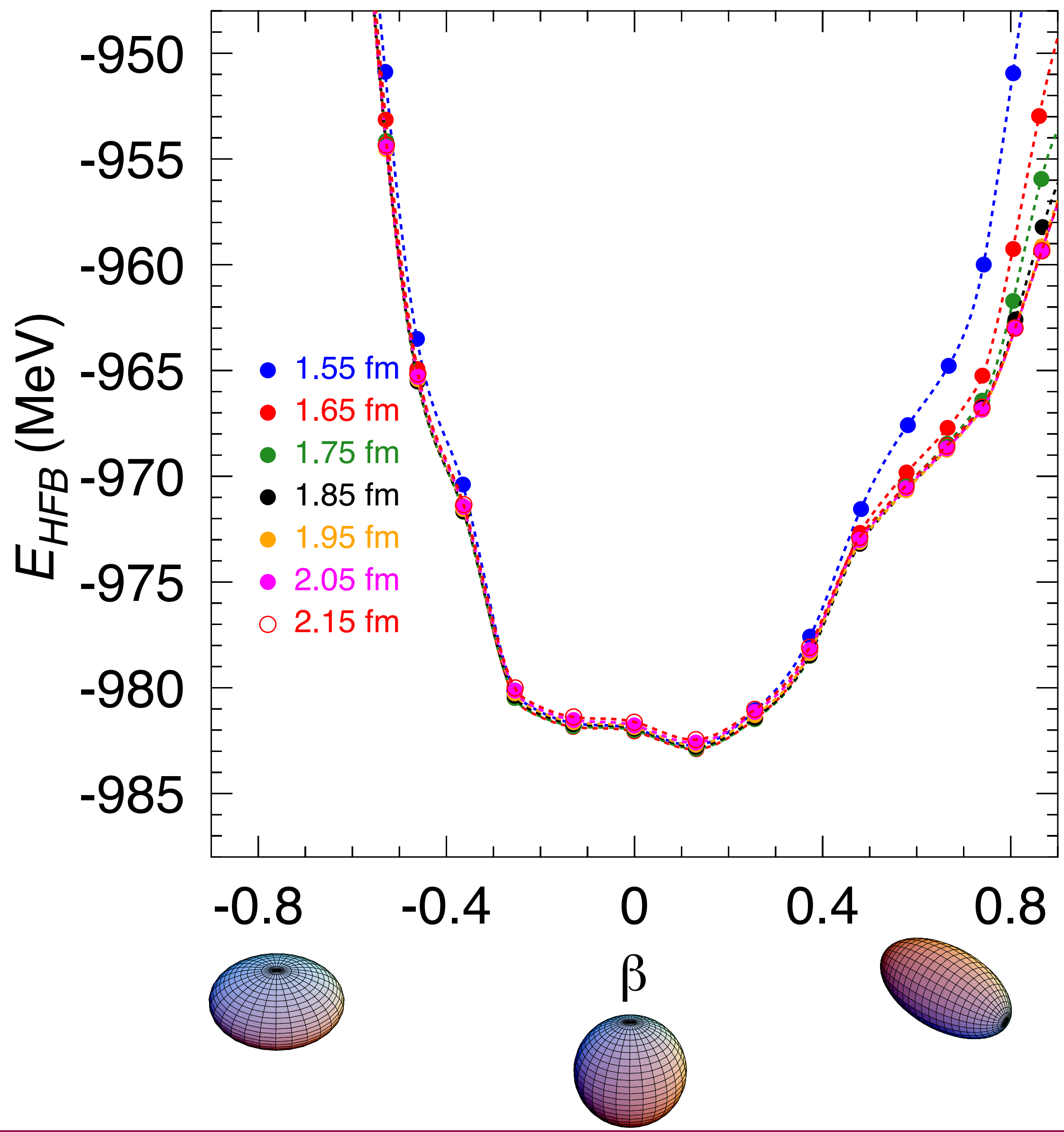
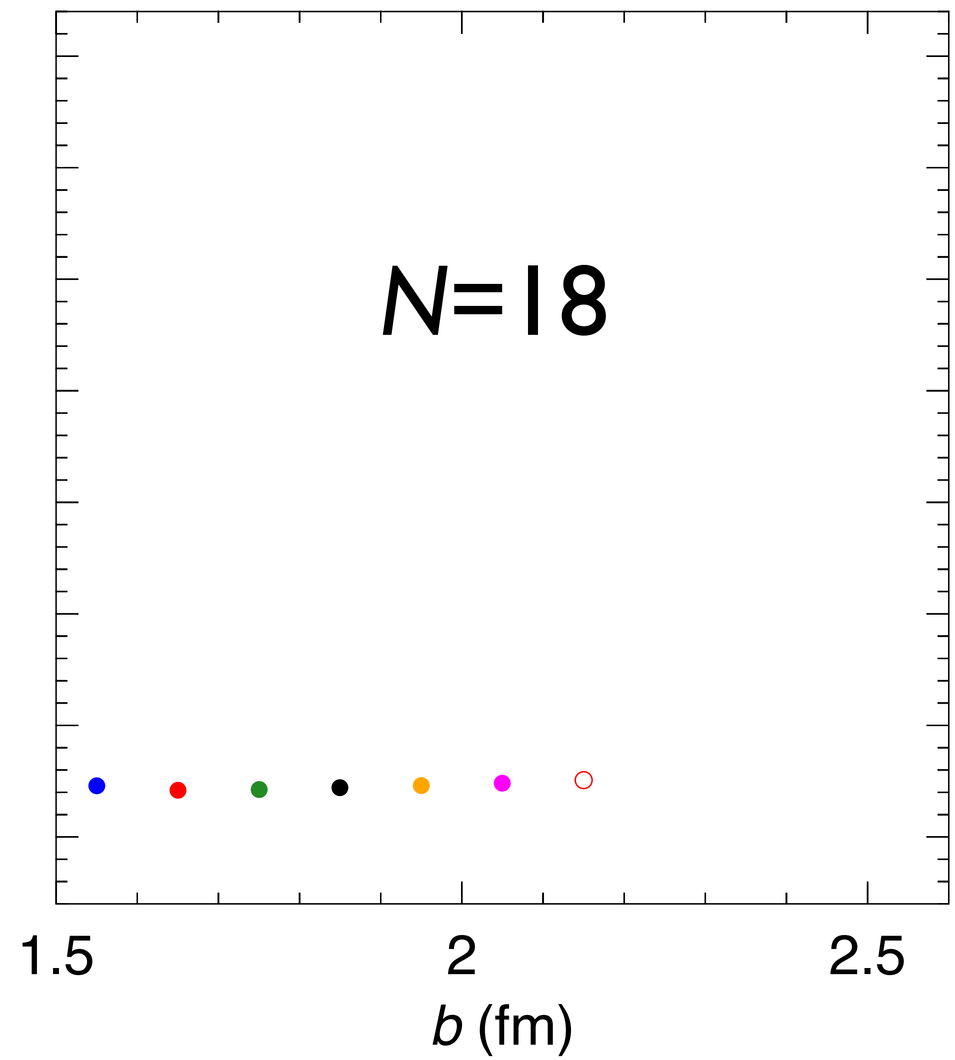
Example: 





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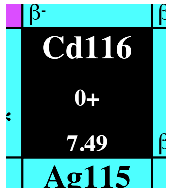
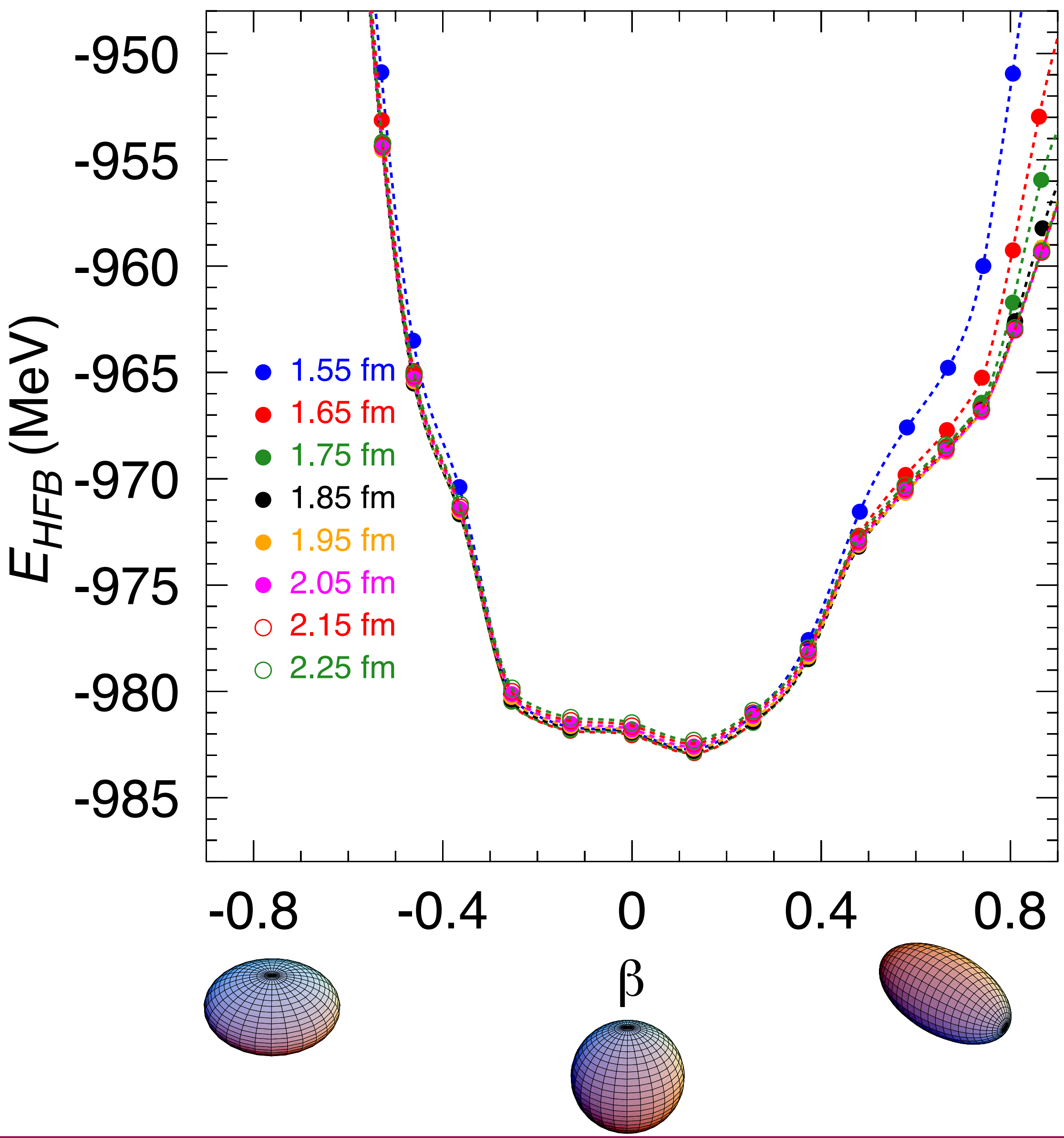
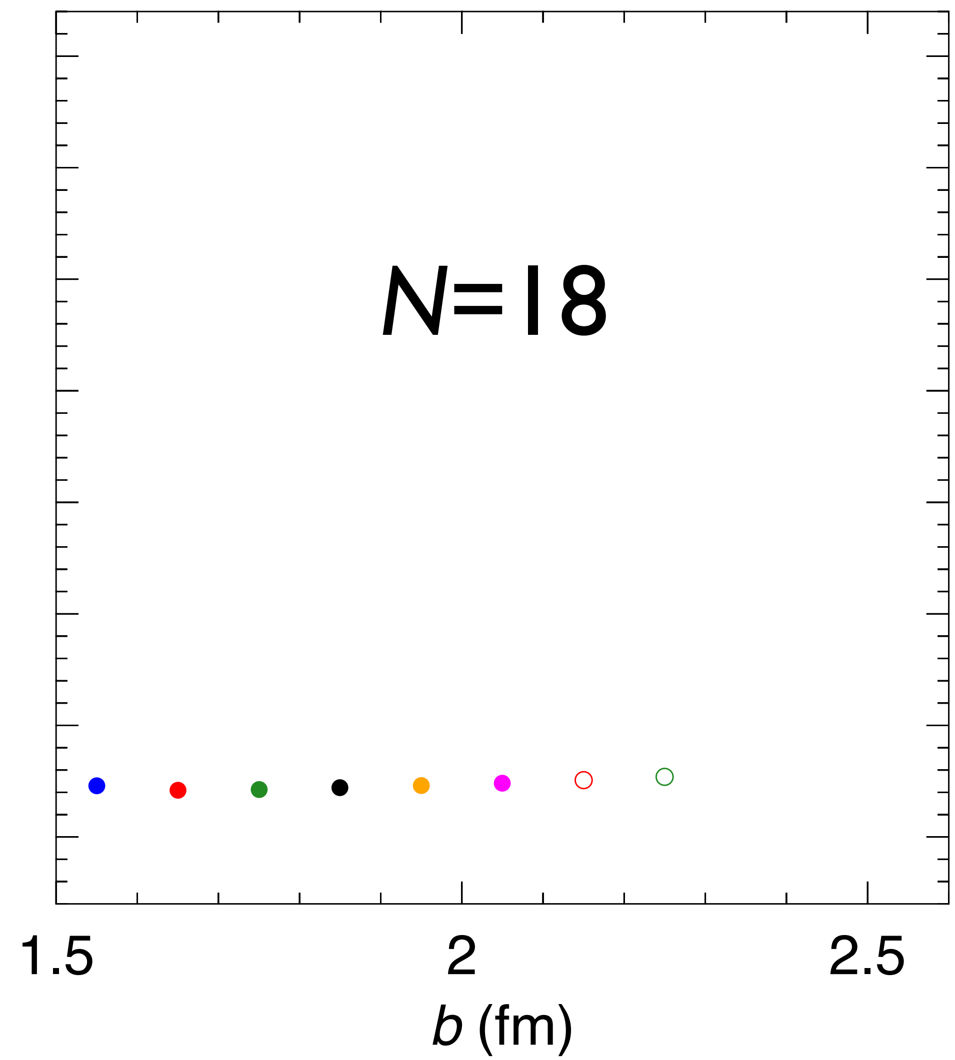
Example: 





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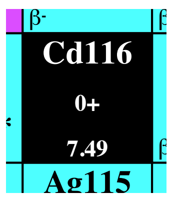
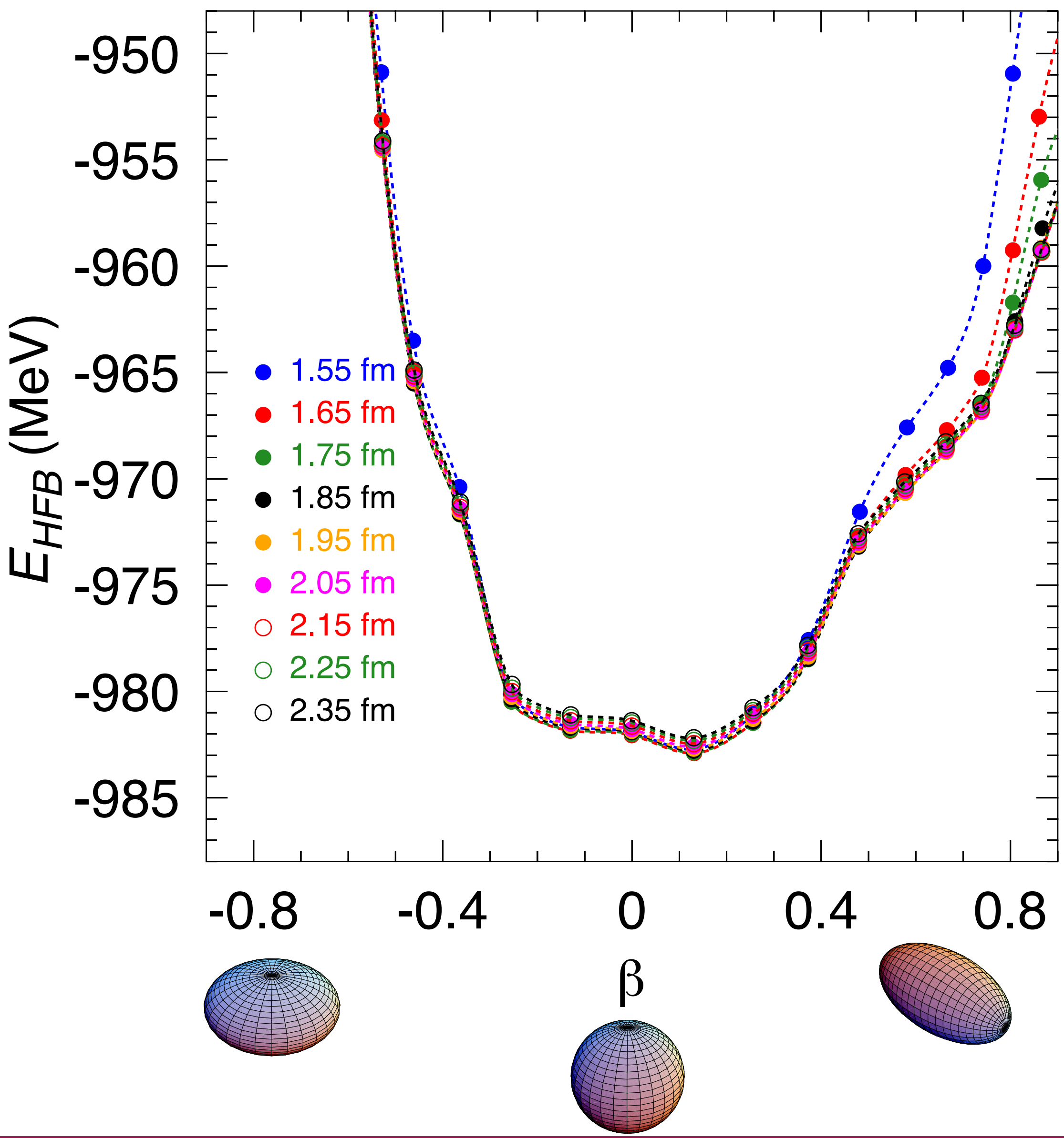
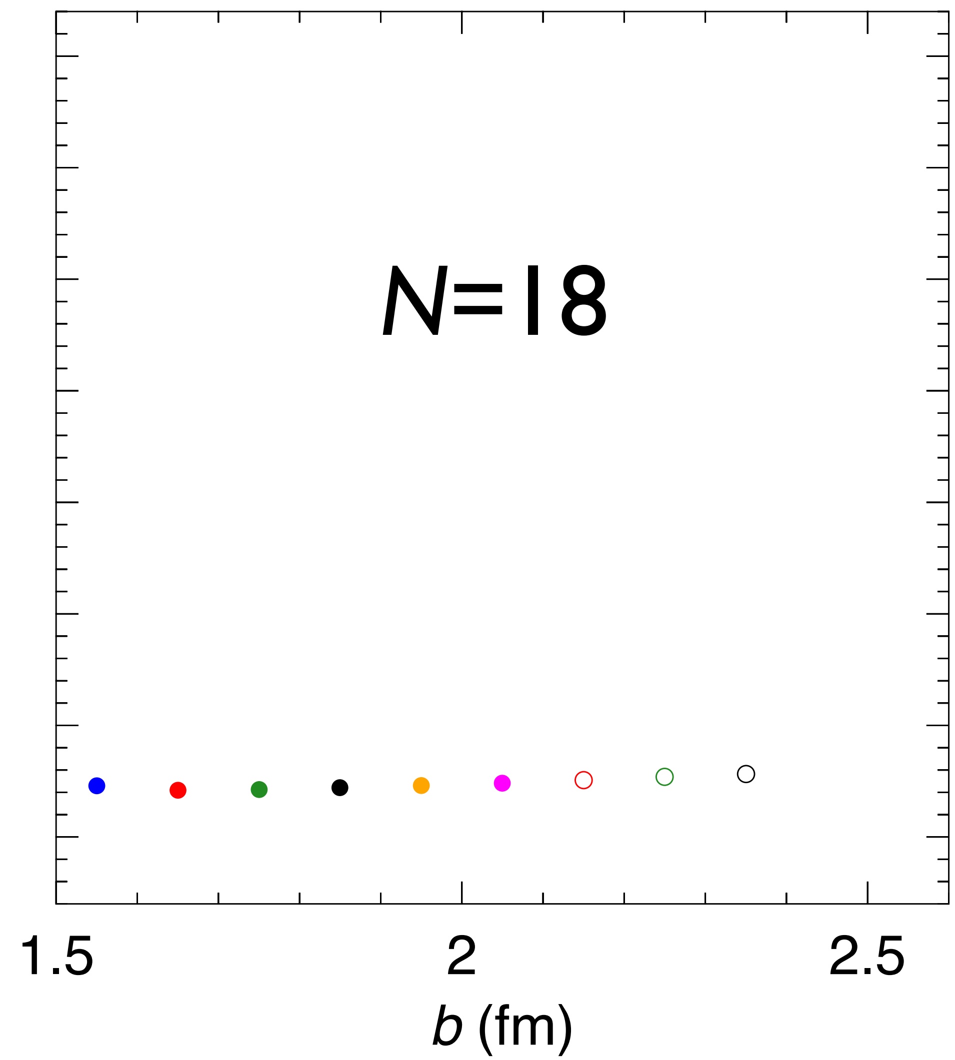
Example: 





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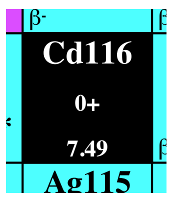
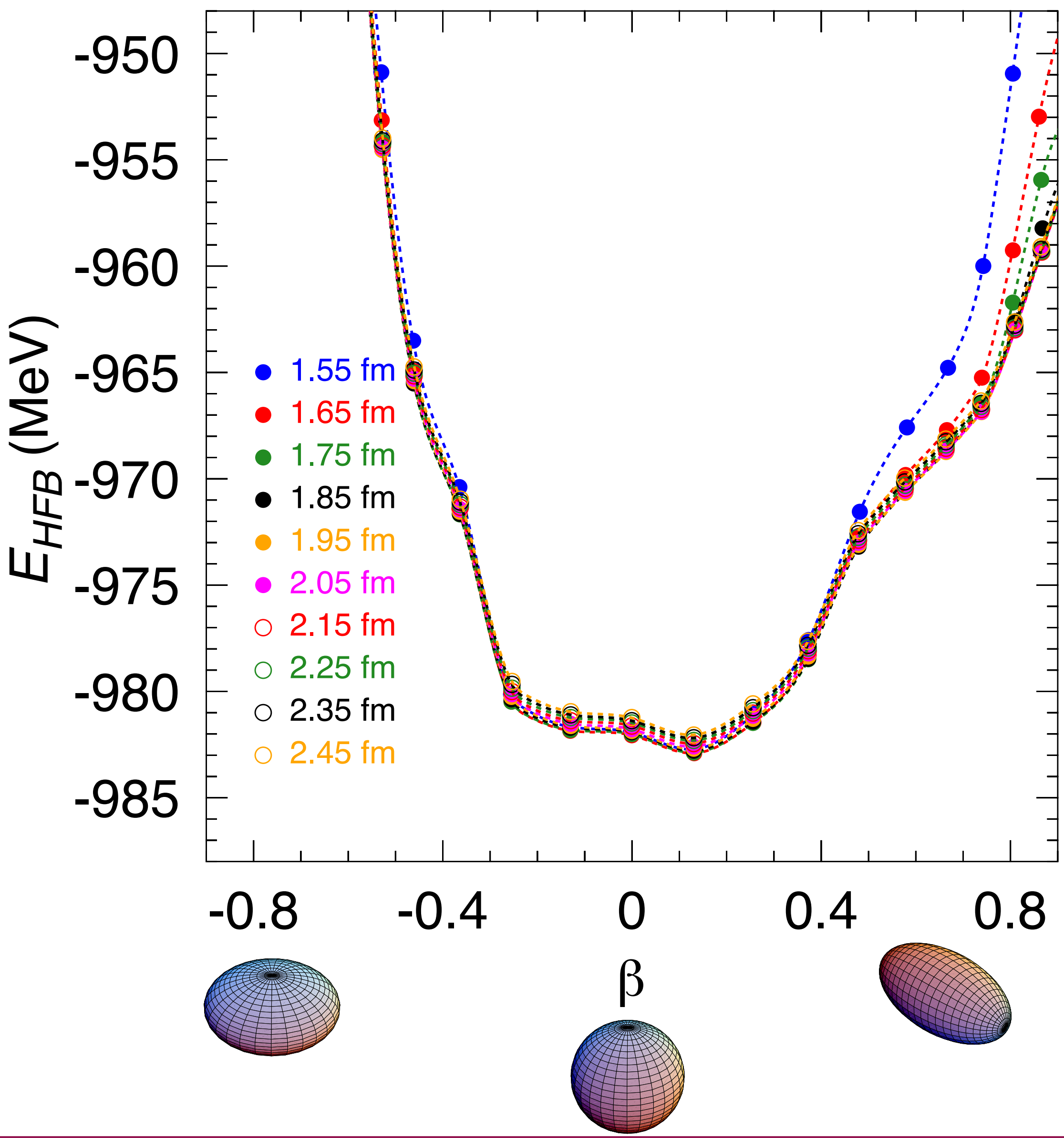
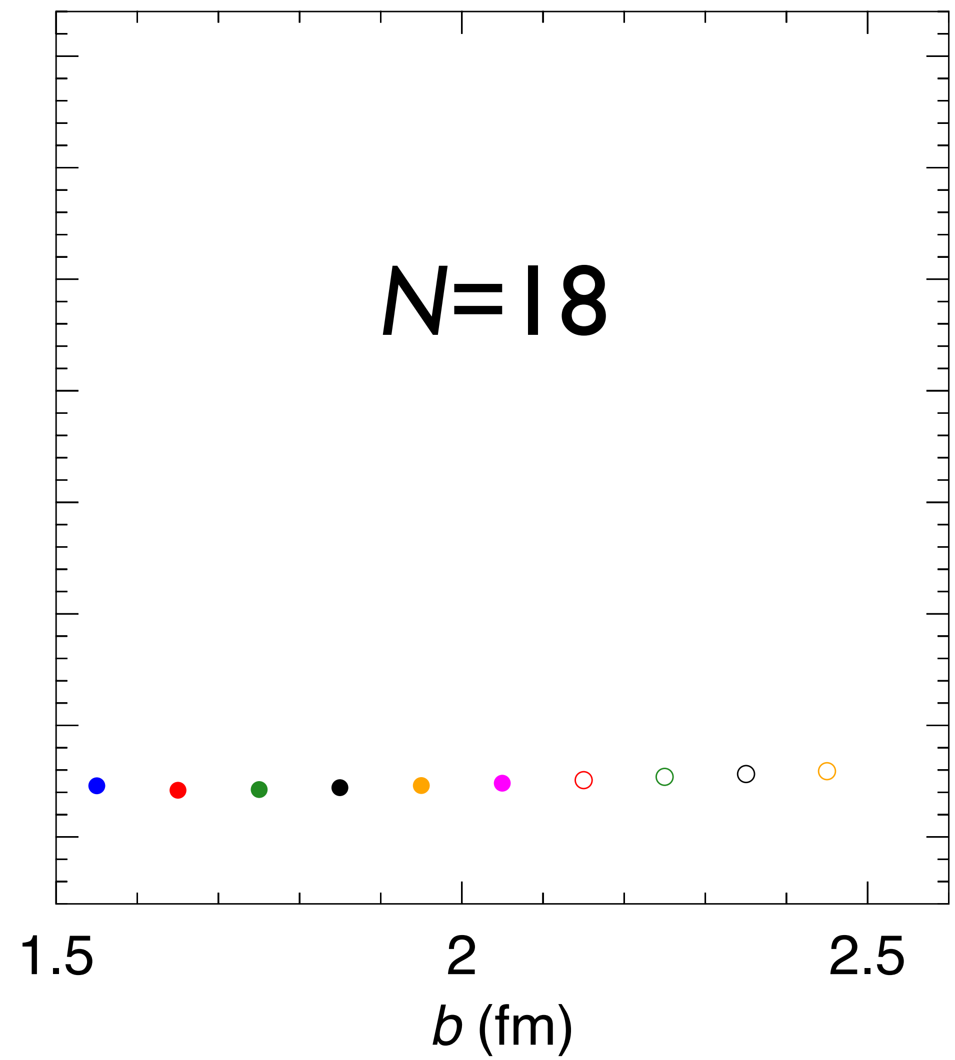
Example: 





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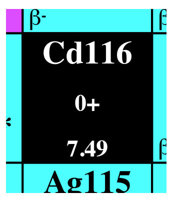
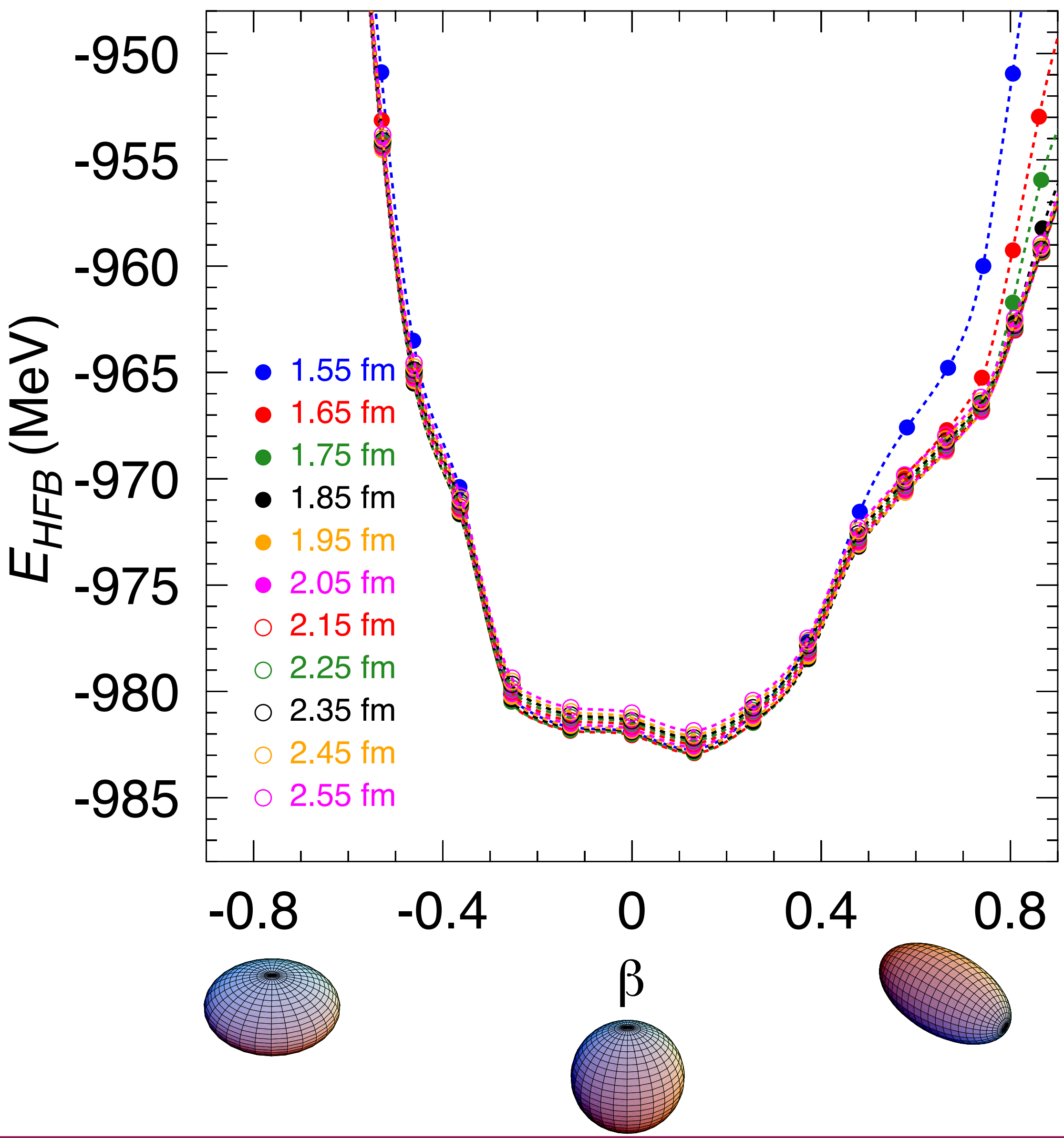
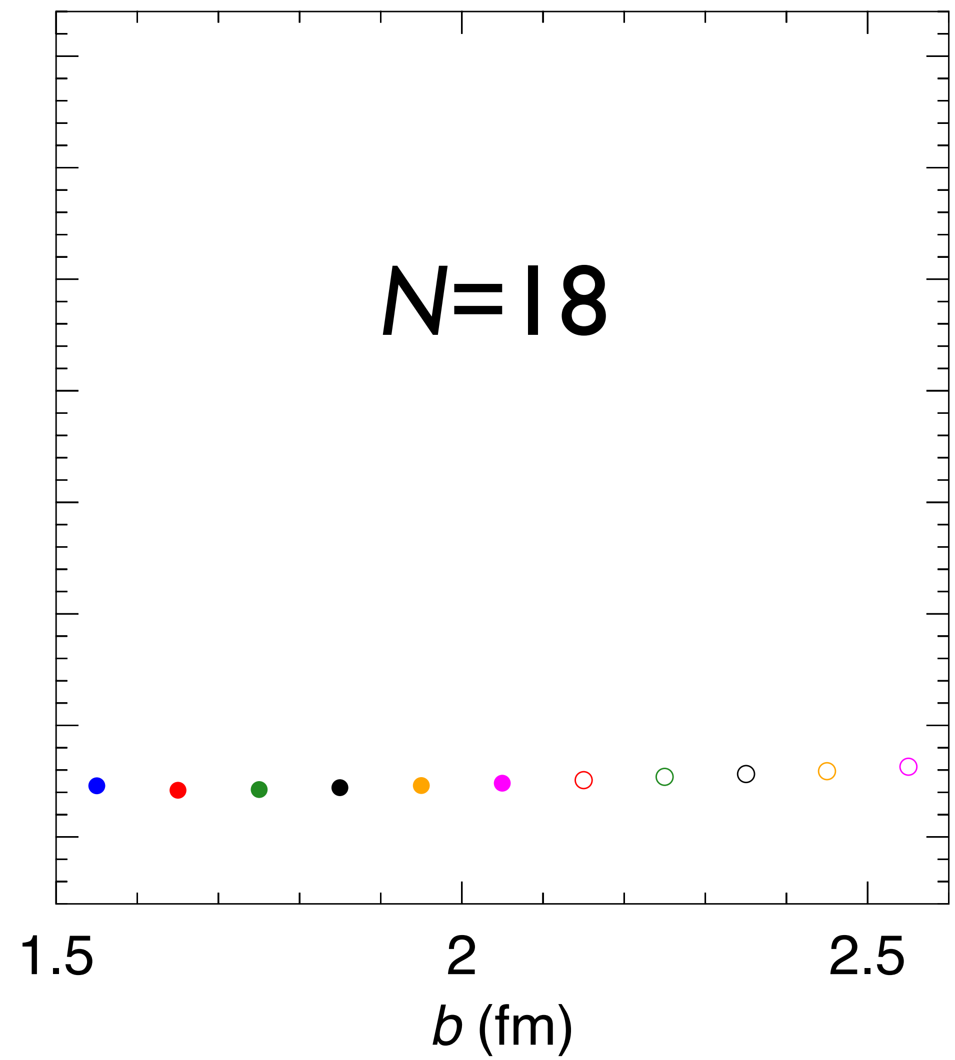
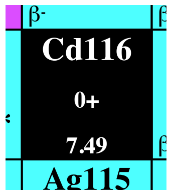
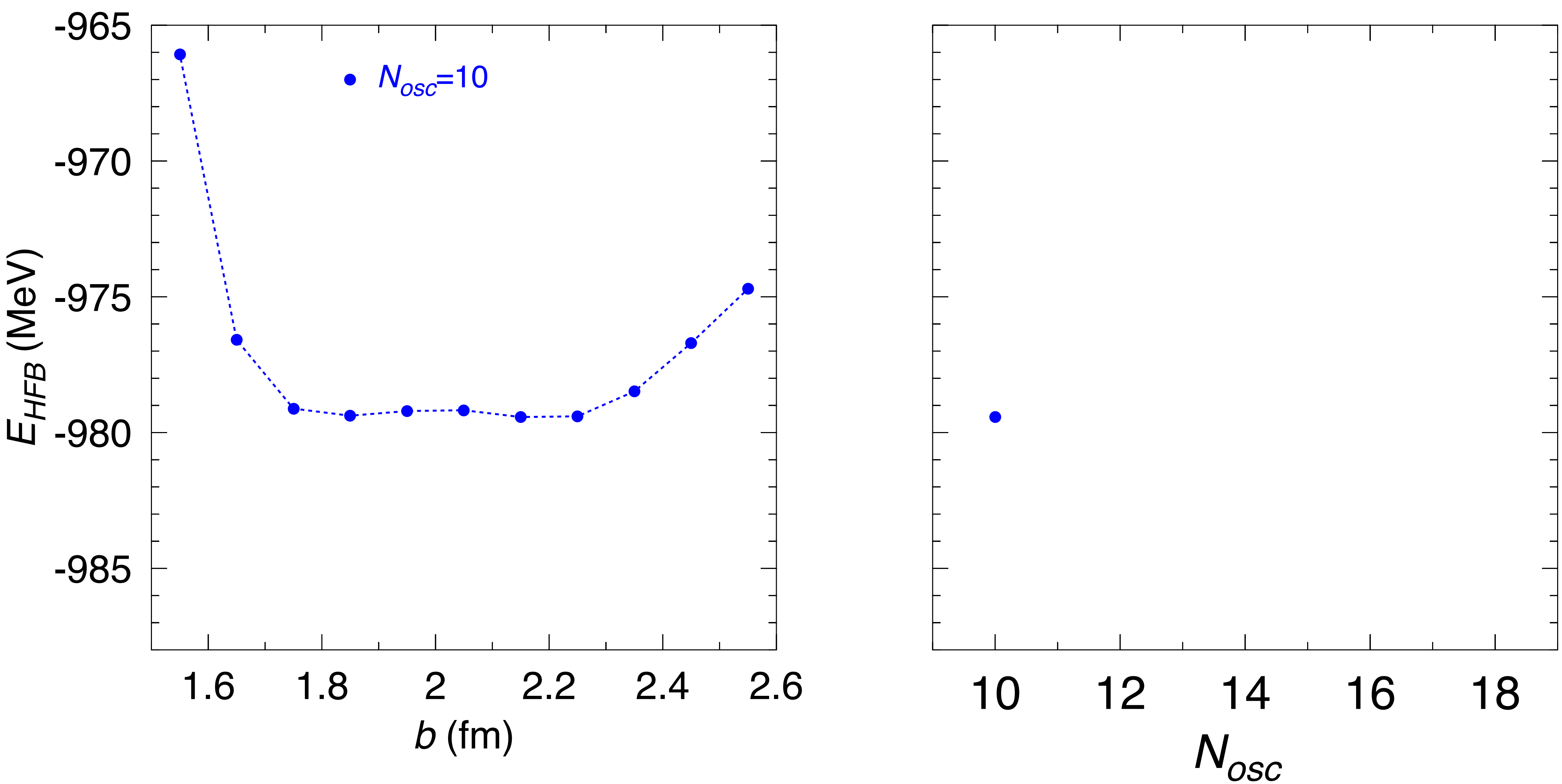
Example: 





Final convergence

Example: 



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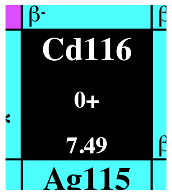
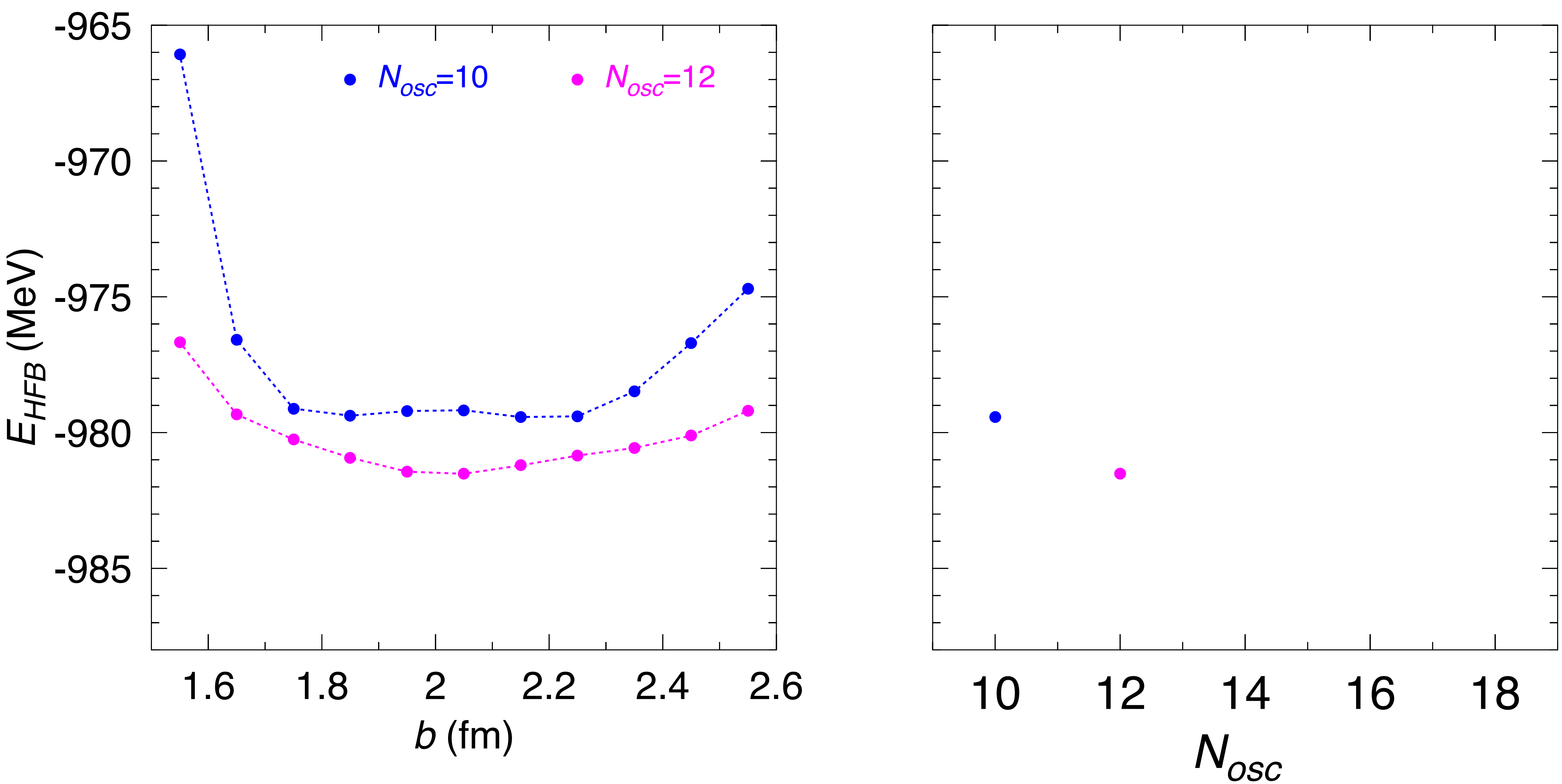
Example: 



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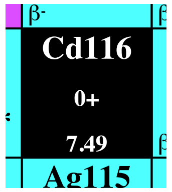

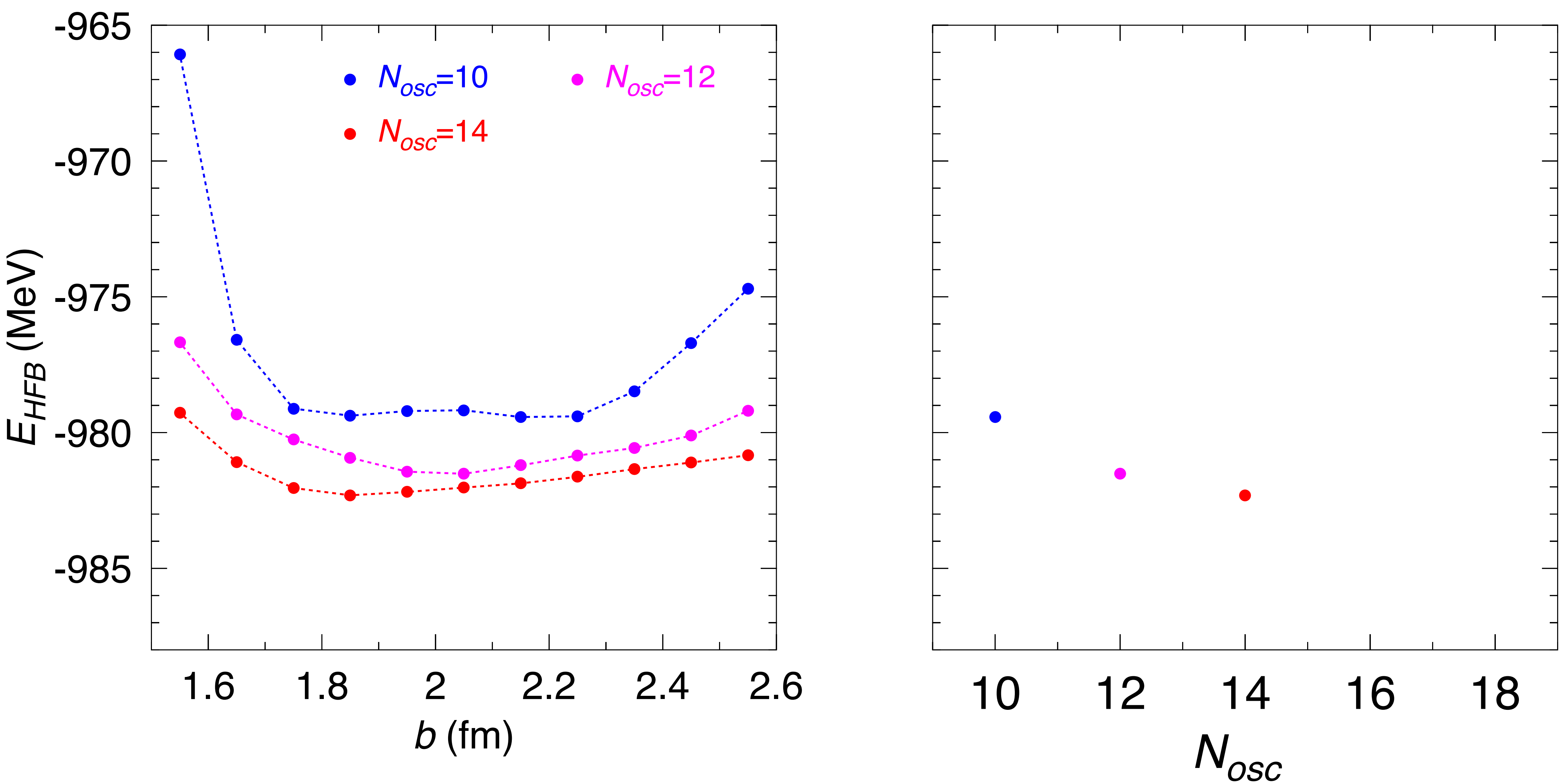

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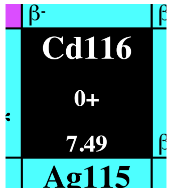

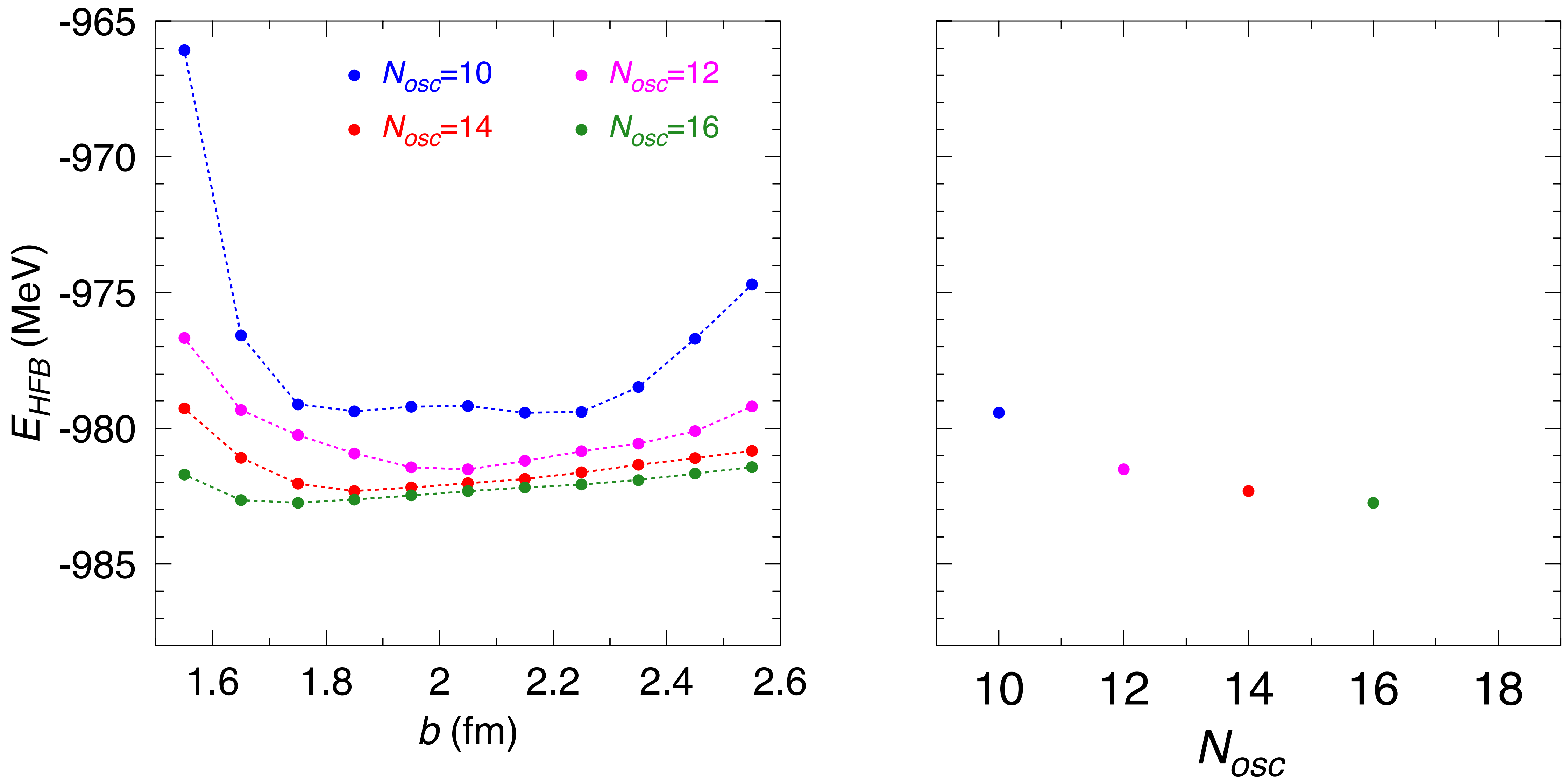

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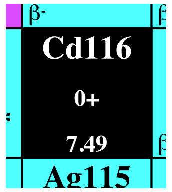
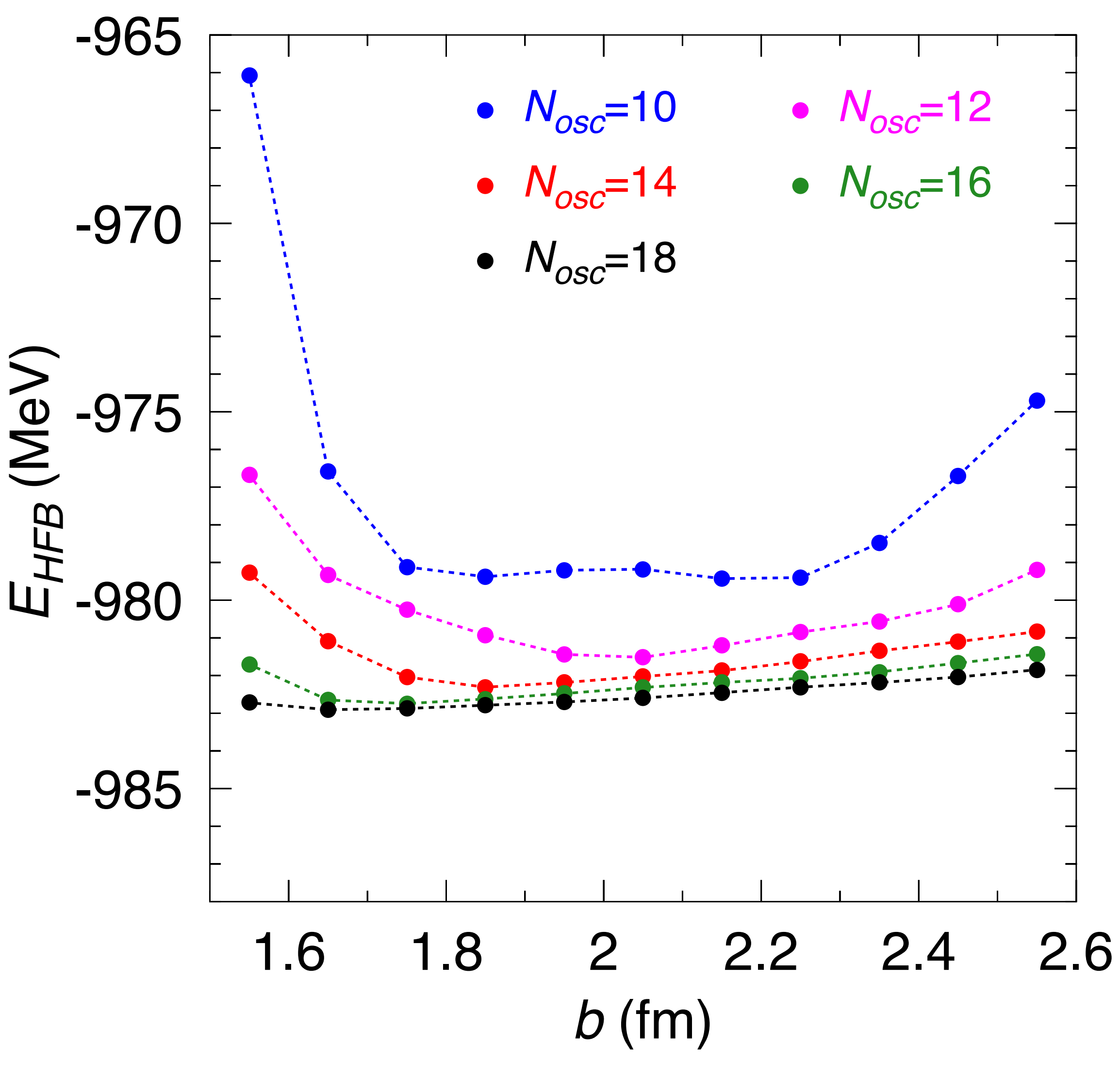
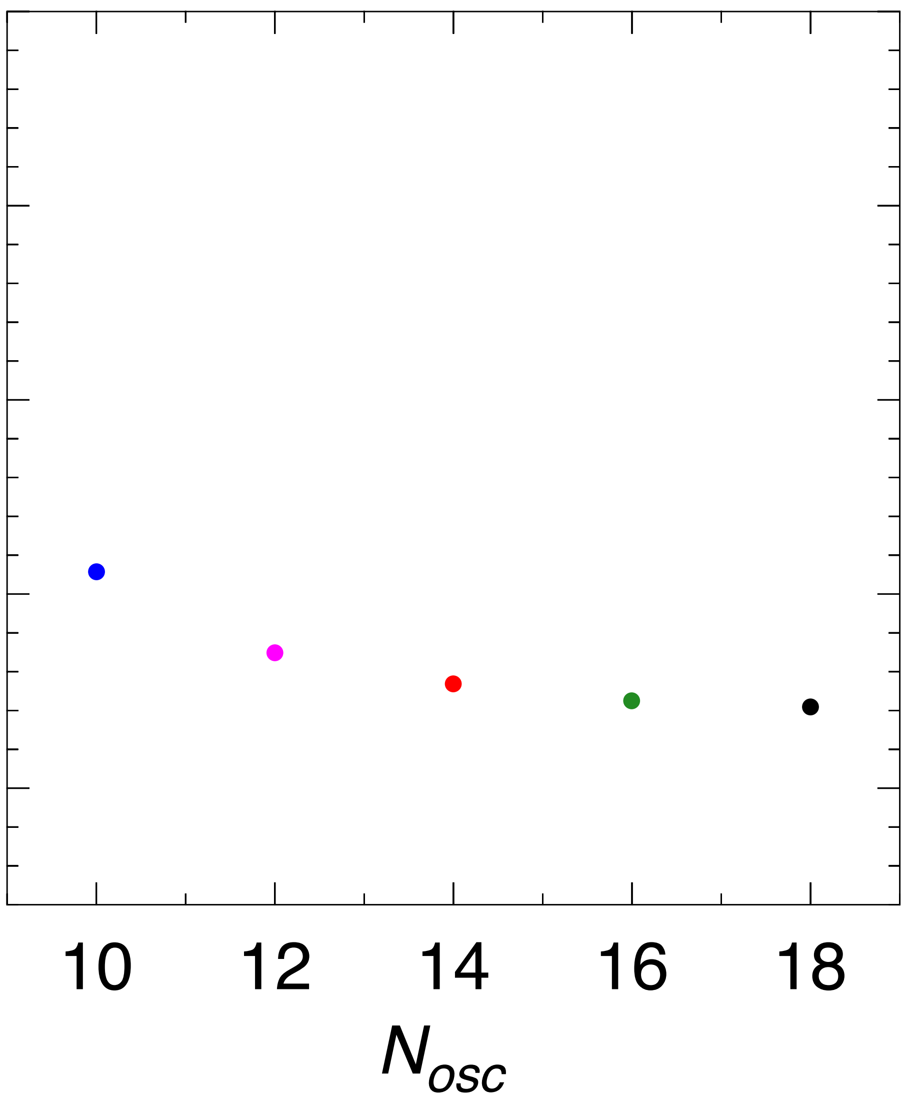


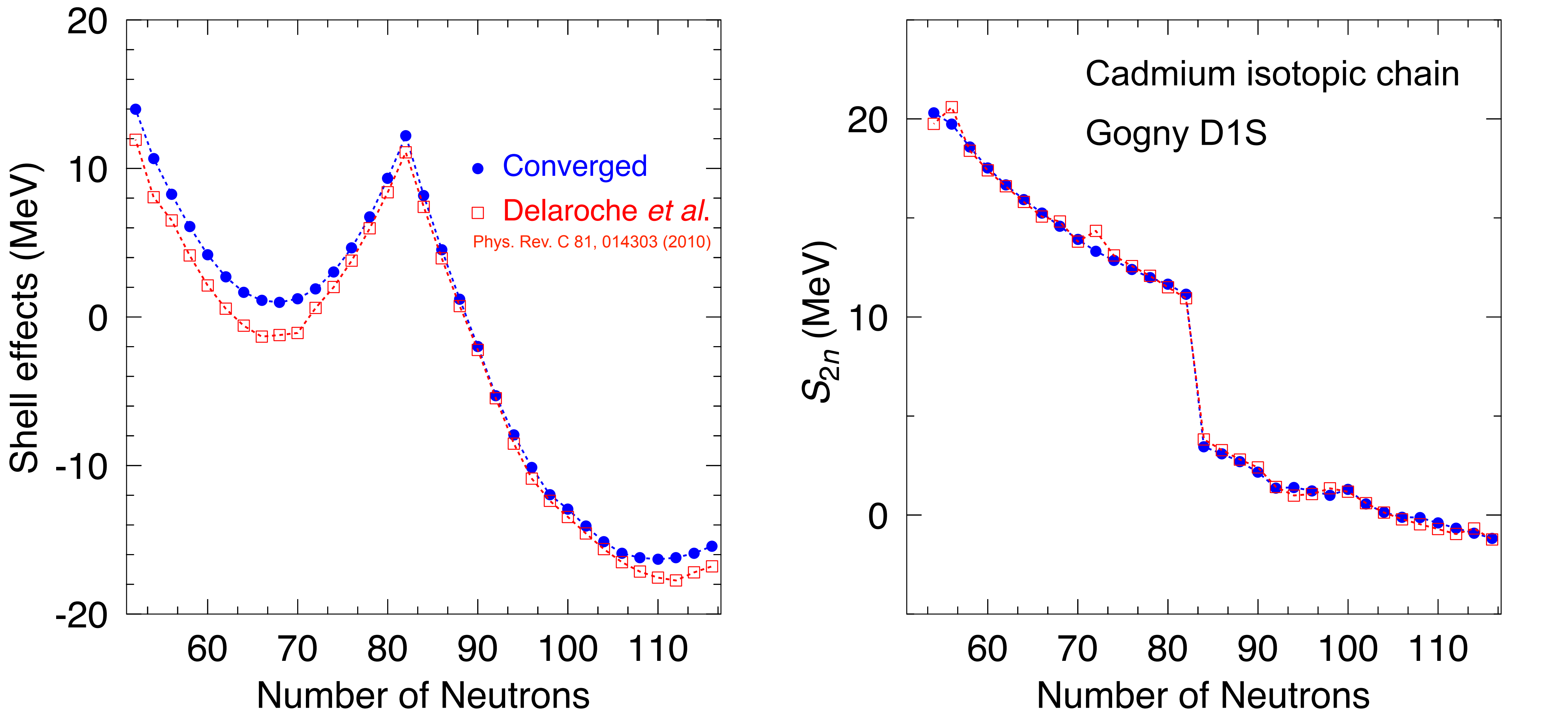




TECHNISCHE UNIVERSITÄT DARMSTADT

Convergence

- Published tables could contain some lack of convergence in the total binding energy.
- Two neutron separation energies are better converged.
- Artificial ‘jumps’ or ‘noise’ could appear in the S_{2n} due to lack of convergence.



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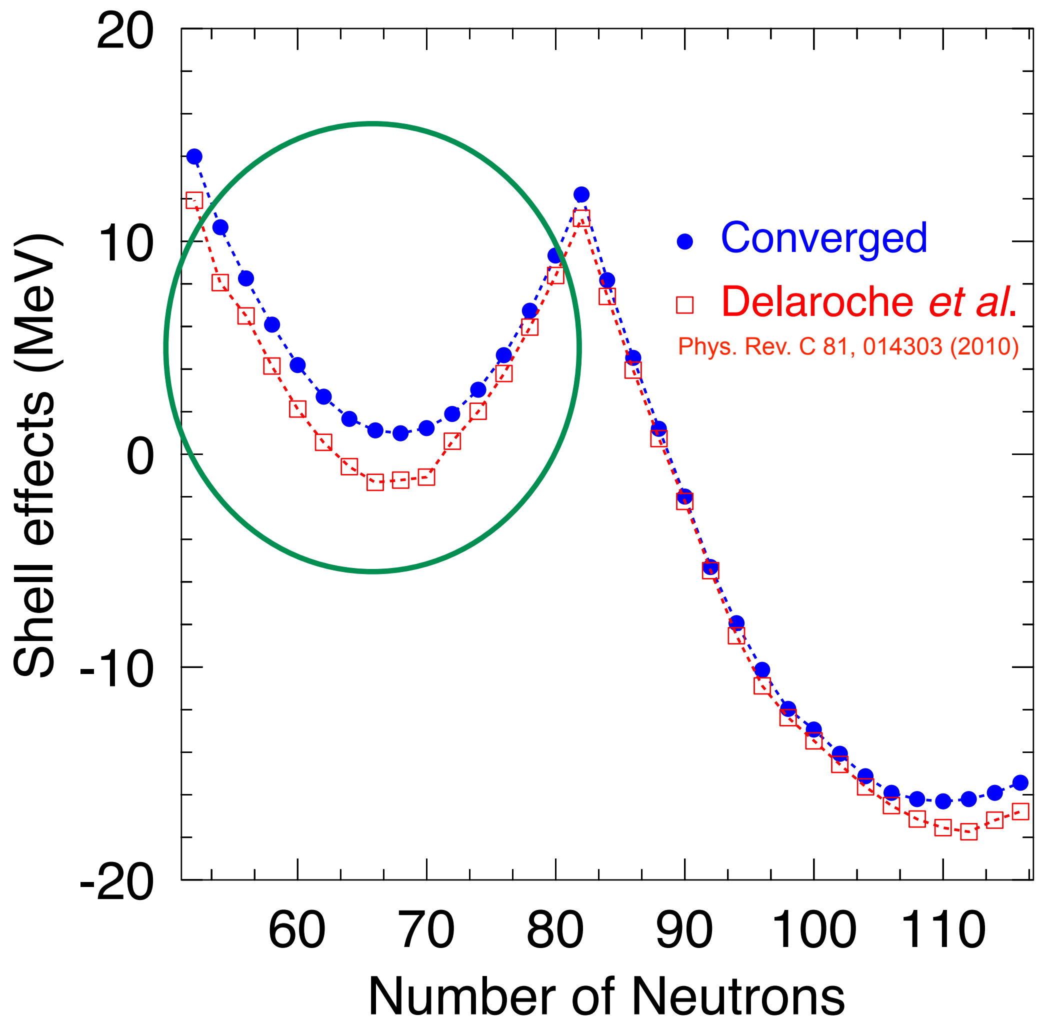

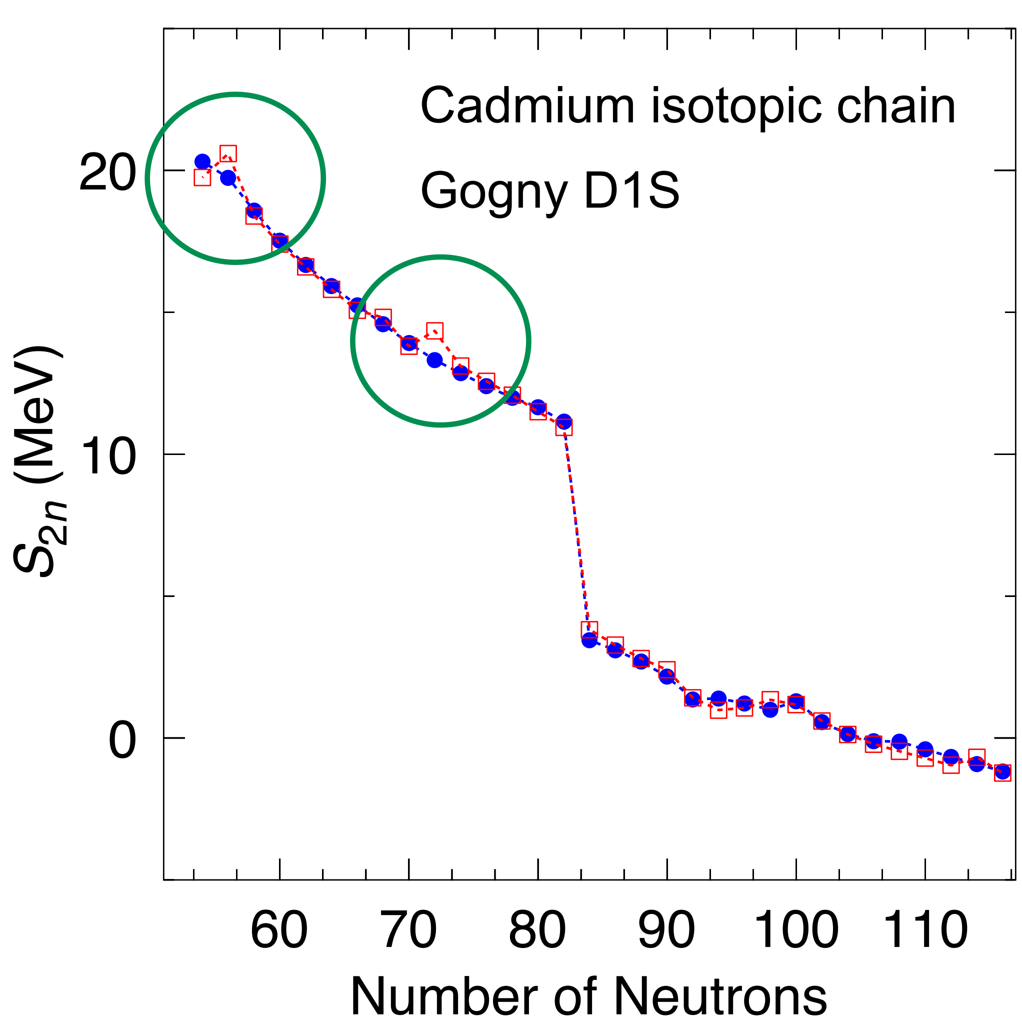

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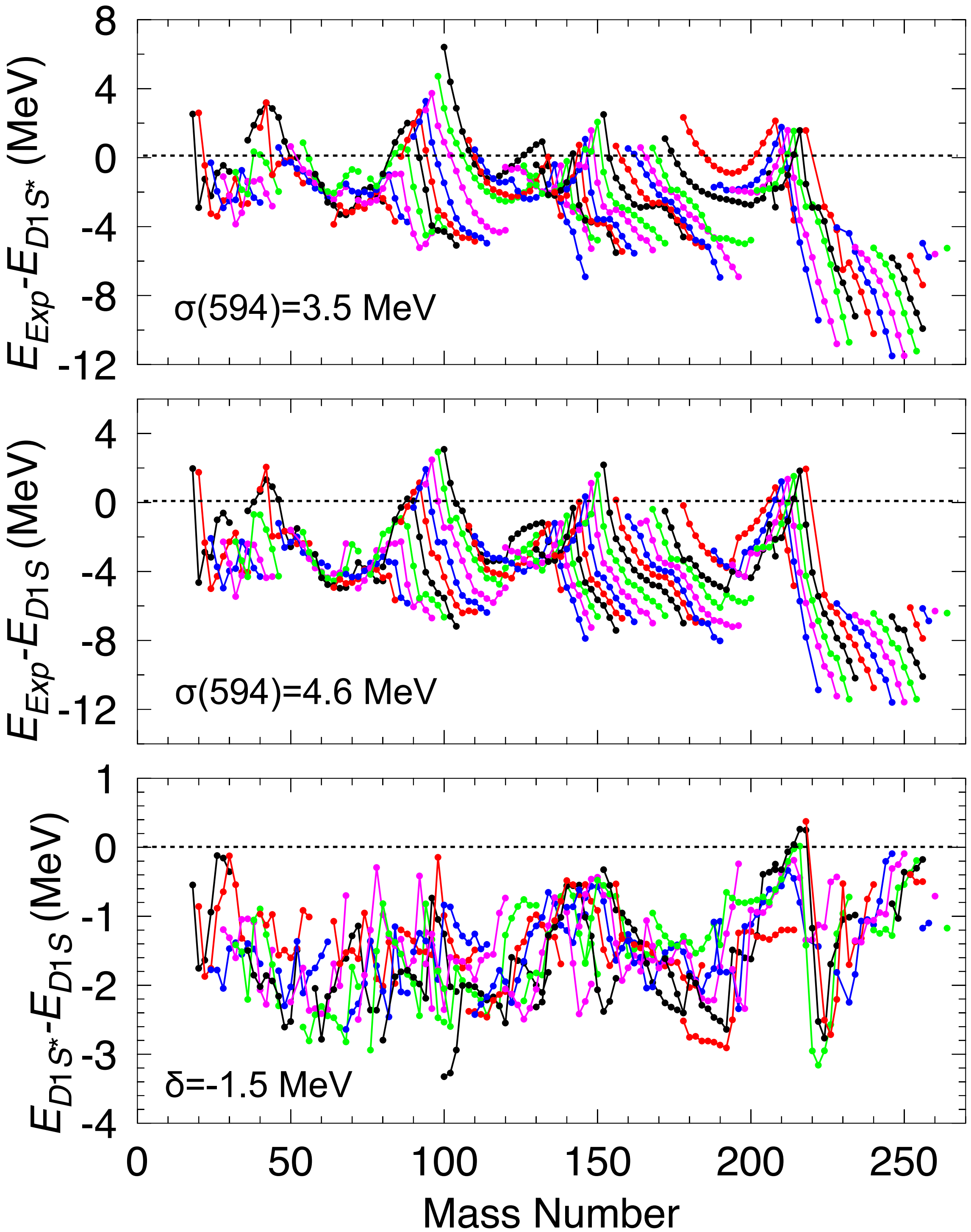

- Experimental data: AME12, only even-even.
- Gogny D1S: Delaroche et al., PRC 81, 014303 (2010).
- Gogny D1S*: N_{osc}=18, *b* optimized, β_2 explored.

- Gogny D1S **is not** a good parametrization for masses (overbinding of double magic nuclei, underbinding of neutron rich nuclei, poor r.m.s.).

- Better convergence gives smaller r.m.s. and smoother behavior along the whole AME12 even-even data.
- ~1.5 MeV average gain in energy by improving the convergence.

A. Arzhanov, Master Thesis

Hartree-Fock-Bogoliubov (HFB) with blocking

Variational space: $\{|\Phi_b\rangle \equiv \alpha_b^\dagger |\Phi\rangle\}$ set of **product-type** wave functions which fulfill:

- Quasiparticle vacua: $\bar{\alpha}_k|\Phi_b\rangle = 0$
- Most general linear combination of the arbitrary single particle basis:

$$\bar{\alpha}_k^\dagger = \sum_l \bar{U}_{lk} c_l^\dagger + \bar{V}_{lk} c_l$$

- Fermionic operators: $\{\bar{\alpha}_k^\dagger, \bar{\alpha}_{k'}\} = \delta_{kk'}; \{\bar{\alpha}_k^\dagger, \bar{\alpha}_{k'}^\dagger\} = \{\bar{\alpha}_k, \bar{\alpha}_{k'}\} = 0$

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Variational principle: $$\delta \left[E_b^{\prime\,\mathrm{HFB}} = \langle \Phi_b | \hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} | \Phi_b \rangle \right]_{|\Phi_b\rangle = |\mathrm{HFB}_b\rangle} = 0$$

$$\lambda_Z \rightarrow \langle \Phi_b | \hat{Z} | \Phi_b \rangle = Z$$

$$\lambda_N \rightarrow \langle \Phi_b | \hat{N} | \Phi_b \rangle = N$$

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$$\lambda_Z \to \langle\Phi_b|\hat{Z}|\Phi_b\rangle = Z$$

$$\lambda_N \to \langle\Phi_b|\hat{N}|\Phi_b\rangle = N$$

$$E_b^{\mathrm{HFB}} = \langle\mathrm{HFB}_b|\hat{H}|\mathrm{HFB}_b\rangle$$

$|\mathrm{HFB}_b\rangle$ **Product Type**

Hartree-Fock-Bogoliubov (HFB) with blocking

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- Most general linear combination of the arbitrary single particle basis: $\bar{\alpha}_k^\dagger = \sum_l \bar{U}_{lk}c_l^\dagger + \bar{V}_{lk}c_l$ **Breaks time reversal symmetry!**
- Fermionic operators: $\{\bar{\alpha}_k^\dagger, \bar{\alpha}_{k'}\} = \delta_{kk'}; \{\bar{\alpha}_k^\dagger, \bar{\alpha}_{k'}^\dagger\} = \{\bar{\alpha}_k, \bar{\alpha}_{k'}\} = 0$

Variational principle: $\delta\left[E_b^{'\mathrm{HFB}} = \langle\Phi_b|\hat{H} - \lambda_N\hat{N} - \lambda_Z\hat{Z}|\Phi_b\rangle\right]_{|\Phi_b\rangle=|\mathrm{HFB}_b\rangle} = 0$

$\lambda_Z \rightarrow \langle\Phi_b|\hat{Z}|\Phi_b\rangle = Z$

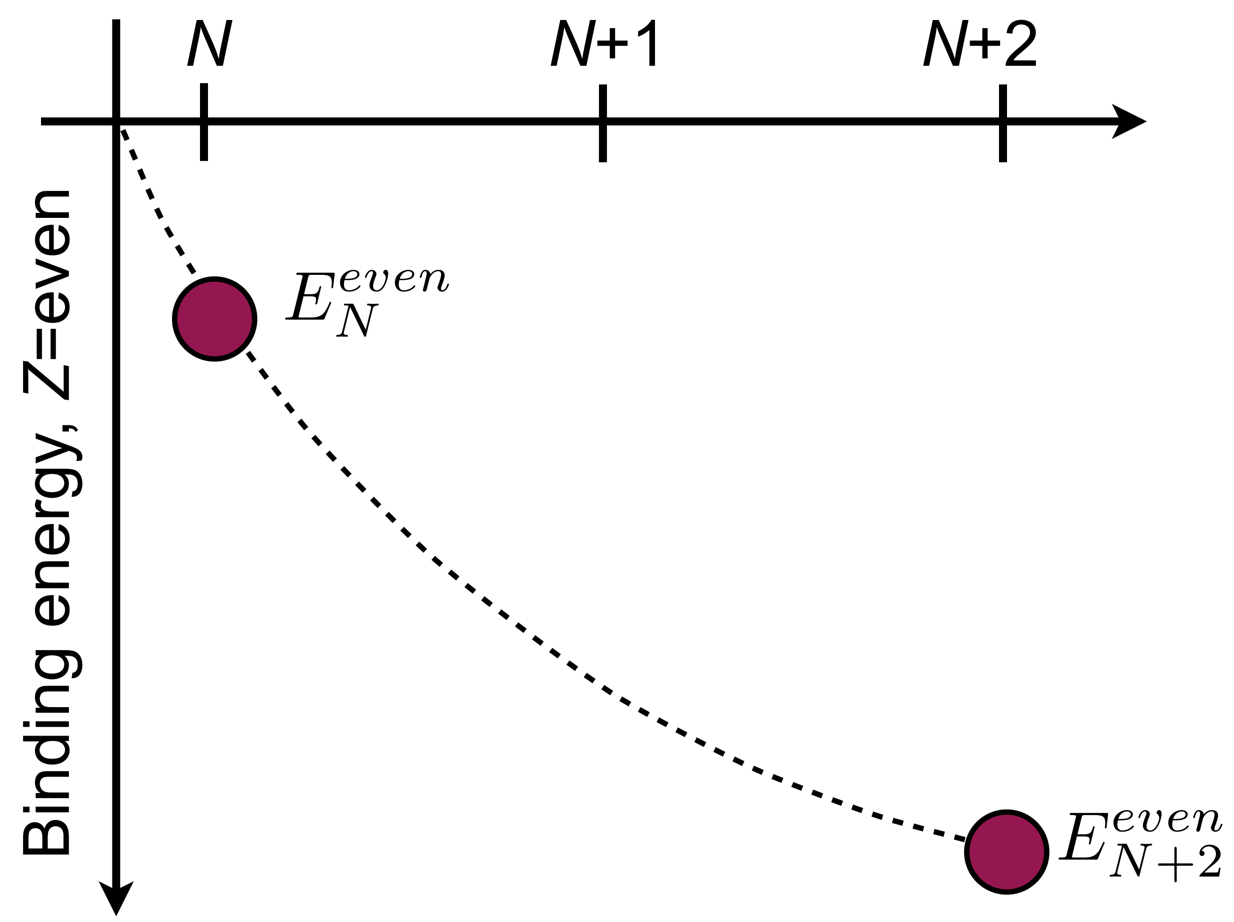
$\lambda_N \rightarrow \langle\Phi_b|\hat{N}|\Phi_b\rangle = N$

$$E_b^{\mathrm{HFB}} = \langle\mathrm{HFB}_b|\hat{H}|\mathrm{HFB}_b\rangle$$

$|\mathrm{HFB}_b\rangle$ **Product Type**

Perturbative nucleon addition method

T. Duguet et al., Phys. Rev. C 65, 014301 (2001)



Perturbative nucleon addition method

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1. Find an even HFB wave function (no blocking) constrained to have an odd number of particles

$$\lambda_N \rightarrow \langle \Phi_{N+1} | \hat{N} | \Phi_{N+1} \rangle = N+1$$

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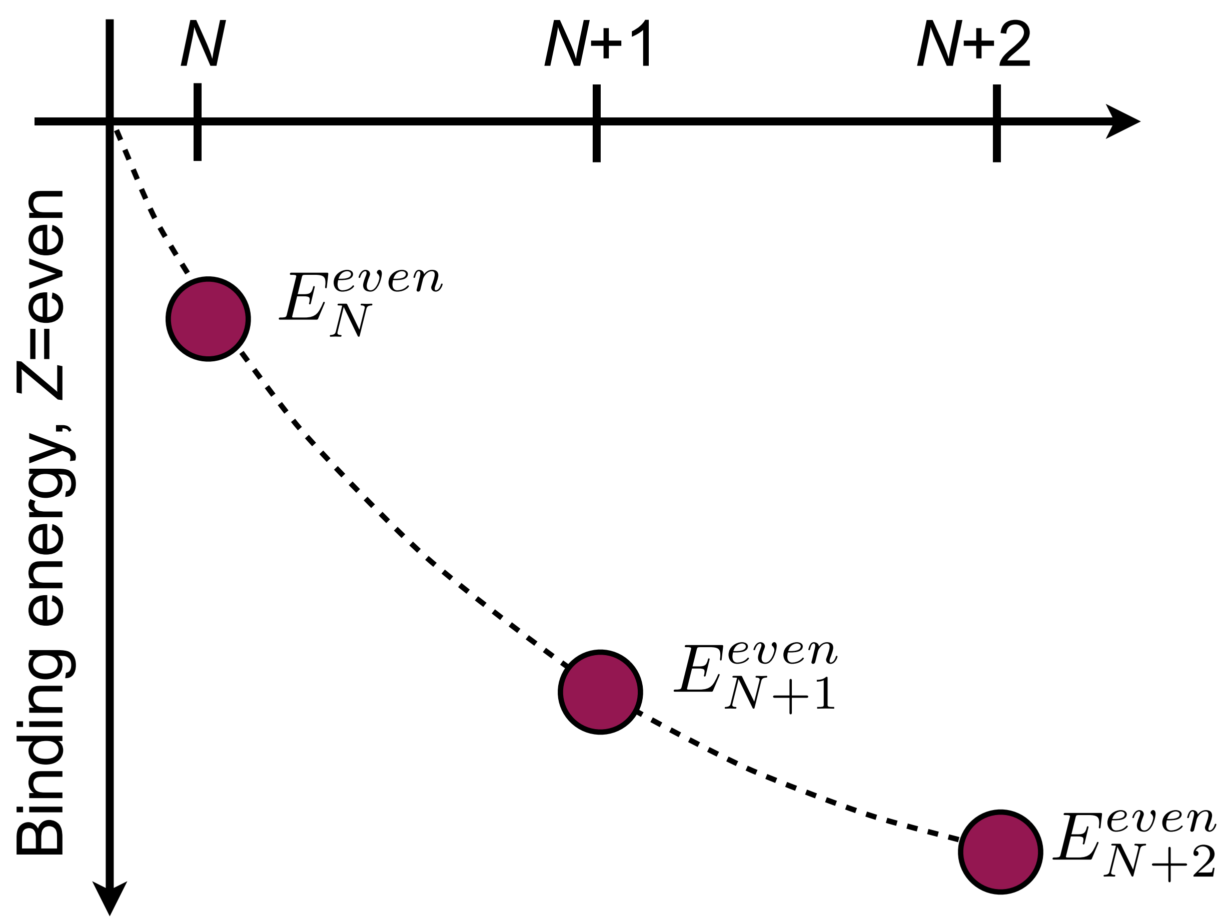

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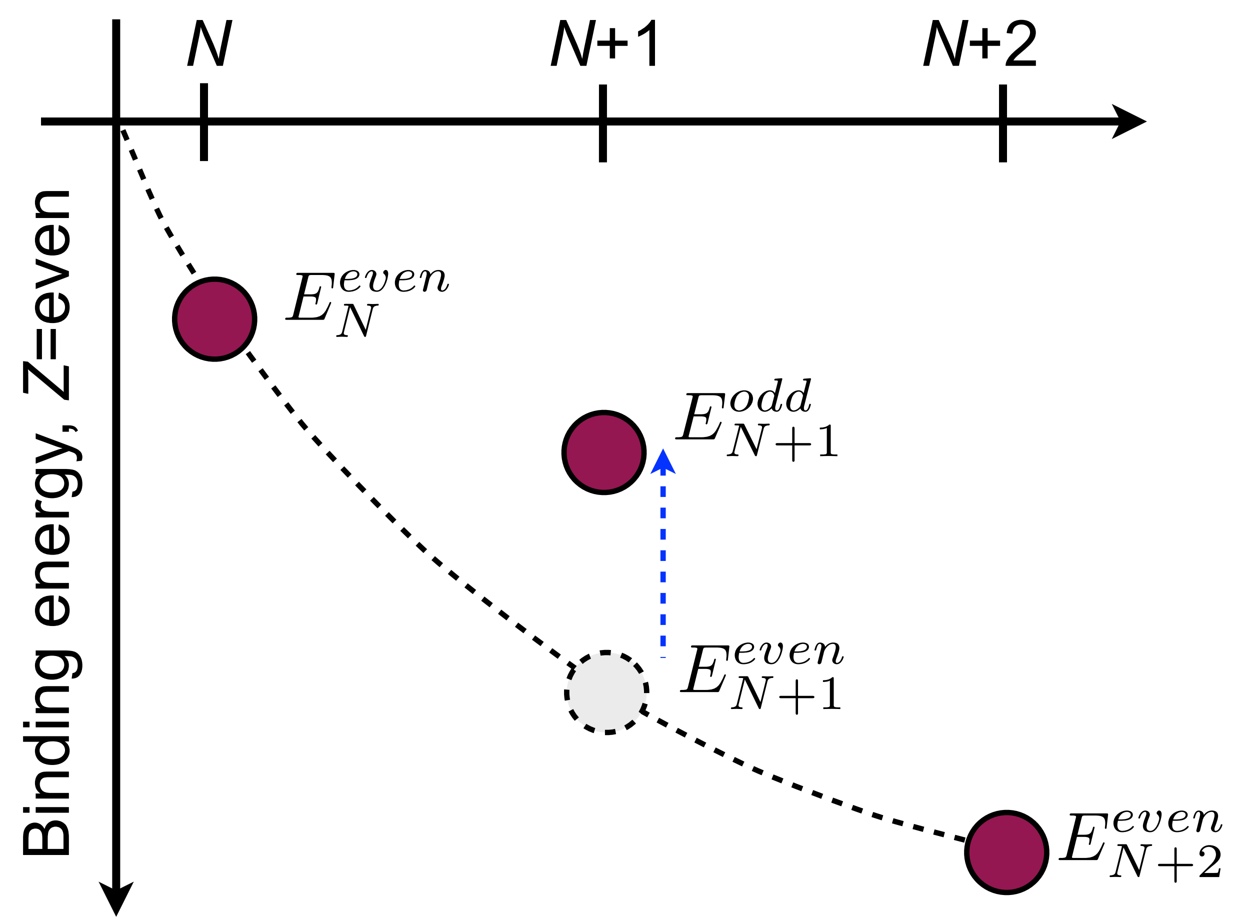
$$E_{N+1}^{even} = \langle \Phi_{N+1} | \hat{H} | \Phi_{N+1} \rangle$$

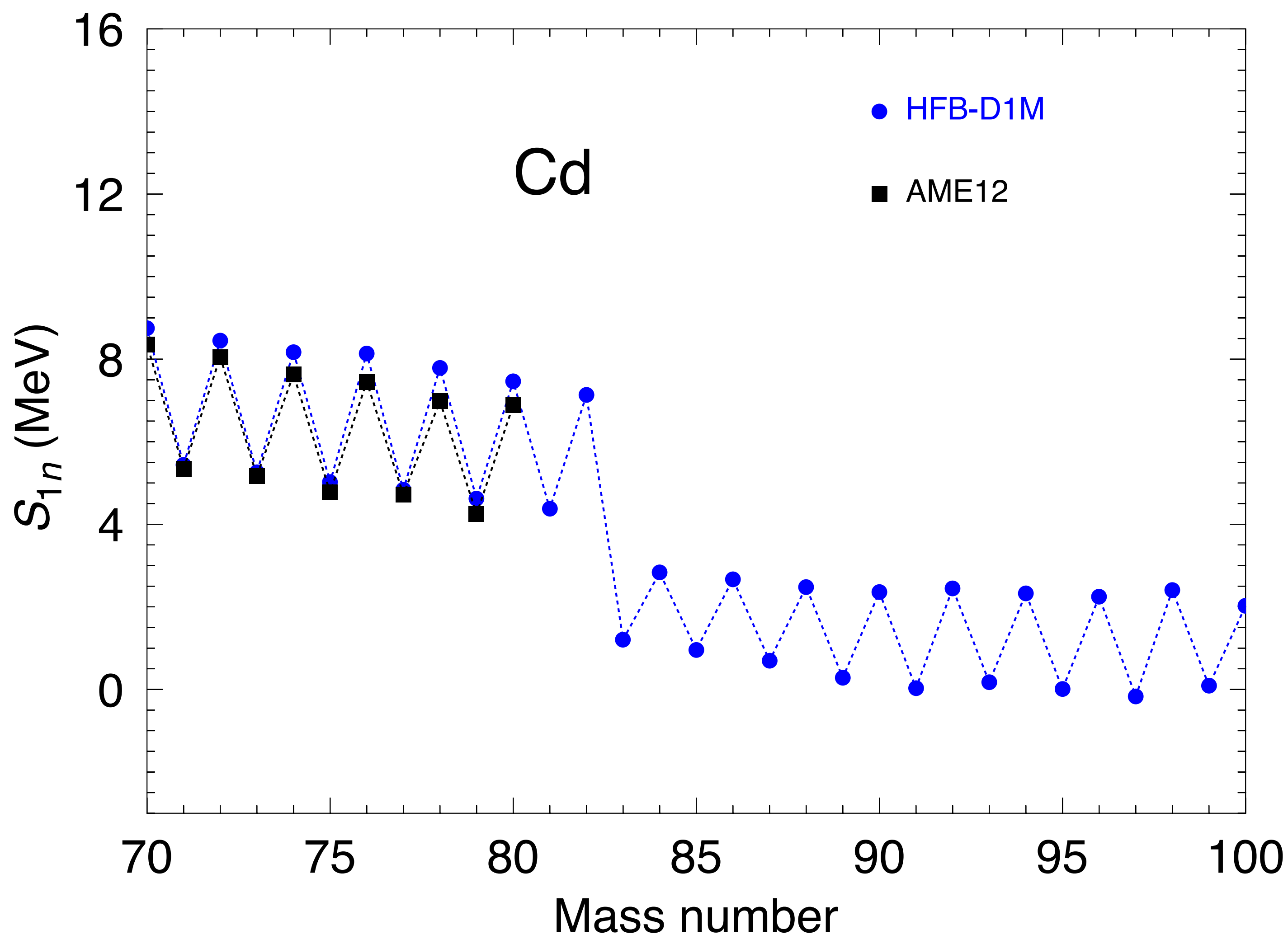
2. Add the energy of the lowest quasiparticle excitation

$$E_{N+1}^{odd} = E_{N+1}^{even} + \varepsilon_b^{qp}$$



Perturbative nucleon addition method

A. Arzhanov, Master Thesis



- ✦ Overestimation of the pairing gap.
- ✦ Overestimation of *N*=82 shell gap.

→

- True blocking.
- Beyond mean field effects.

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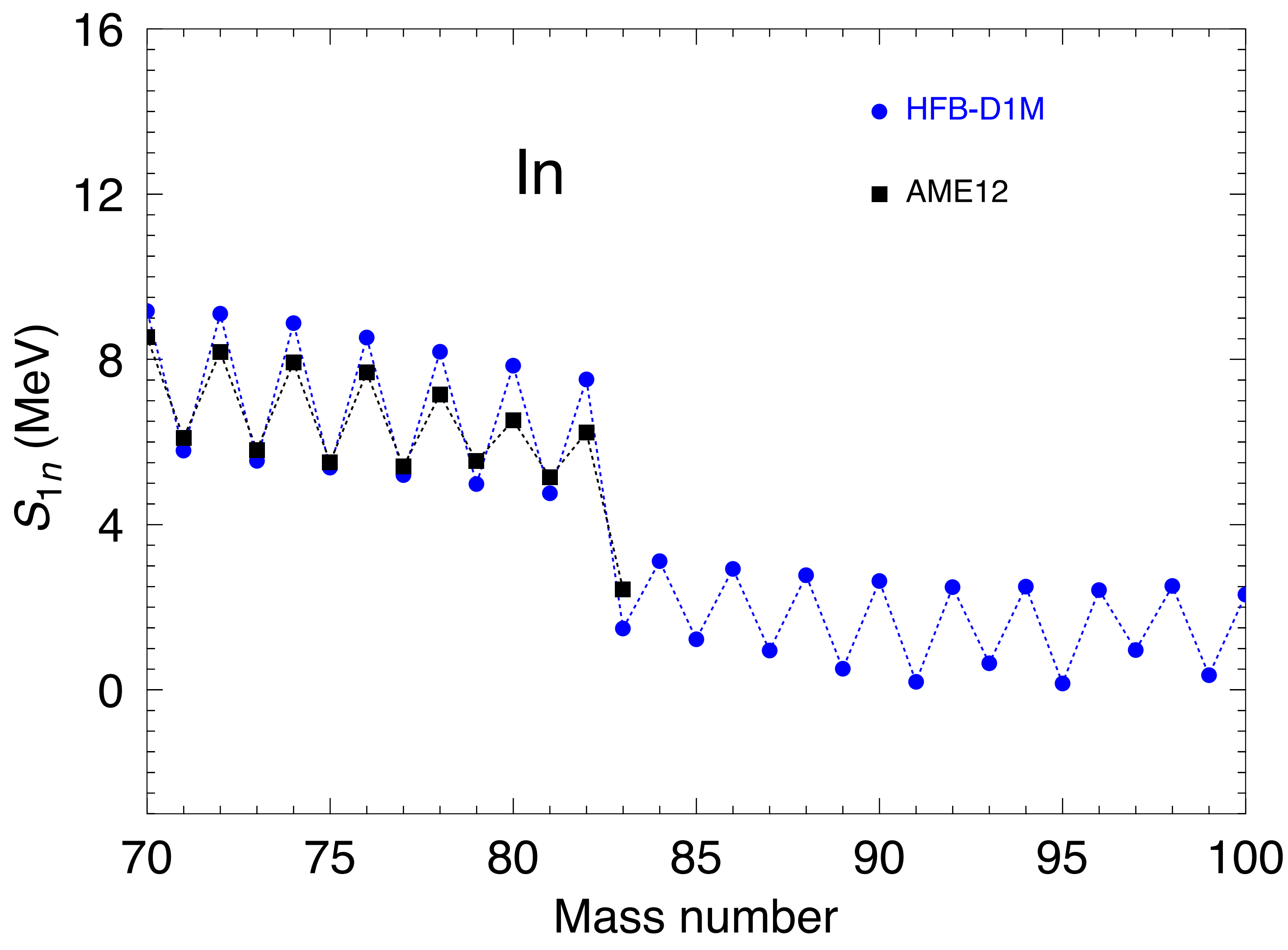

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Approaching odd-nuclei

Perturbative nucleon addition method

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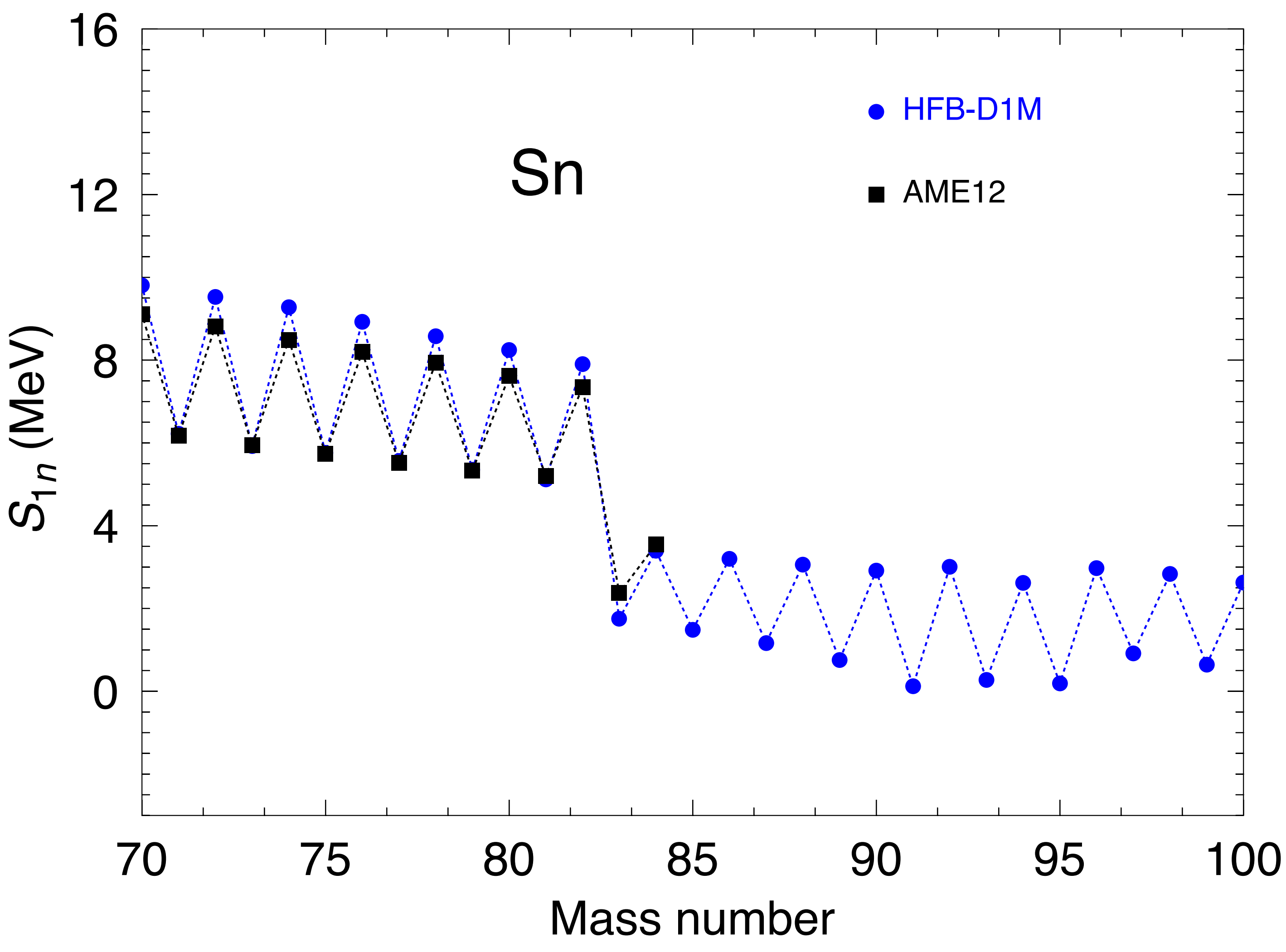

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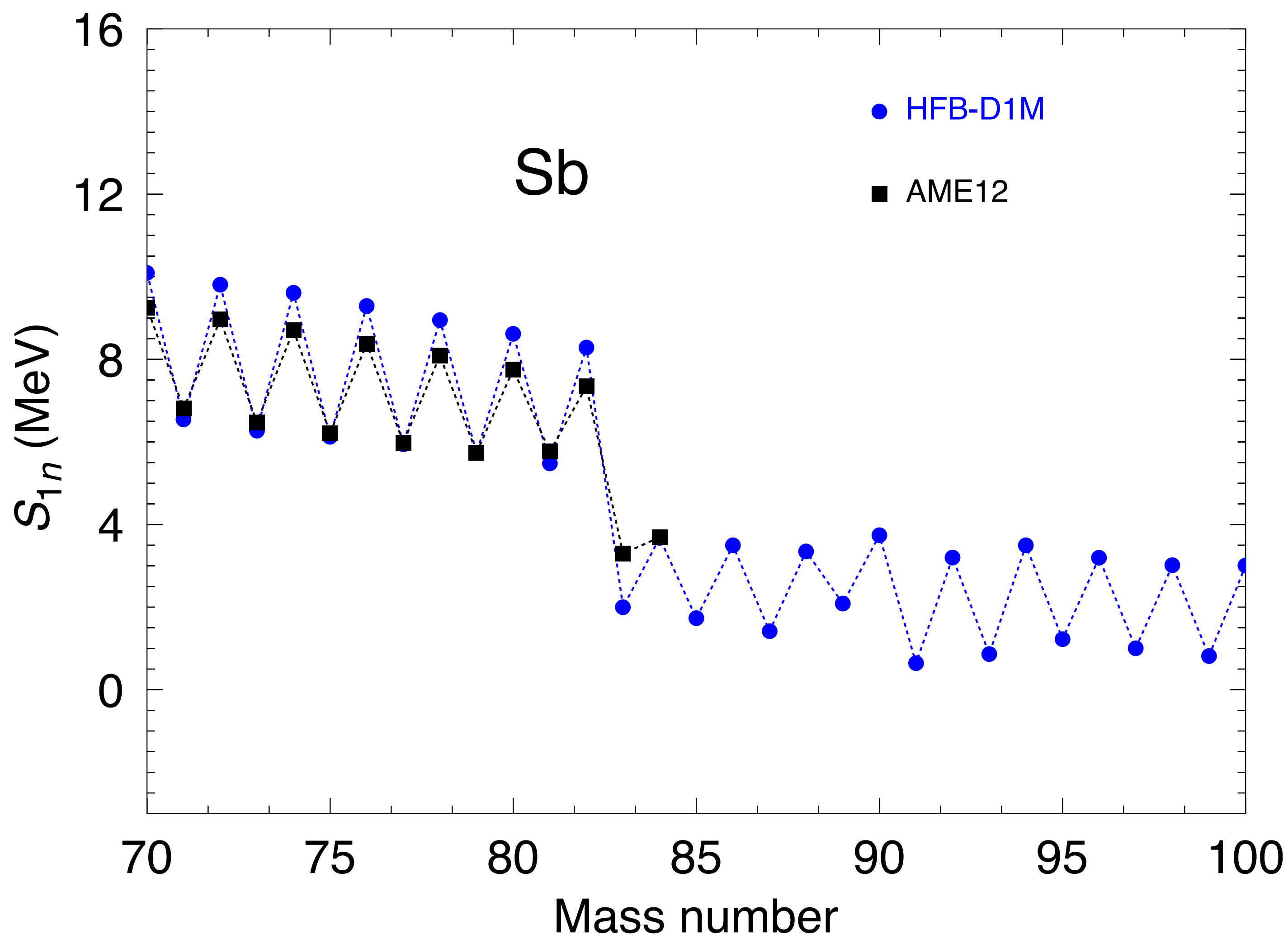

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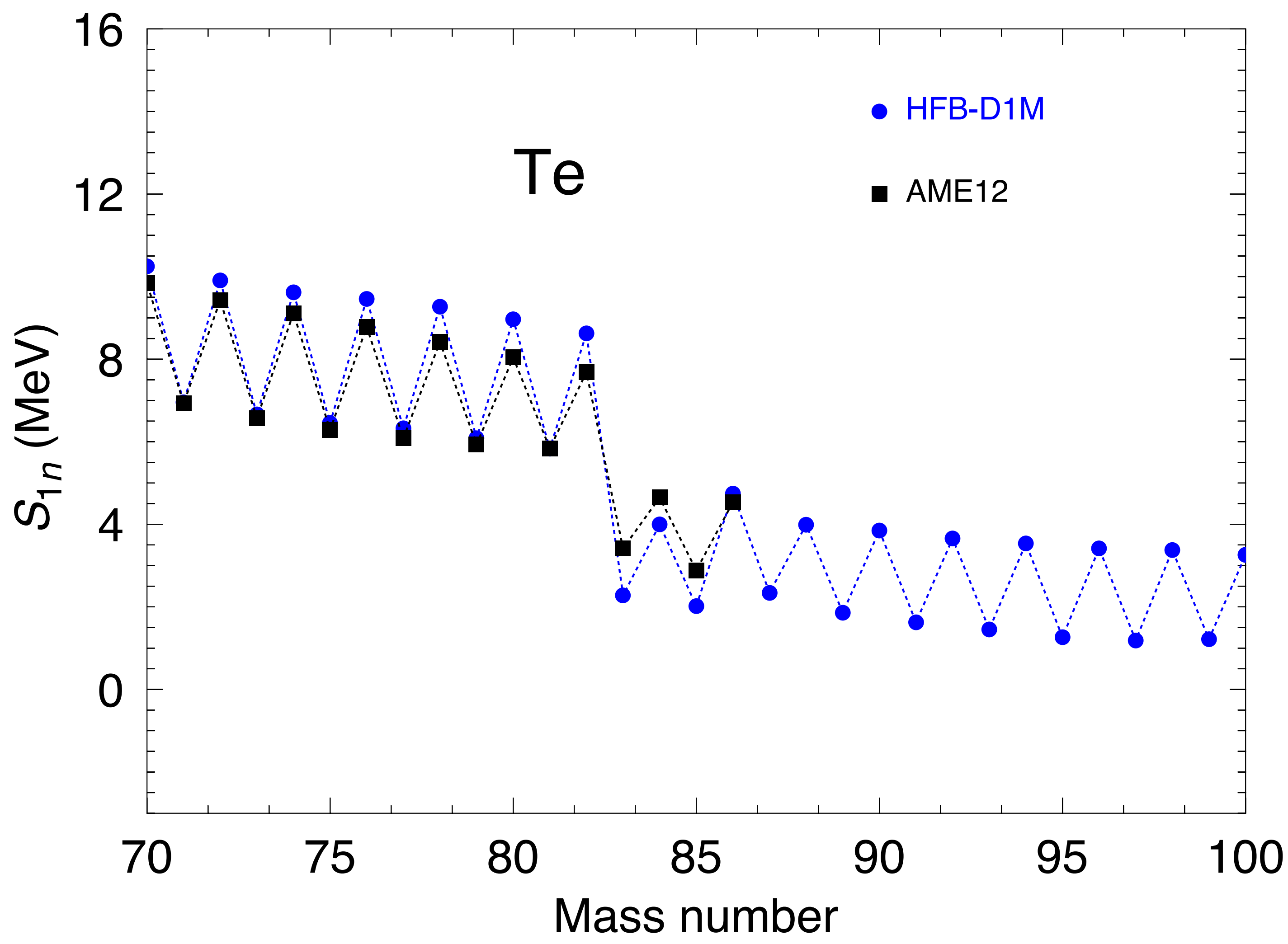

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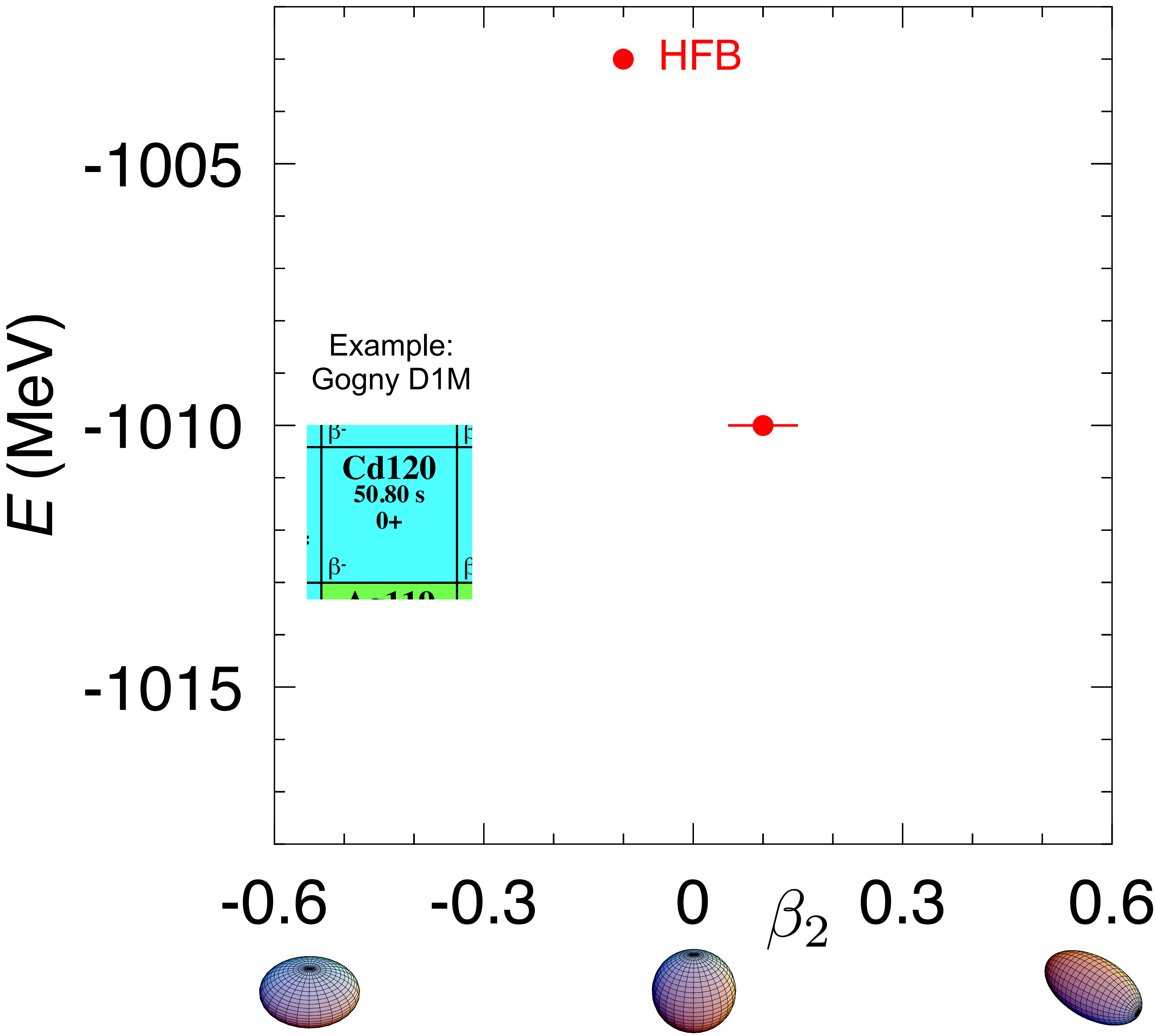
Self-consistent beyond mean field description



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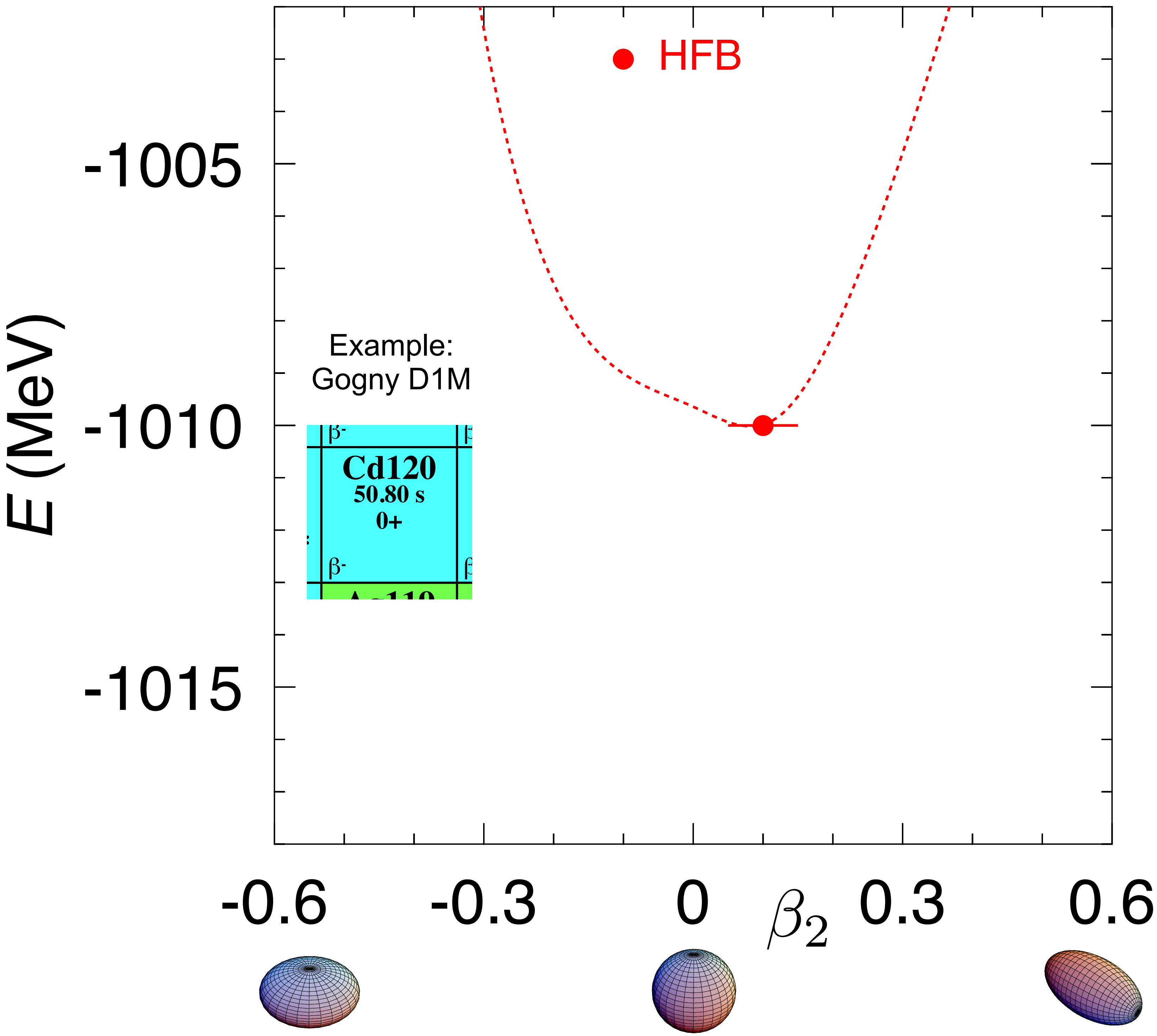

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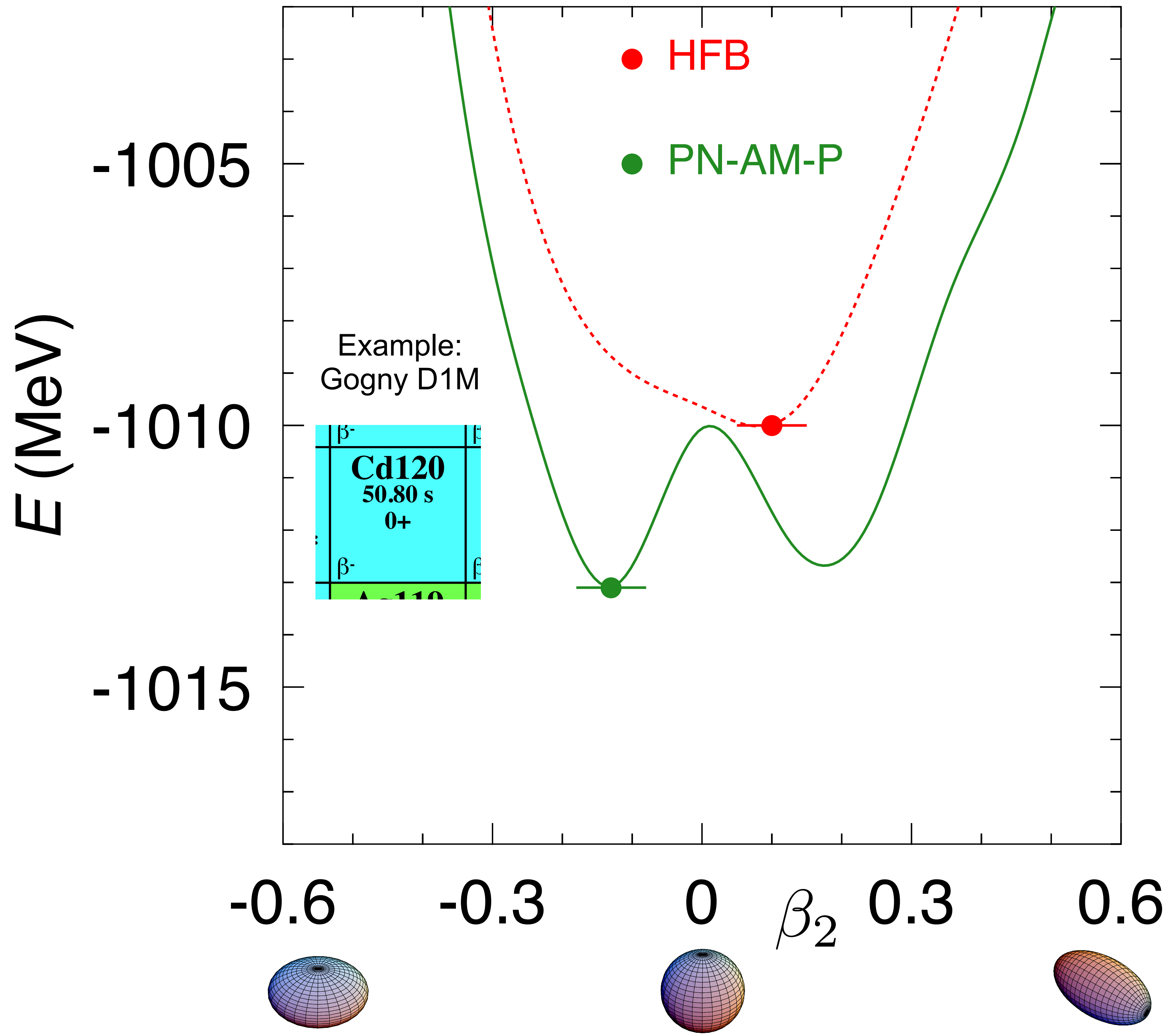

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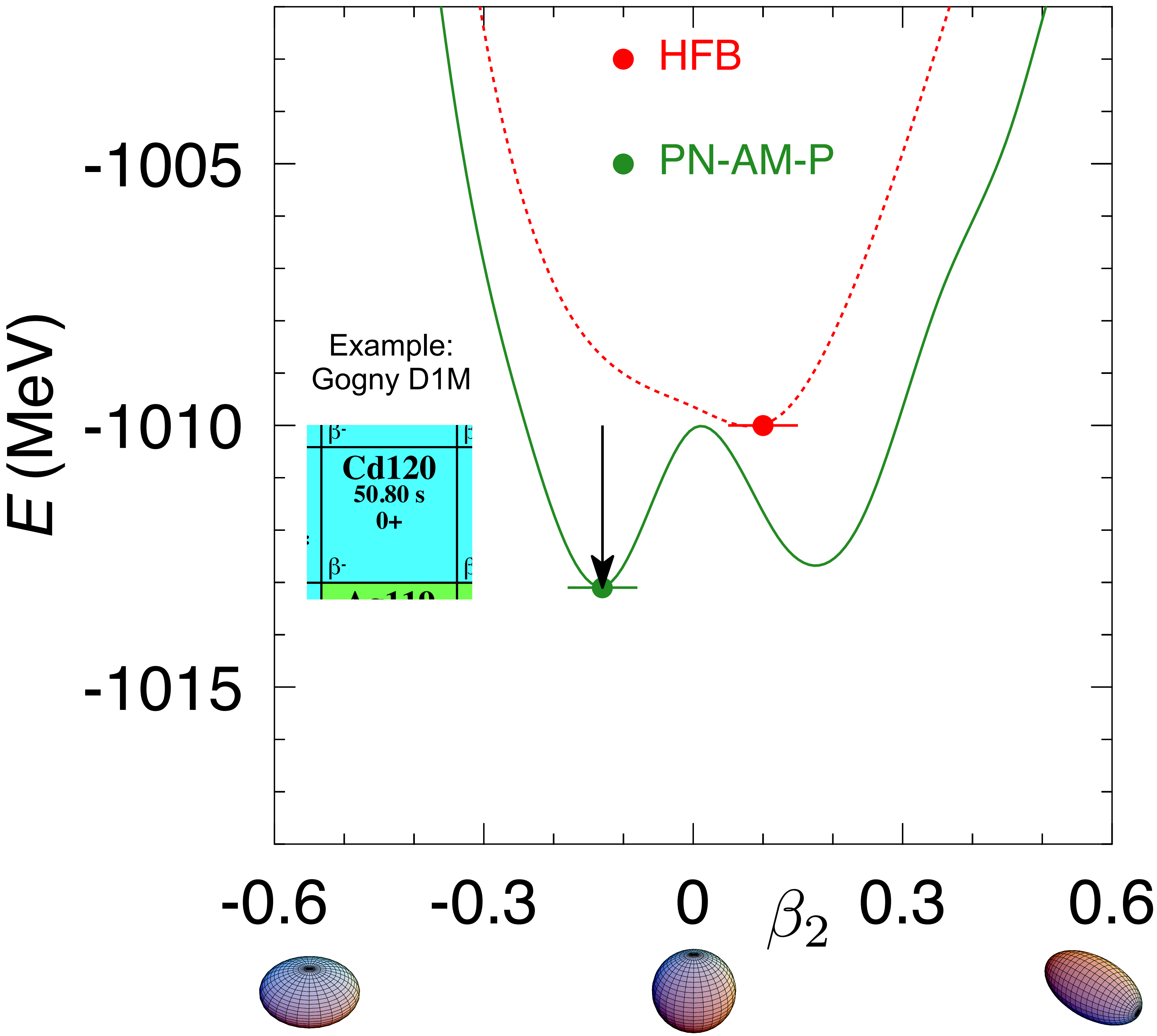

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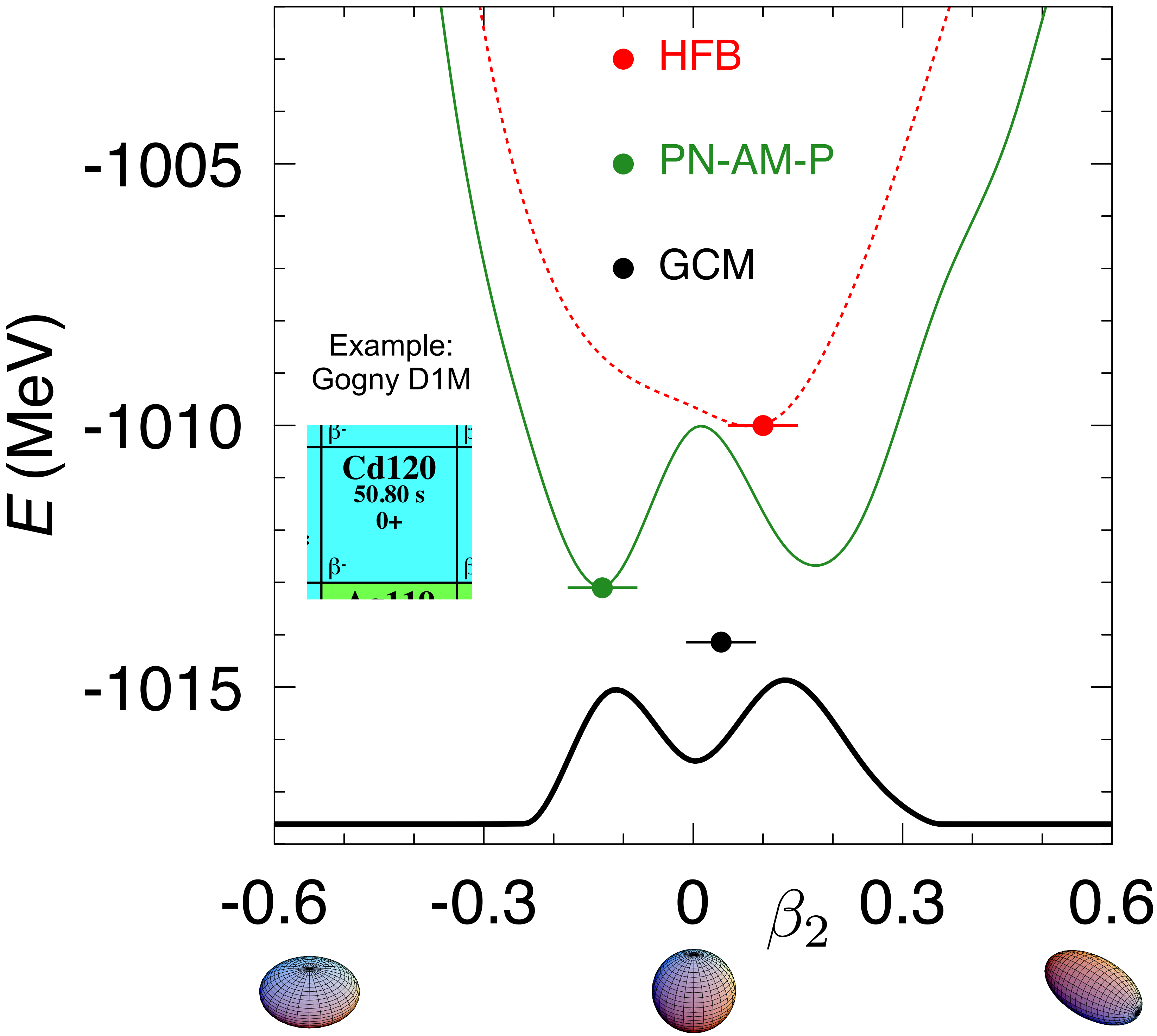

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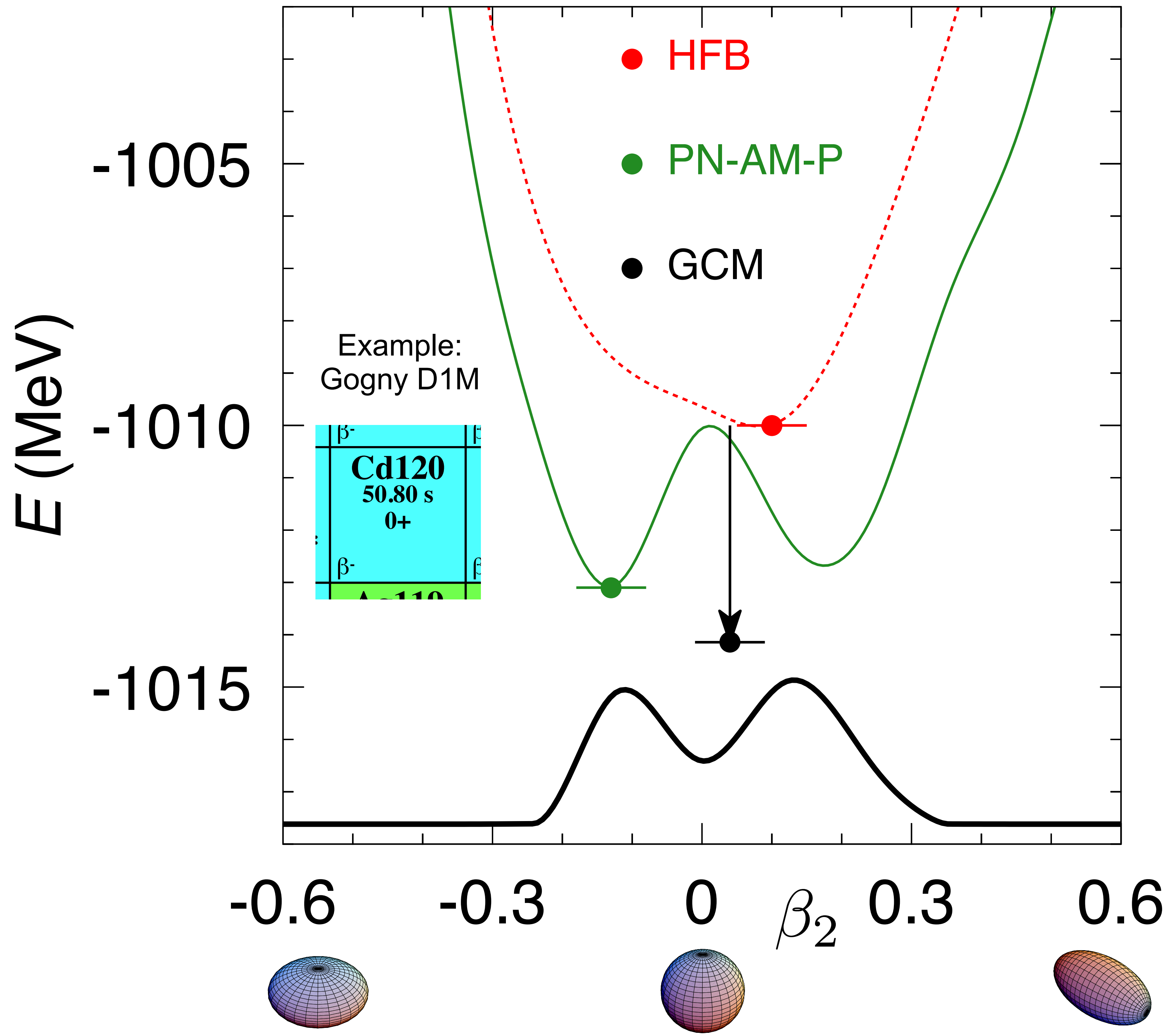

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Self-consistent beyond mean field description

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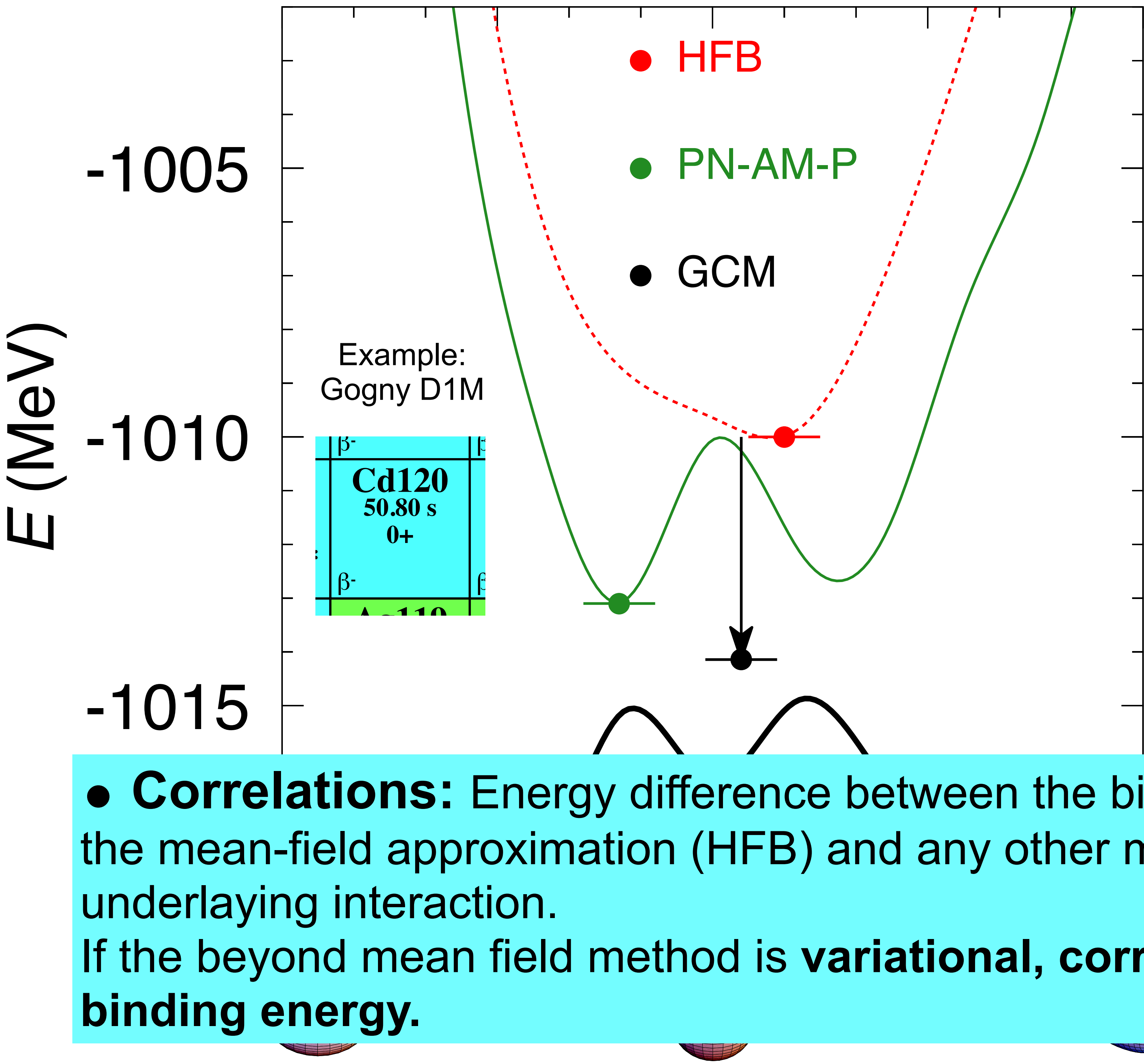

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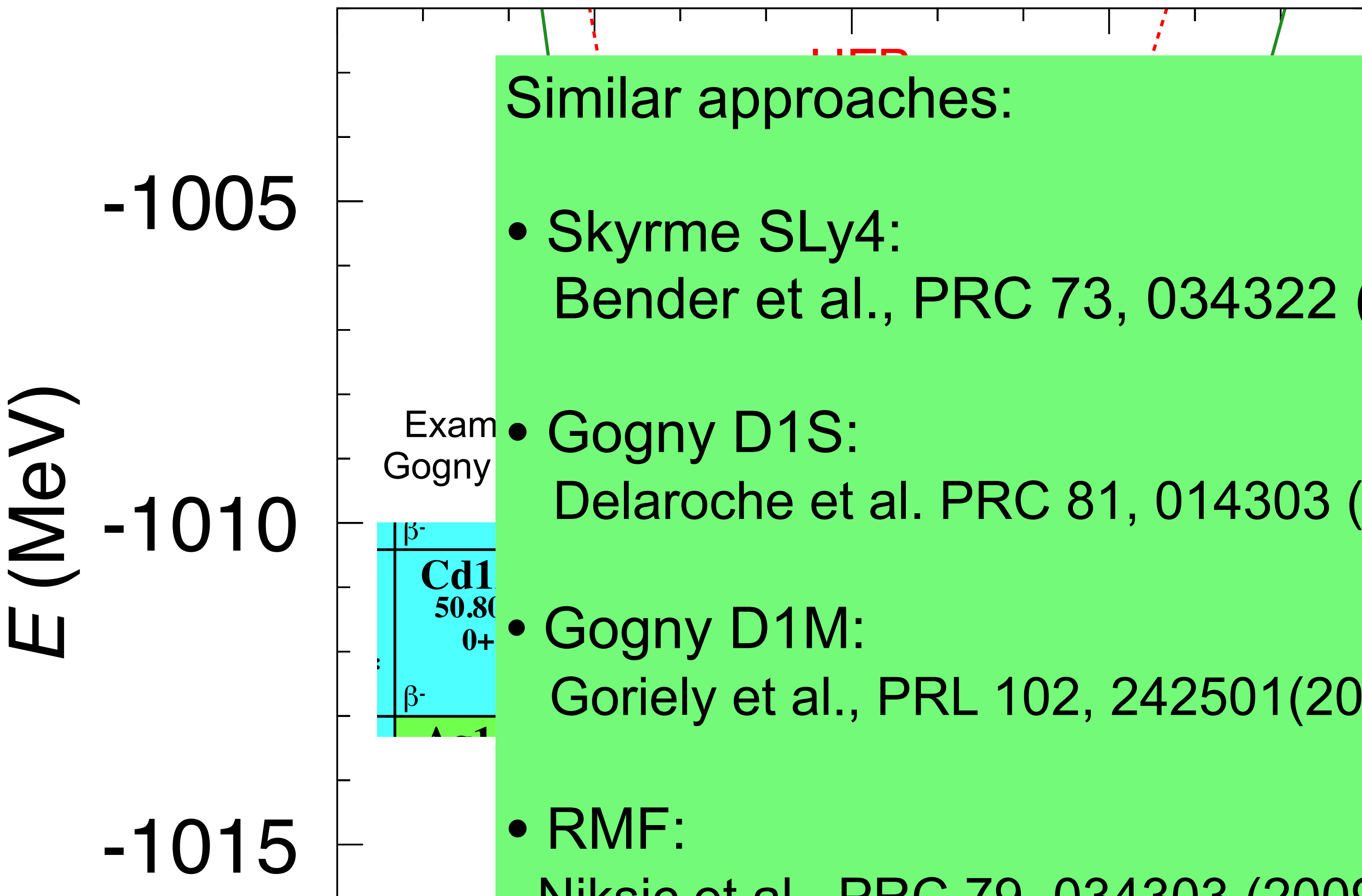
If the beyond mean field method is **variational, correlations must give extra binding energy.**

Self-consistent beyond mean field description



Similar approaches:

- Skyrme SLy4:
  Bender et al., PRC 73, 034322 (2006). GCM
- Gogny D1S:
  Delaroche et al. PRC 81, 014303 (2010). 5DCH
- Gogny D1M:
  Goriely et al., PRL 102, 242501(2009). 5DCH
- RMF:
  Niksic et al., PRC 79, 034303 (2009). 5DCH, local

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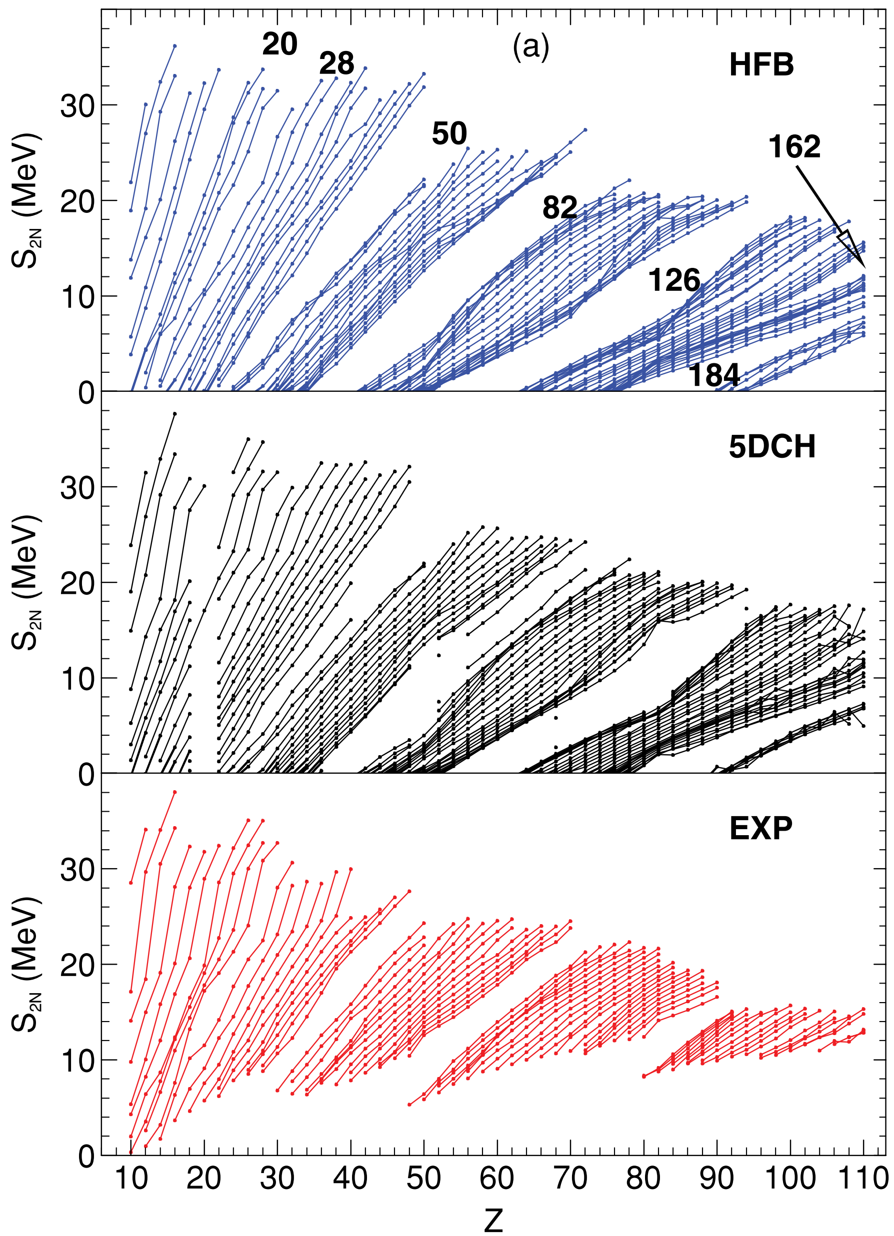
Mean field vs. Beyond mean field. Global systematics

Gogny D1S



Delaroche et al. PRC 81, 014303 (2010)

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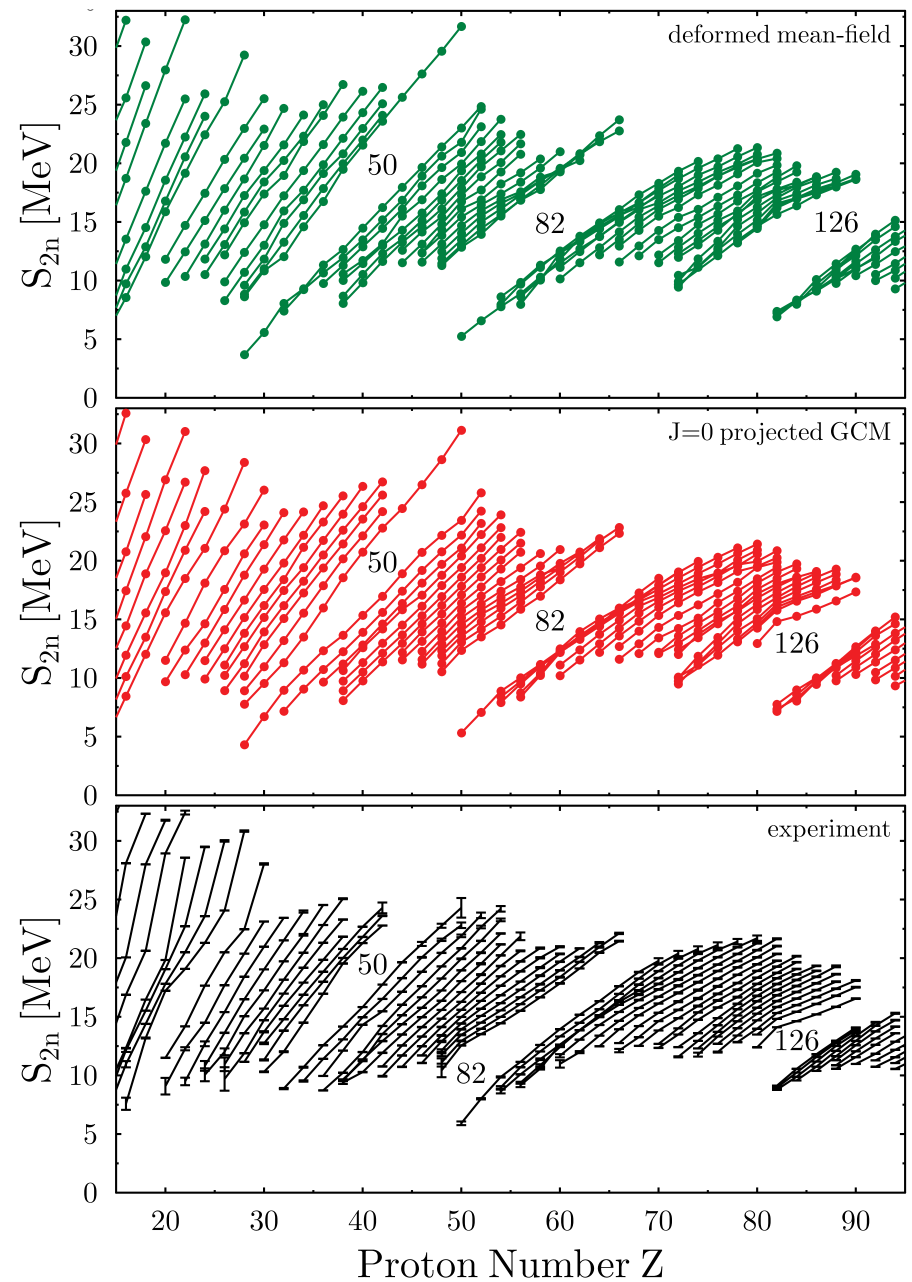

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- Separation energies are smoother when beyond mean field are included.

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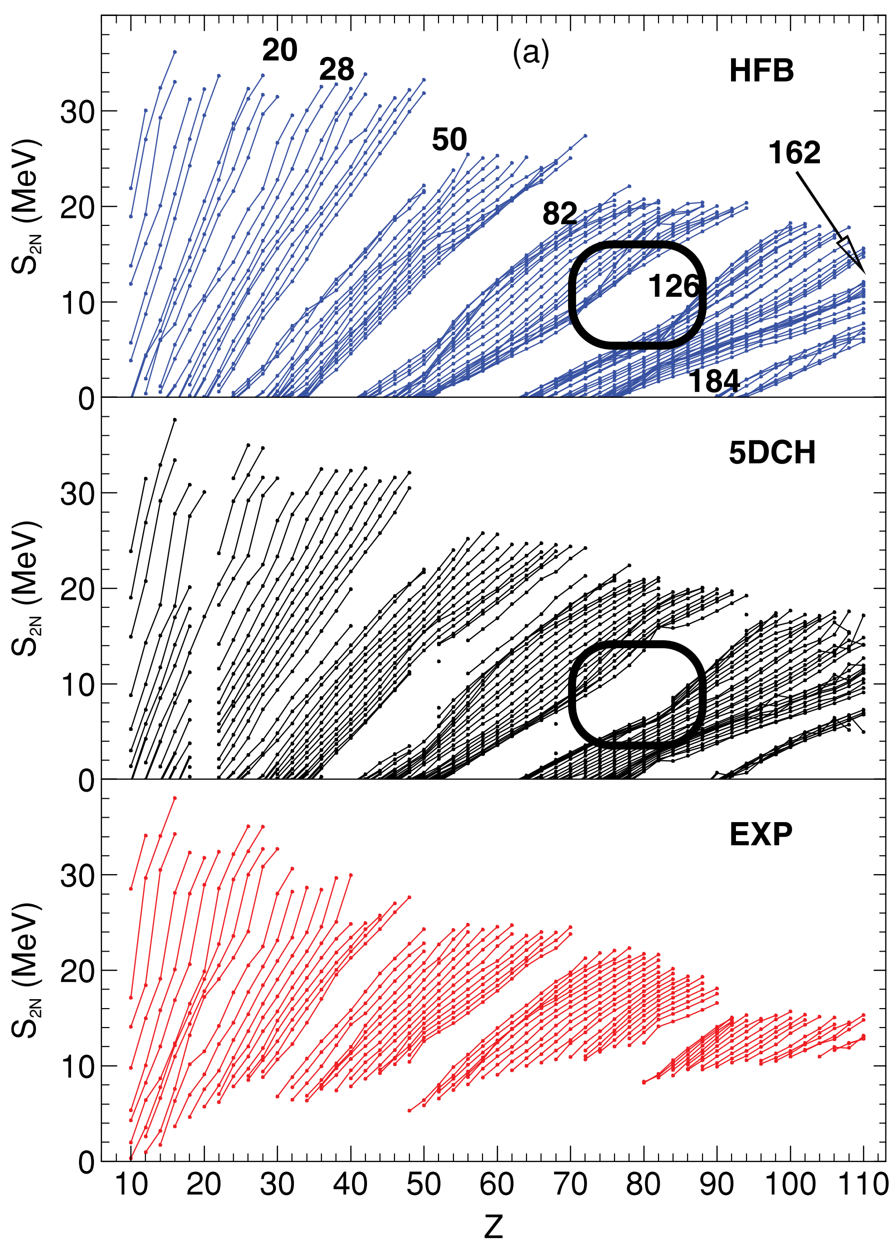

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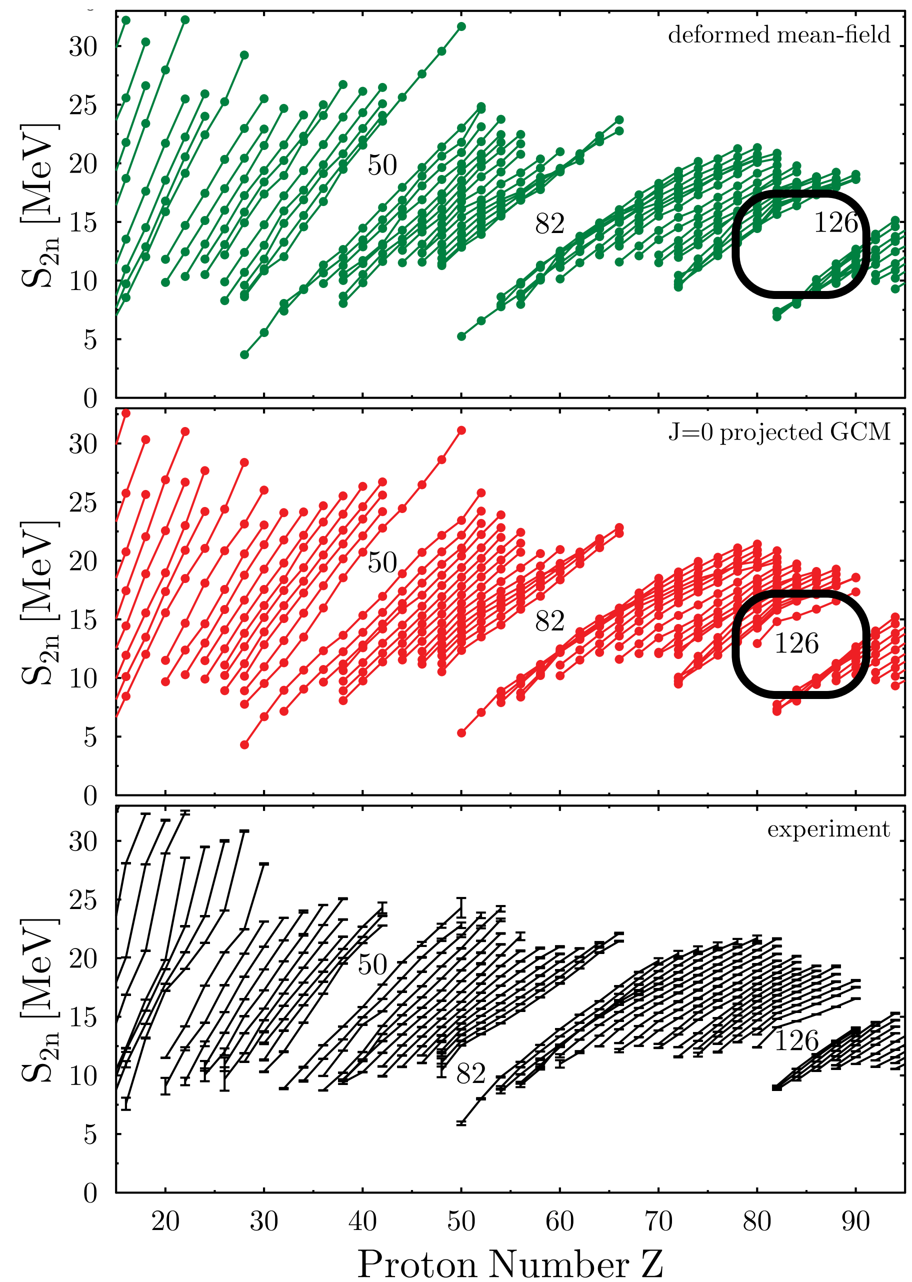

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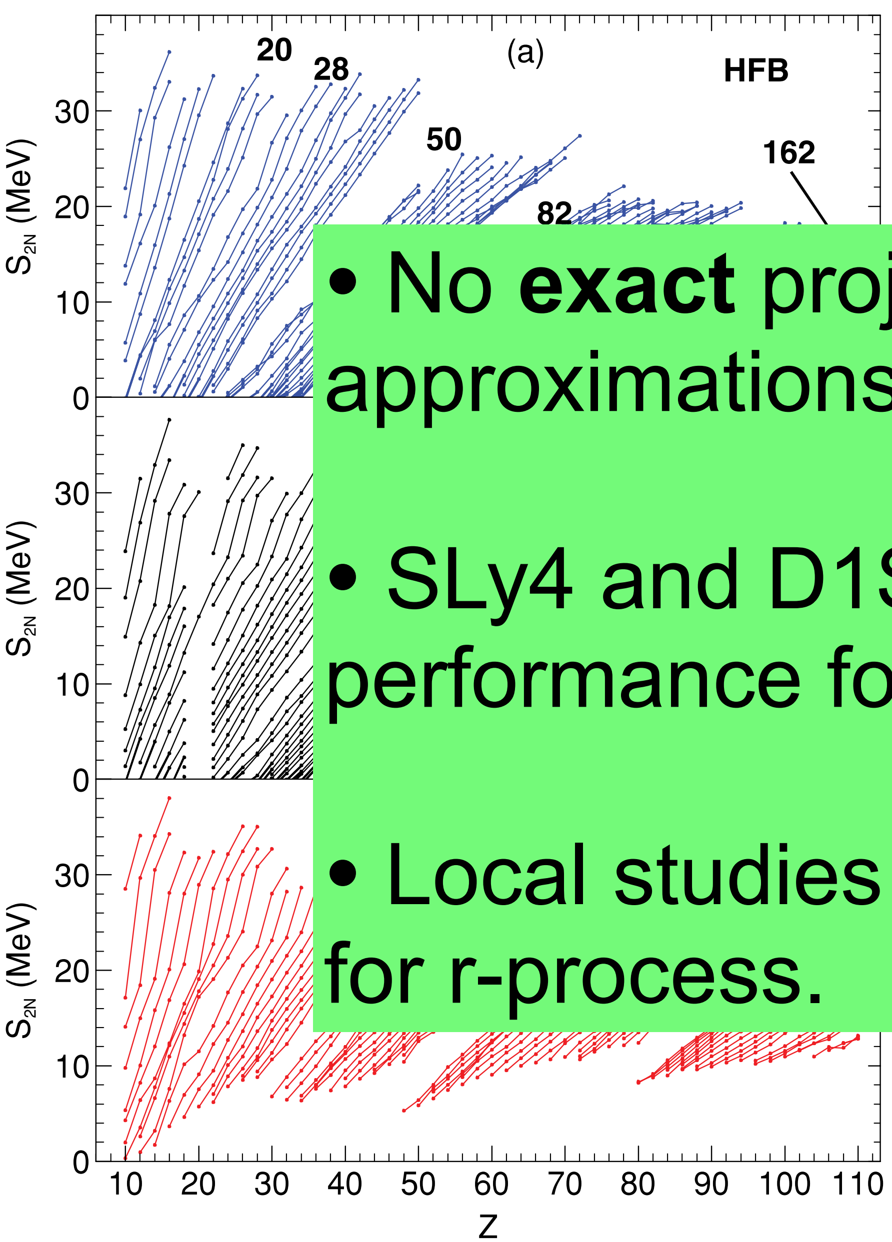

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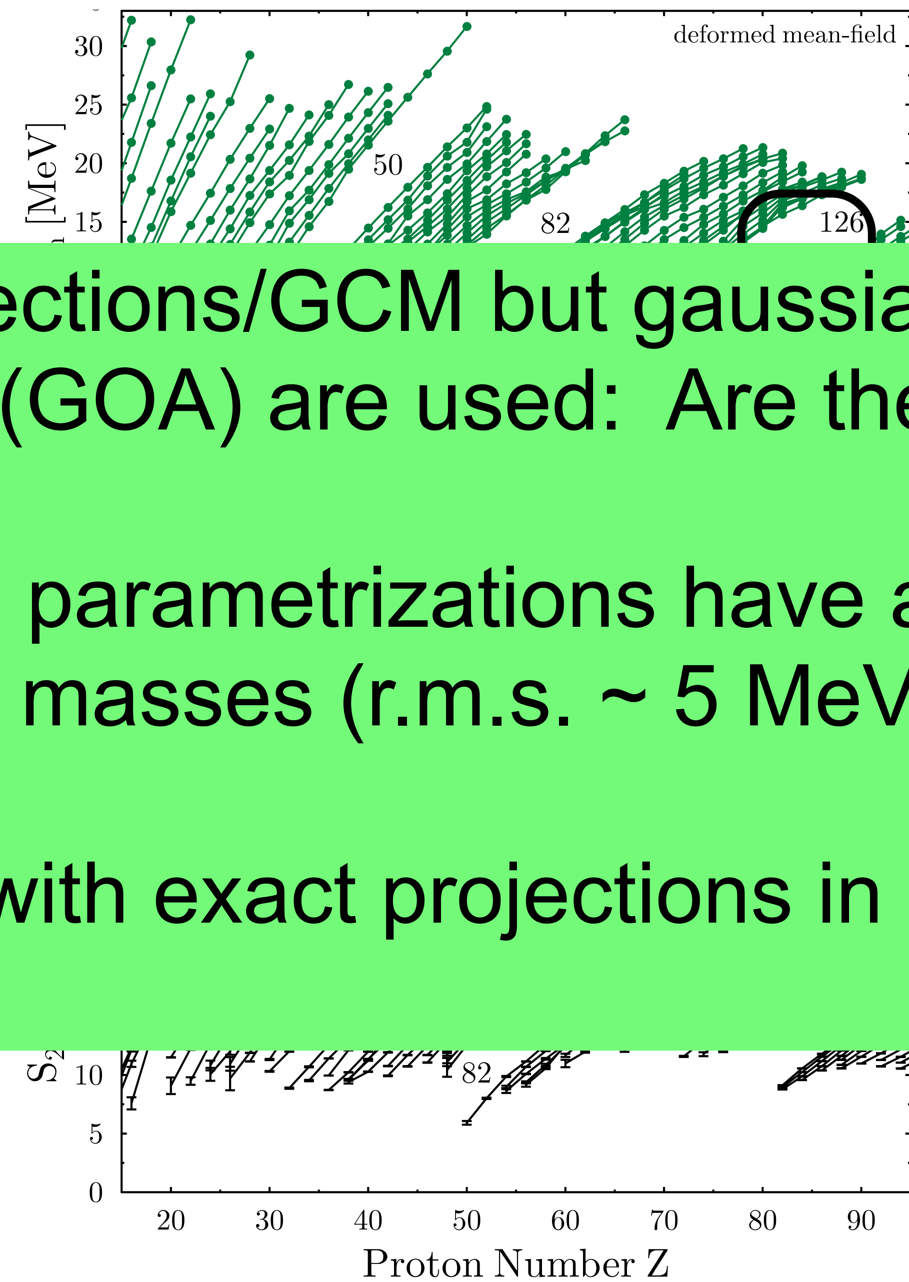

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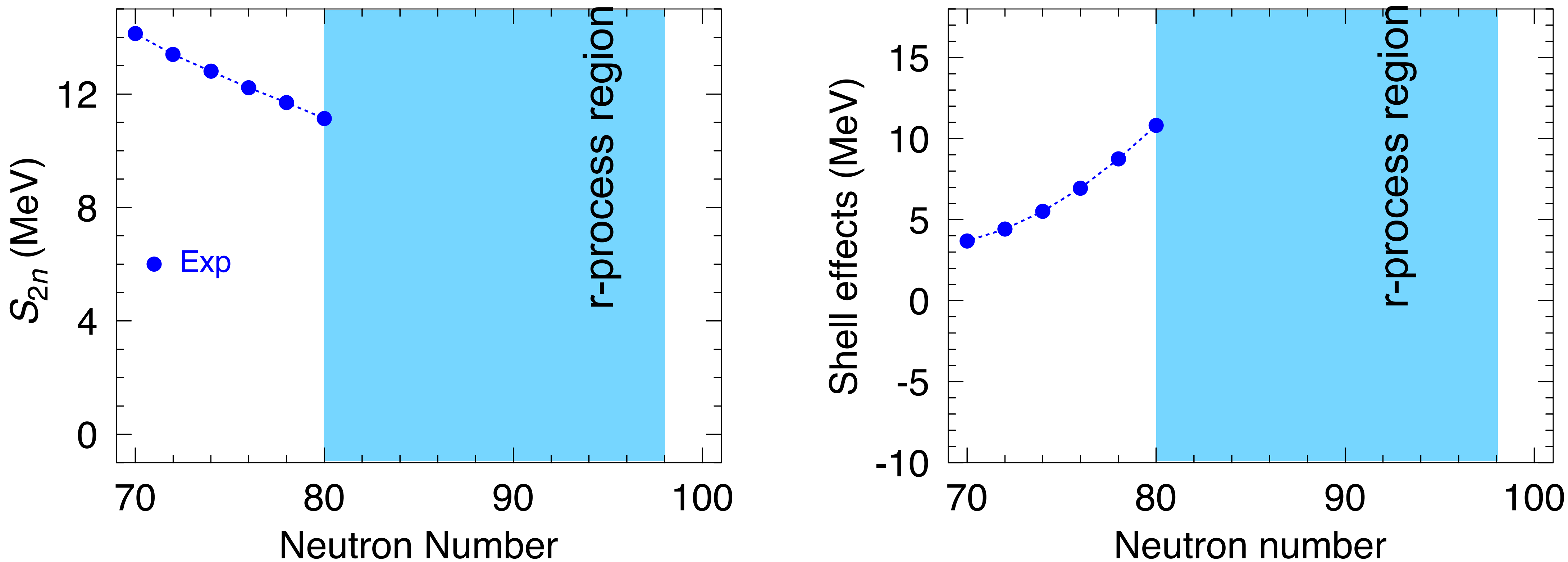
• Beyond mean field

• No **exact** projections/GCM but gaussian overlap approximations (GOA) are used: Are they **variational?**

• SLy4 and D1S parametrizations have a poor performance for masses (r.m.s. ~ 5 MeV).

• Local studies with exact projections in isotopes relevant for r-process.

Cadmium isotopes. Gogny D1S parametrization



- Similar behavior of the two-neutron separation energies in all approaches and close to the experiment in the experimental region.
- GCM approach always includes correlation energies (variational) while 5DCH fails close to the shell closure.
- 5DCH approach removes the shell gap at N=82 while the others still give a sizable gap. This quenching is an artifact of the 5DCH and not an effect of including correlations beyond mean field (NOT VARIATIONAL).

Mean field vs. Beyond mean field. Local systematics

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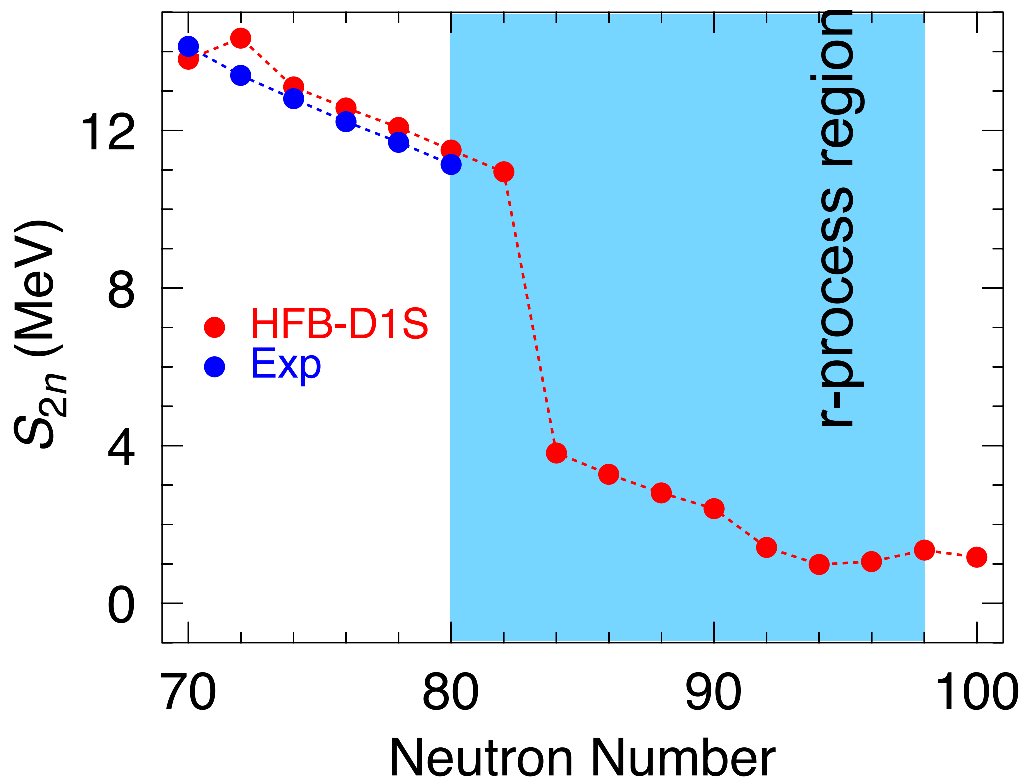

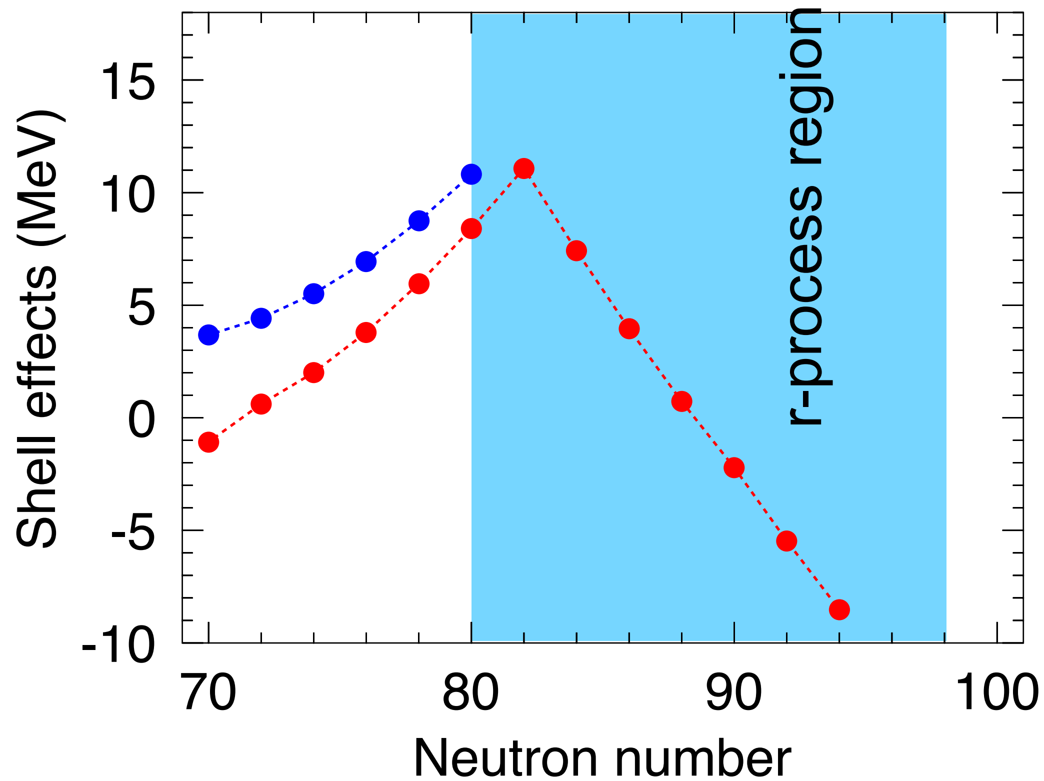

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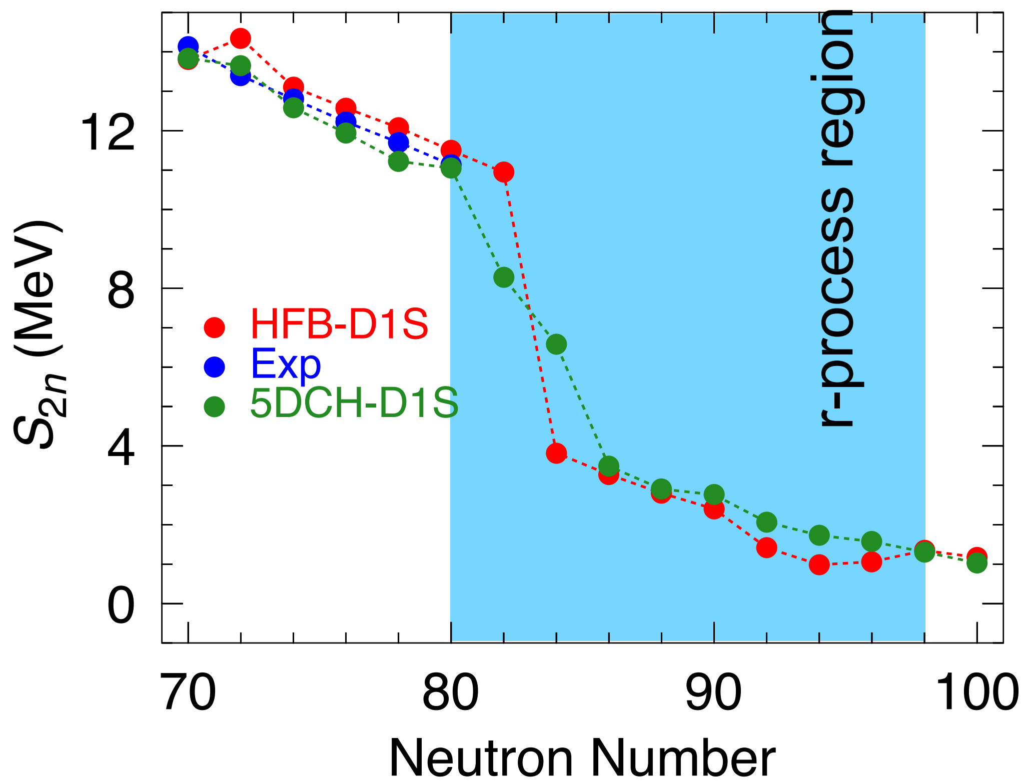

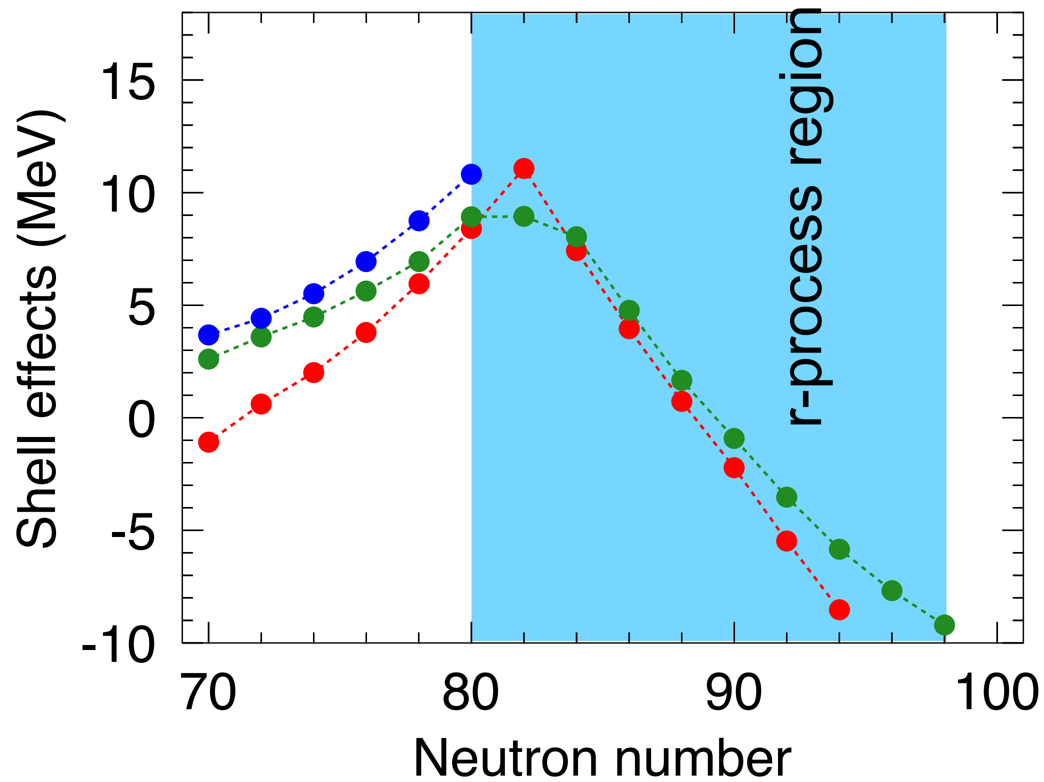

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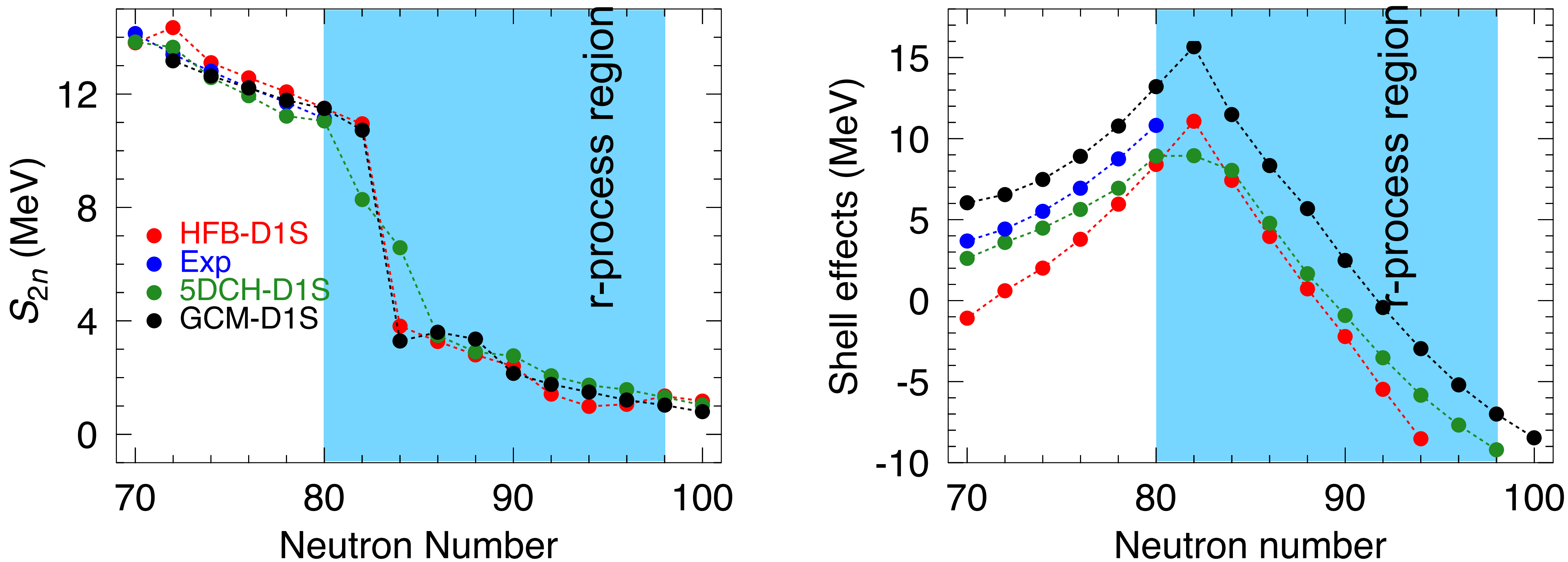

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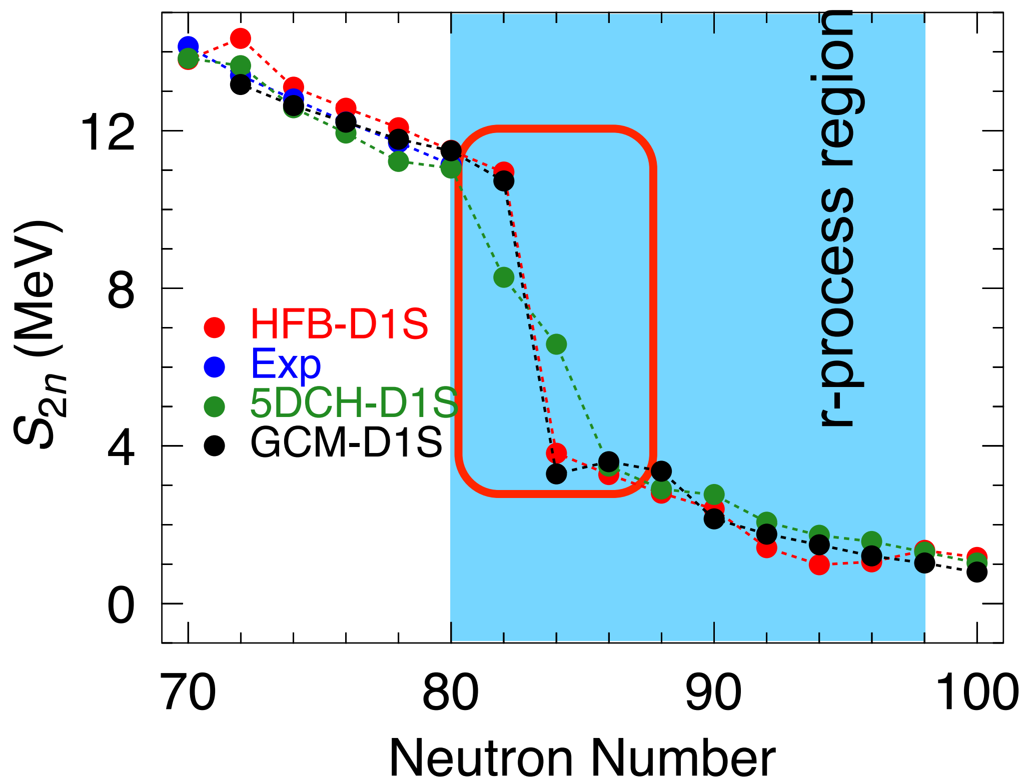

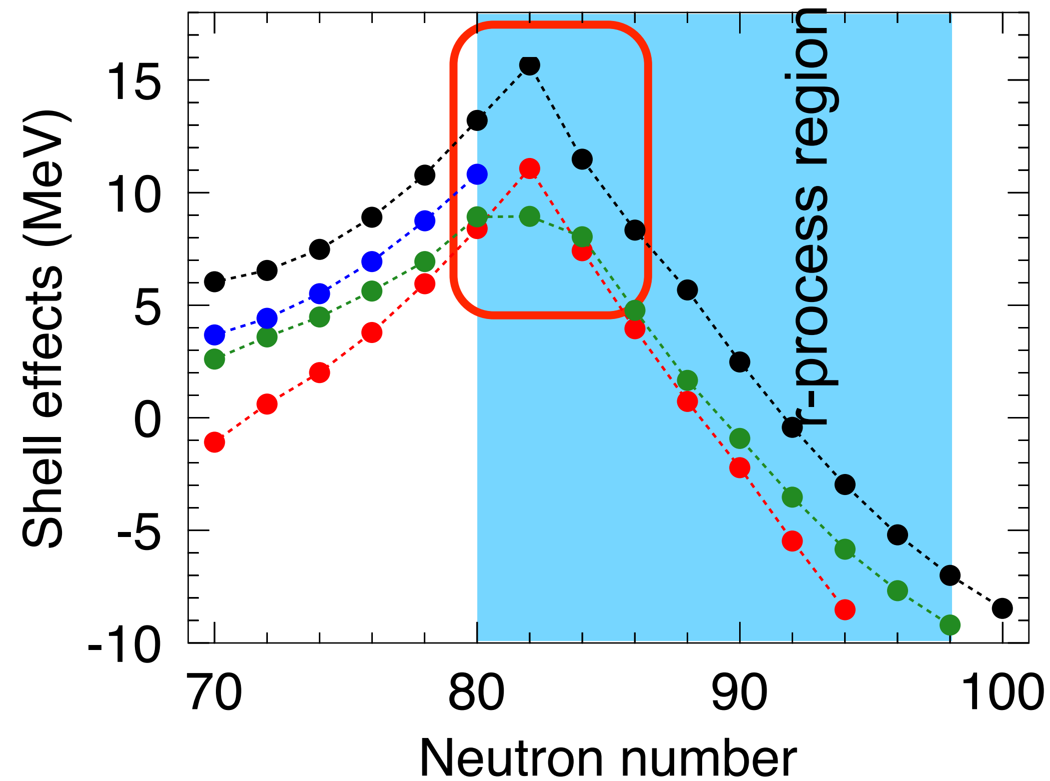

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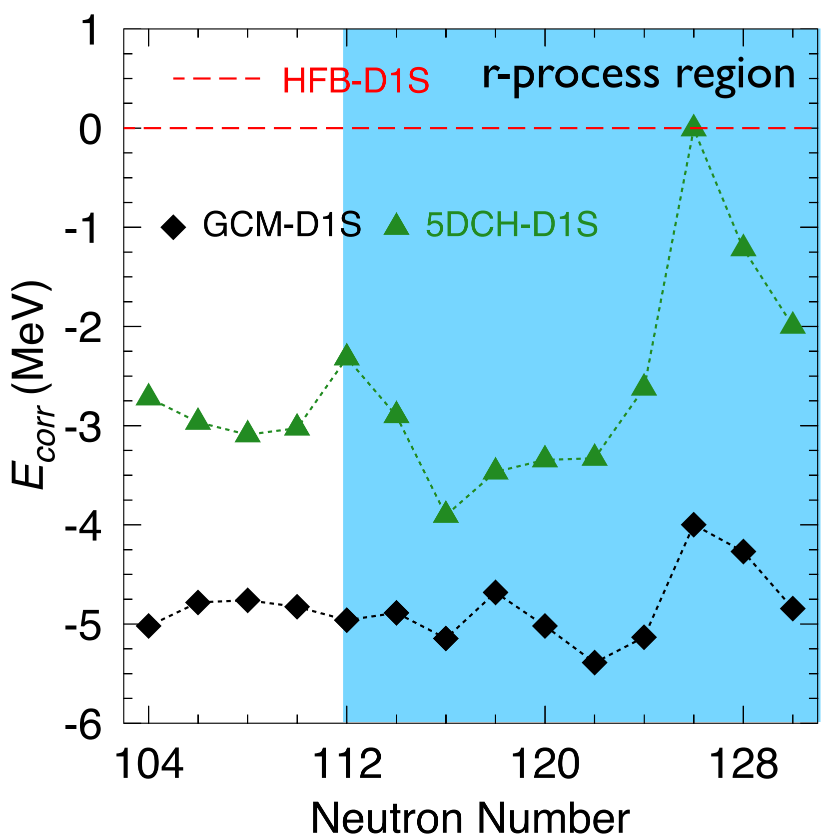
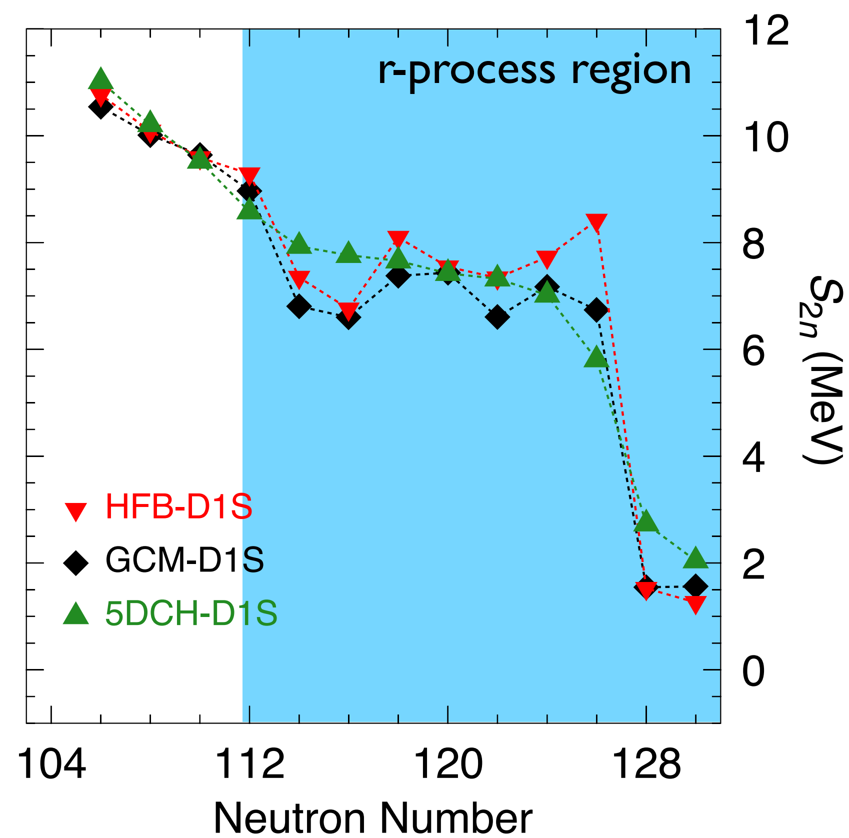
Erbium isotopes. Gogny D1S parametrization





- 5DCH fails in accounting for correlations at N=126 shell closure.
- 5DCH artificially smooths out the trough and the shell gap in the S_{2n}.
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Mean field vs. Beyond mean field. Local systematics

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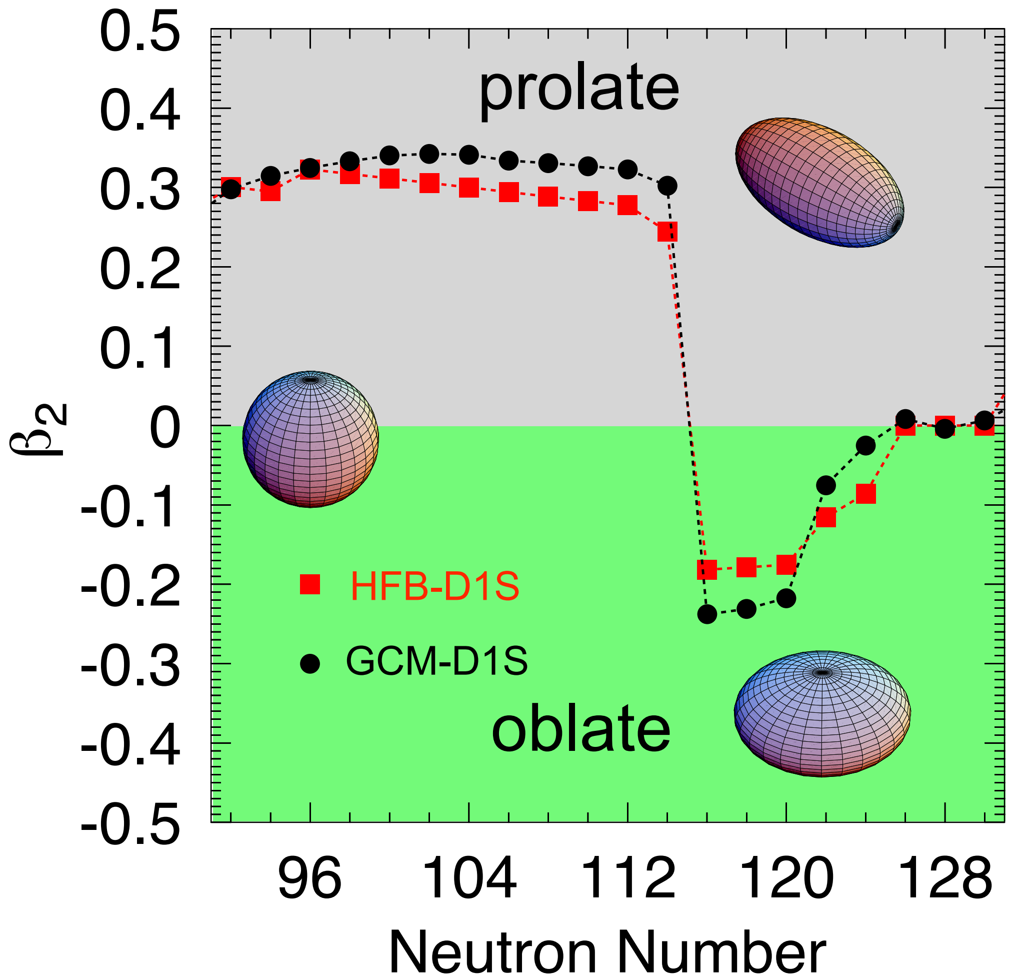

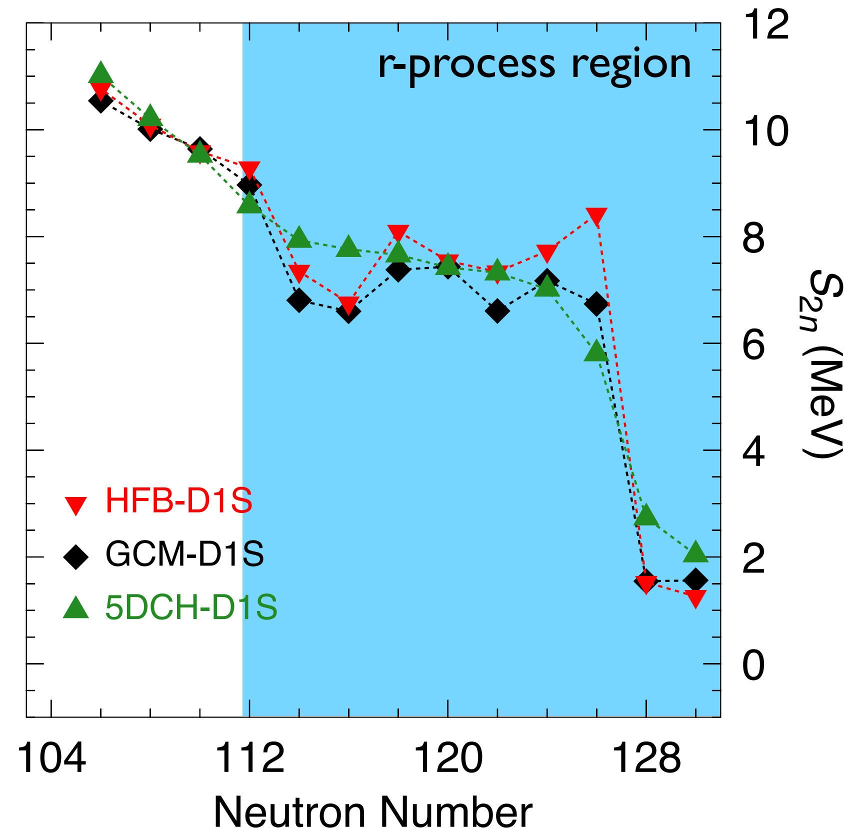

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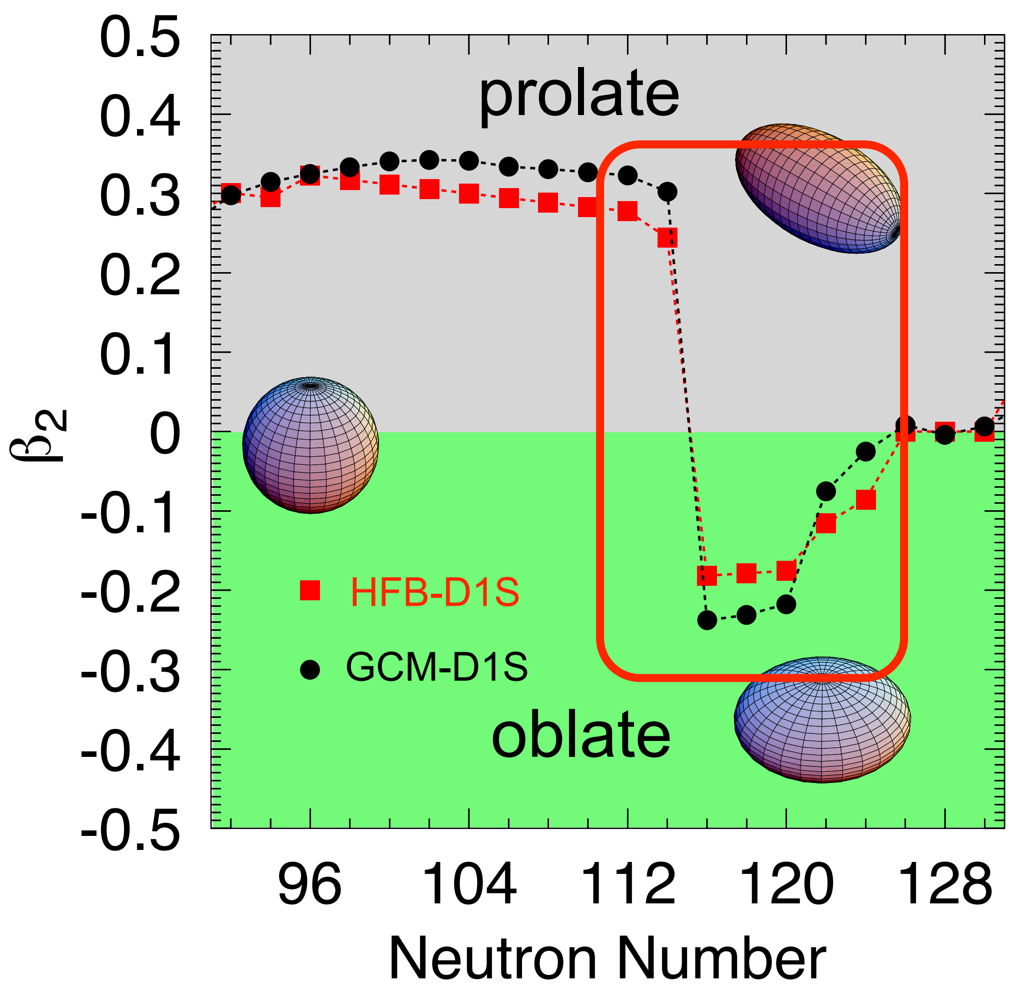

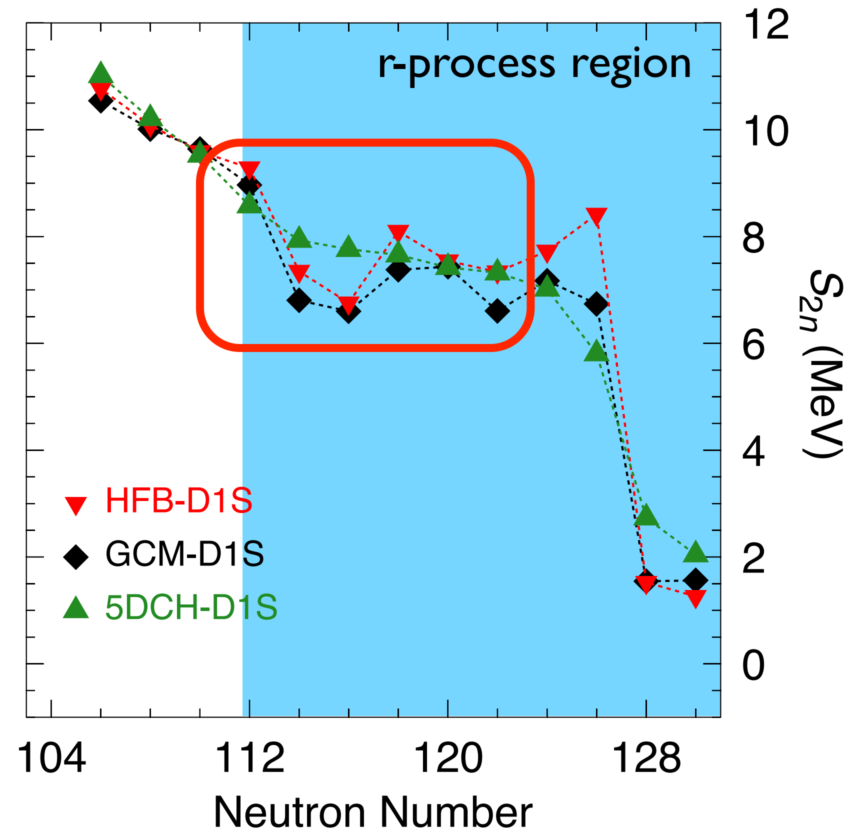

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Summary

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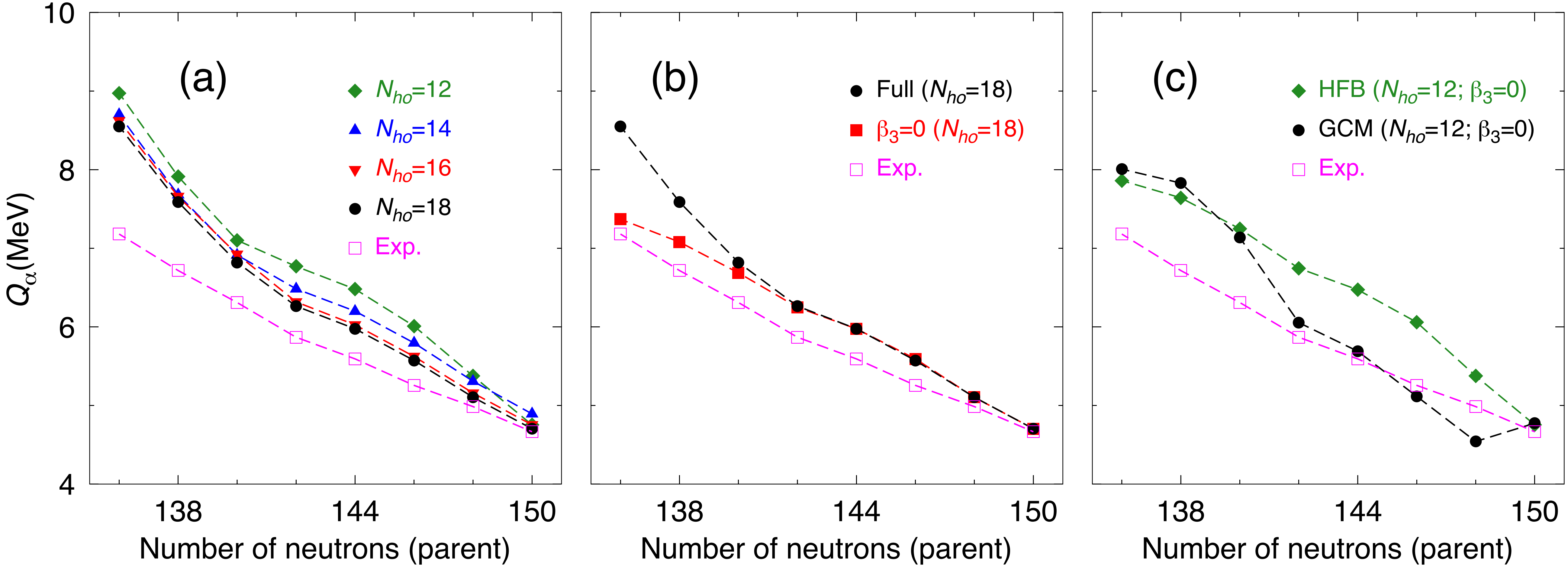
- **Current global calculations including BMF effects** have assumed certain approaches/ interactions that **could produce unphysical results** whenever local analyses are performed:
  - 5DCH is not always variational/consistent with the underlying mean-field and fails near the shell closures: spurious rather than BMF effects in these regions.

Summary

Pu isotopes. Gogny D1M parametrization



Convergence affects the results

Addition of new degrees of freedom affects the results

Beyond mean field effects affects the results

Need to reduce the ***physical*** and ***numerical*** uncertainties in energy density functional calculations

Outlook

- Systematic analysis of the convergence/numerical noise.
- Perform global studies ensuring convergence of the results with the present variational BMF method.
- Study the impact on nucleosynthesis simulations.
- In the long-range plan:
  - Description of the odd systems at the same level of BMF approach.
  - Development of parametrizations of the interaction fitted with BMF functionals.

Acknowledgments

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Alexander Arzhanov (TU-Darmstadt, Germany)

Joel Mendoza-Temis (TU-Darmstadt, Germany)

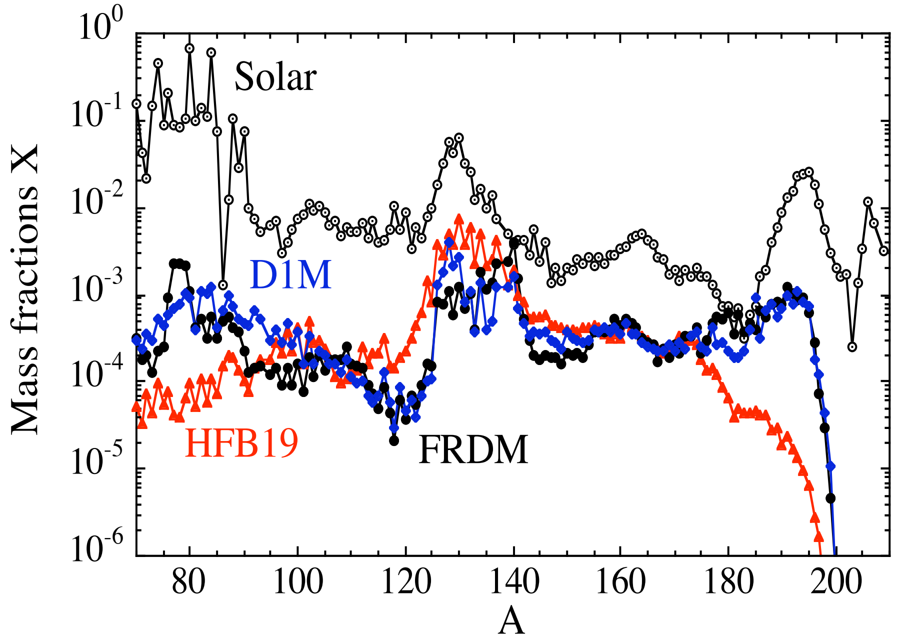
Gabriel Martínez-Pinedo (TU-Darmstadt, Germany)

J. Luis Egido (UAM, Spain)

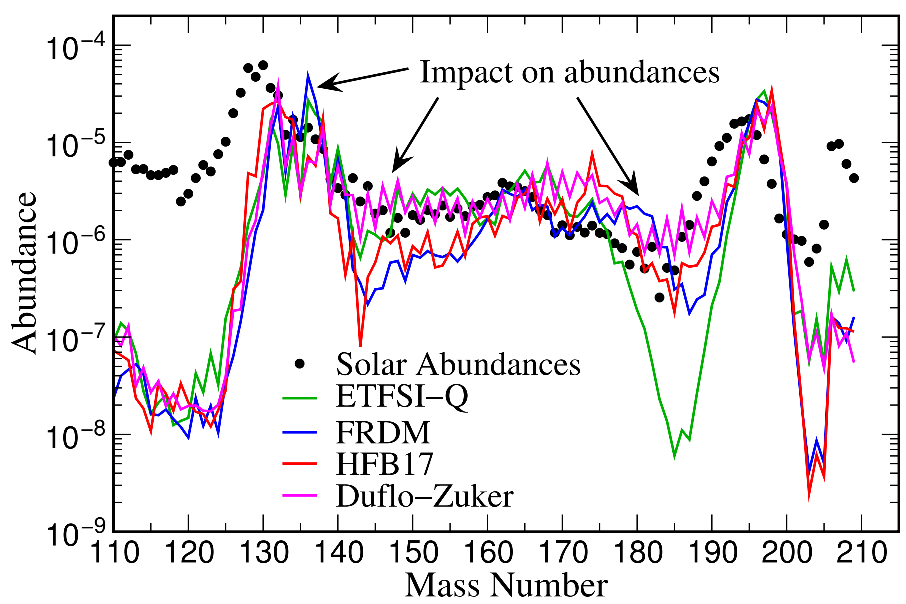
L. M. Robledo (UAM, Spain)

• Impact of the nuclear mass model on r-process nucleosynthesis calculations:

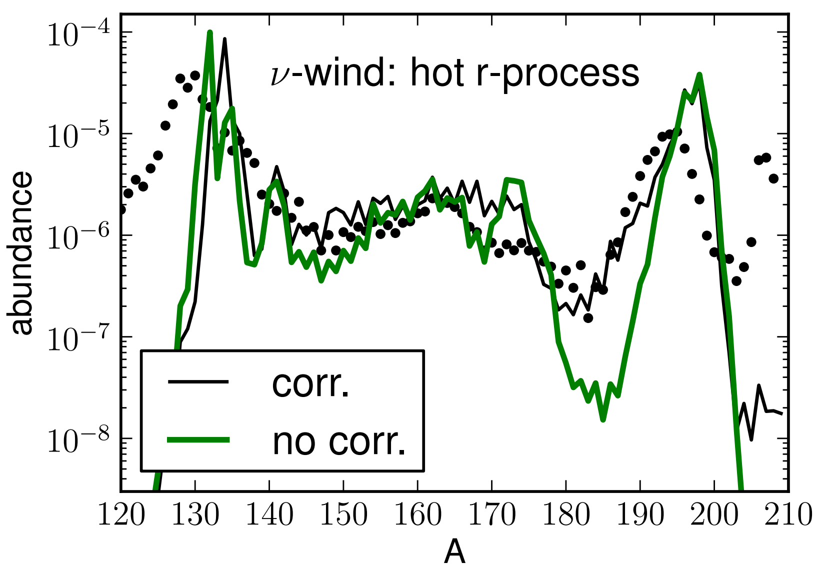
Final abundances depend on the mass model used (for the same astrophysical conditions)



Goriely et al.



Arcones and Martínez-Pinedo, PRC 83, 045809 (2011)



Arcones and Bertsch, PRL 108, 151101(2012)