Ab Initio Theory Outside the Box

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Inside the Box

- this workshop has provided an impressive snapshot of the **progress and perspectives in ab initio nuclear theory** and its links to experiment

- **definition**: everything we have heard so-far is inside the ab initio box

Inside the Box

- **ab initio theory is entering new territory...**
  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT
  - **accuracy frontier**
    control uncertainties, improve convergence, inform extrapolations
  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties
  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum
  - **continuum & clustering frontier**
    include continuum & clustering effects for threshold states & nuclei
  - **reaction frontier**
    describe structure & reaction observables on the same footing

...providing a coherent theoretical framework for nuclear structure & reactions and linking it to experiment

Outside the Box

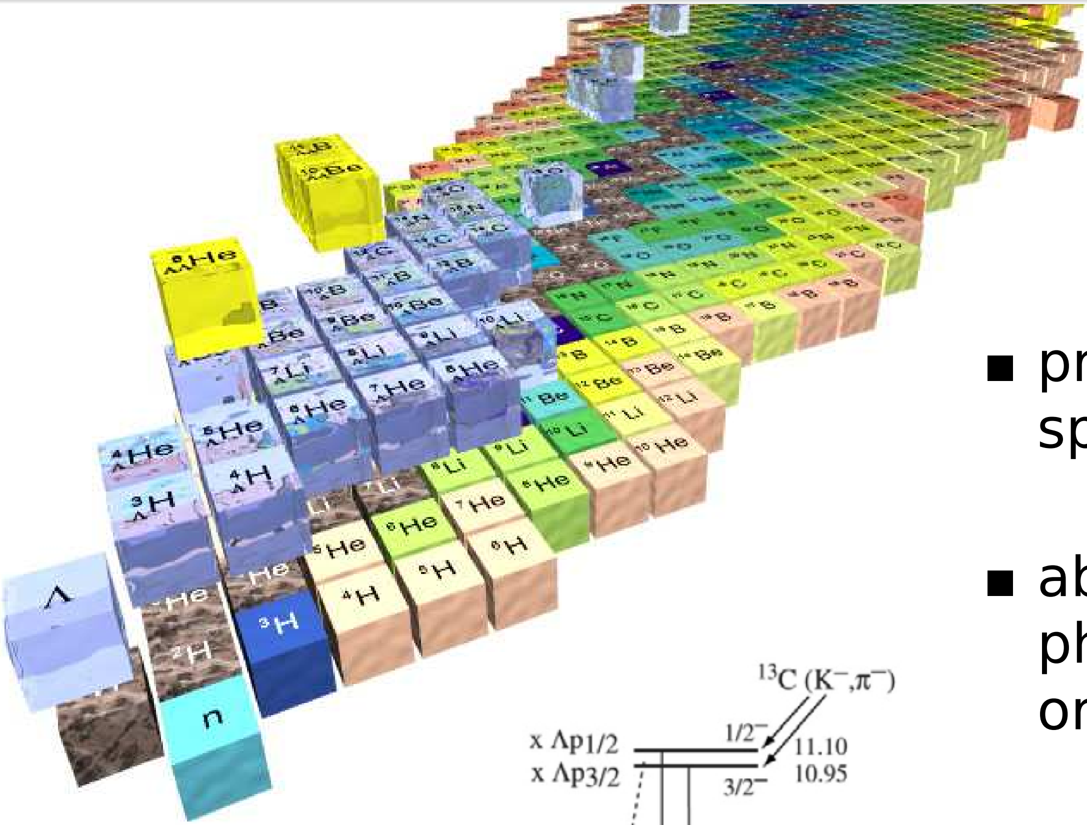
- two more things that are not yet inside the ab initio box:
- **ab initio hypernuclear structure**
  can we describe the spectroscopy of p-shell hypernuclei ab initio ?
- **perturbation theory — ab initio ?**
  wouldn't it be great if MBPT would qualify as ab initio approach ?

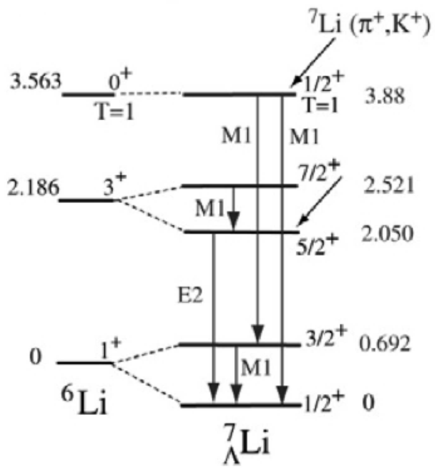
Ab Initio Hypernuclear Structure

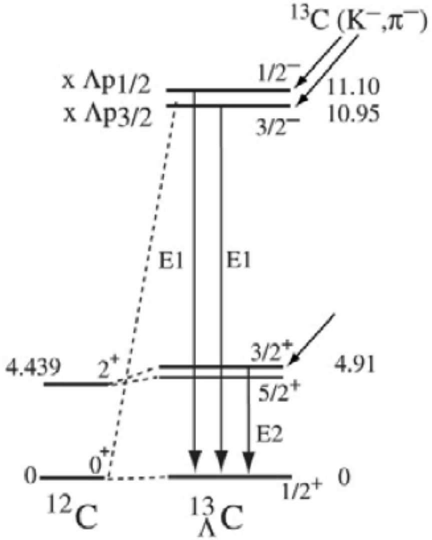
with

Roland Wirth, Daniel Gazda, Petr Navrátil

Ab Initio Hypernuclear Structure



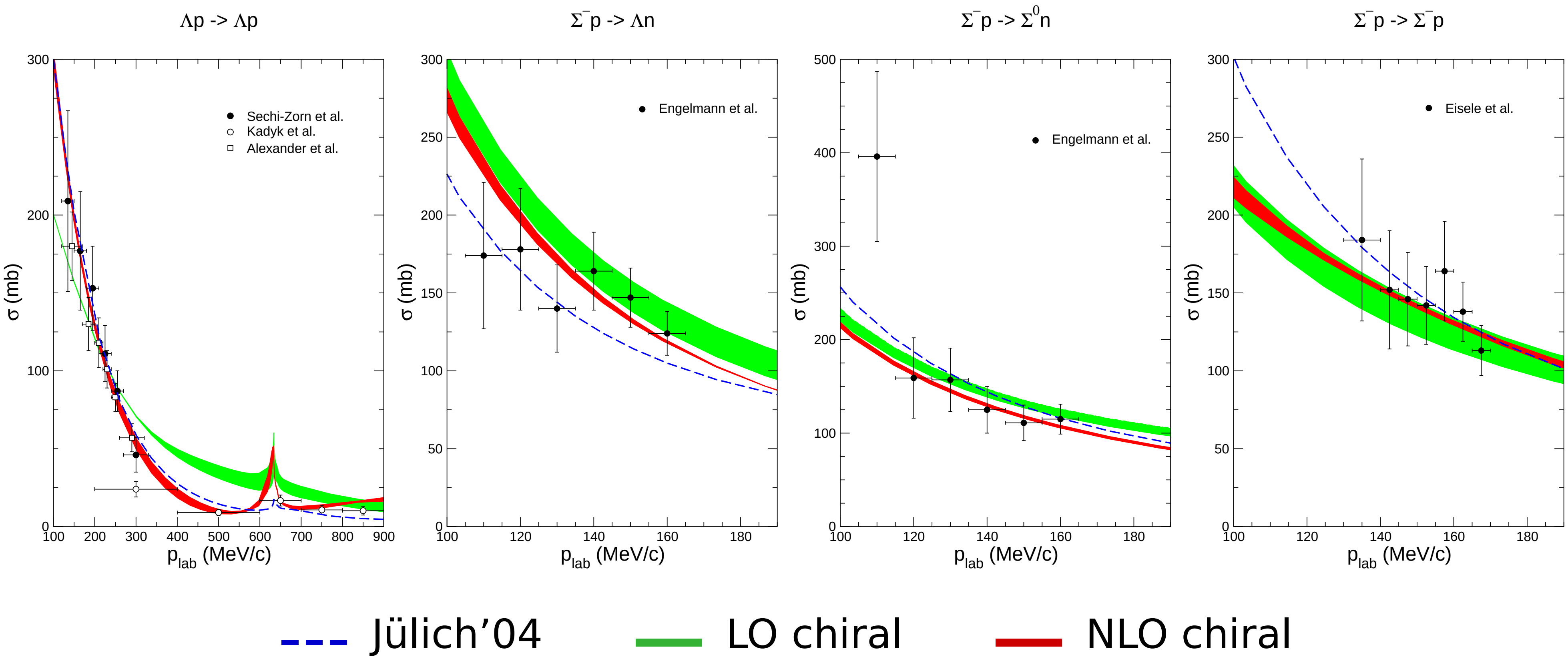




- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations
- chiral YN & YY interactions at (N)LO are available
- constrain YN & YY interactions by ab initio hypernuclear structure calculations

YN Interaction — A Problem

Haidenbauer et al., NPA 915, 24 (2013), Polinder et al., NPA 779, 244 (2006), Haidenbauer et al., PRC 72, 044005 (2005)



- experimental YN scattering data is **scarce** and has **large uncertainties**
- fit of interactions **not well constrained** (invoke symmetries)
- scattering data **cannot discriminate** between different YN potentials

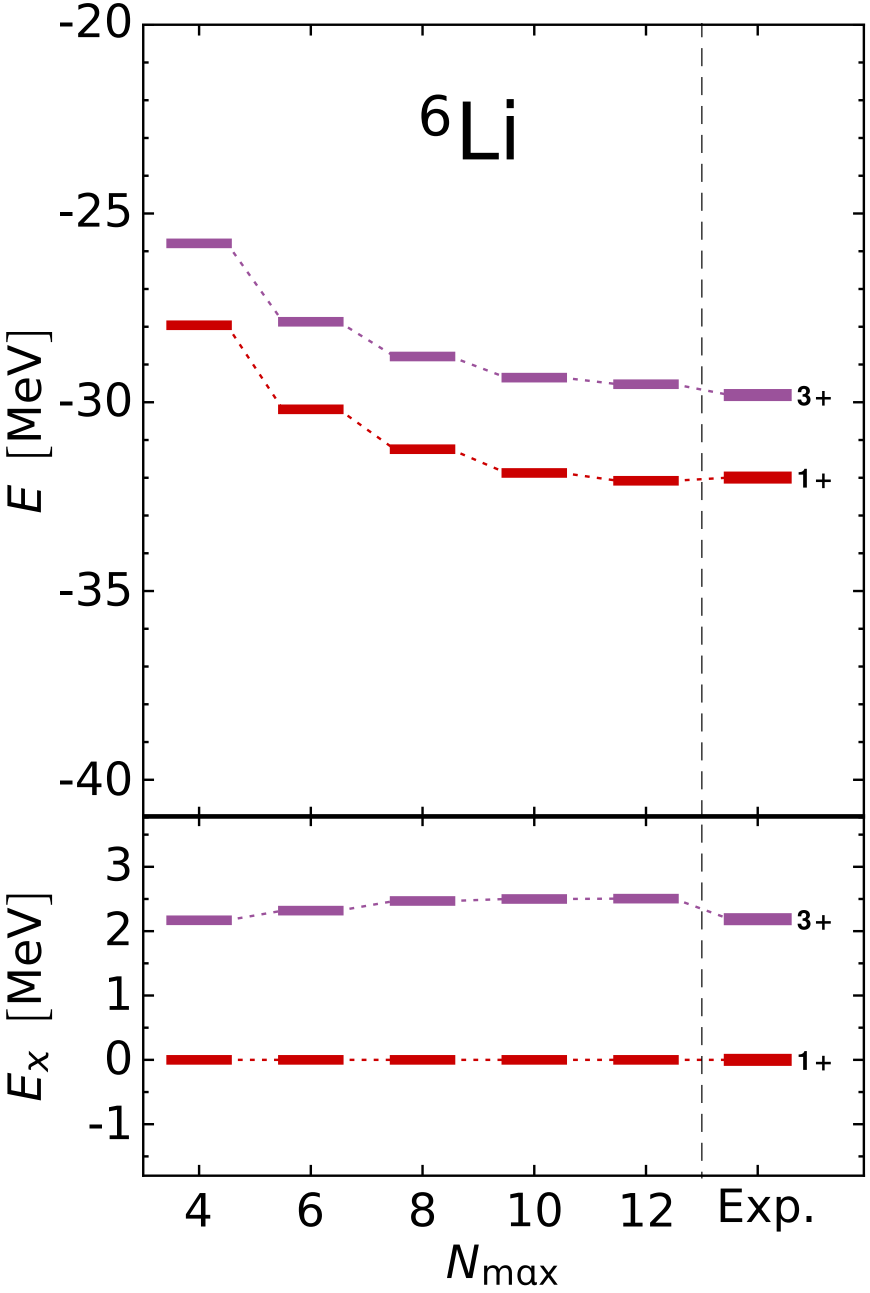
Ab Initio Toolbox

- **Hamiltonian from chiral EFT**
  - NN: chiral N3LO by Entem & Machleidt, $\Lambda_{NN} = 500$ MeV
  - 3N: chiral N2LO by Navrátil, $\Lambda_{3N} = 500$ MeV, $A = 3$ fit
  - YN: chiral LO by Polinder, Haidenbauer & Meißner, $\Lambda_{YN} = 600, 700$ MeV
    Jülich'04 by Haidenbauer & Meißner

- **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including Λ-Σ-coupling (larger matrices)
  - Λ-Σ mass difference and $p\Sigma^{\pm}$ Coulomb included consistently

- **Importance Truncated No-Core Shell Model**
  - include explicit $(p, n, \Lambda, \Sigma^+, \Sigma^0, \Sigma^-)$ with physical masses
  - larger model spaces easily tractable with importance truncation
  - all p-shell single-Λ hypernuclei are accessible

Application: ${}^{7}_{\Lambda}$Li



NN @ N3LO
Λ_{NN} = 500 MeV
Entem&Machleidt

3N @ N2LO
Λ_{3N} = 500 MeV
Navratil
A = 3 fit

$\alpha_N = 0.08\,\text{fm}^4$

$\hbar\Omega$ = 20 MeV

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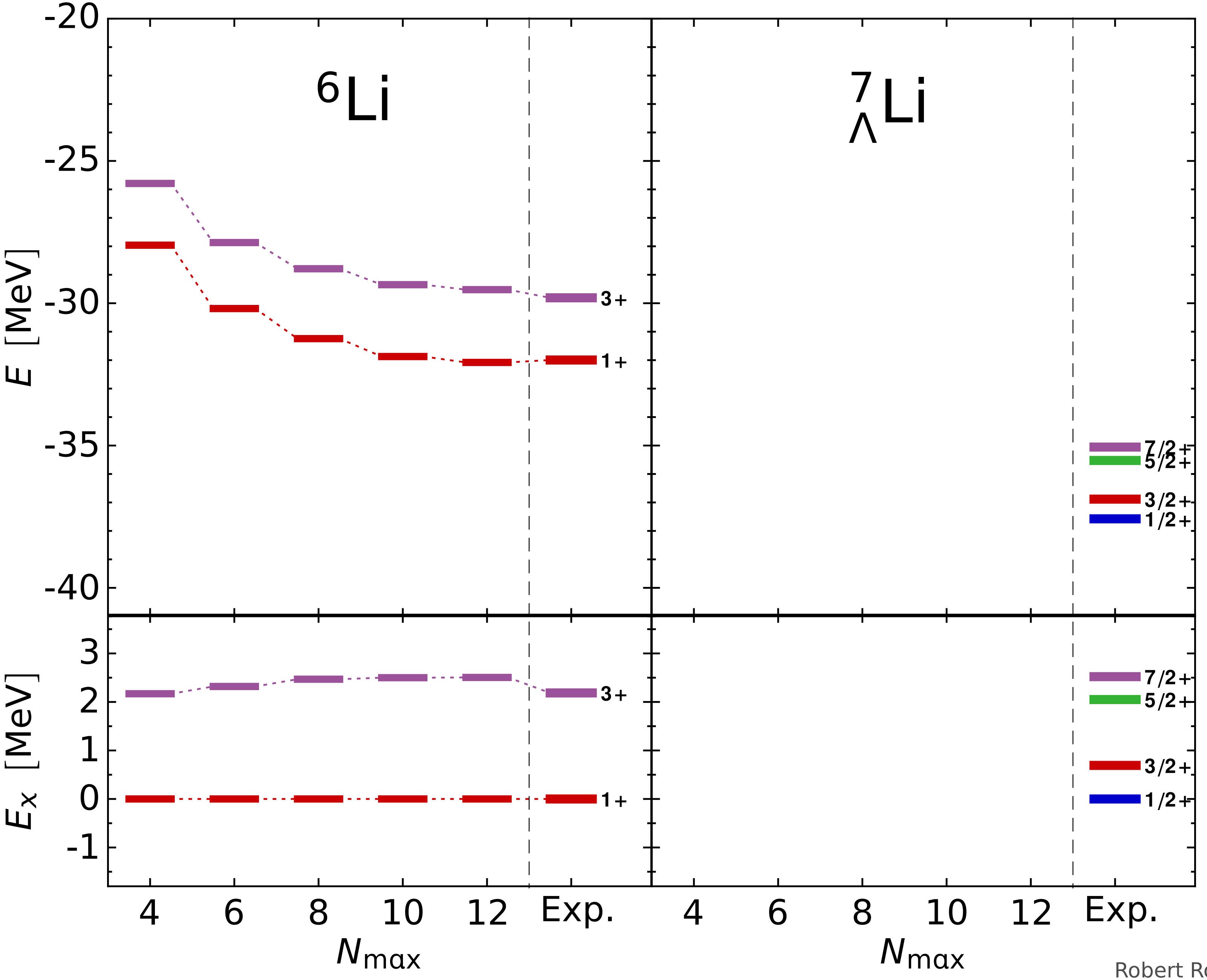

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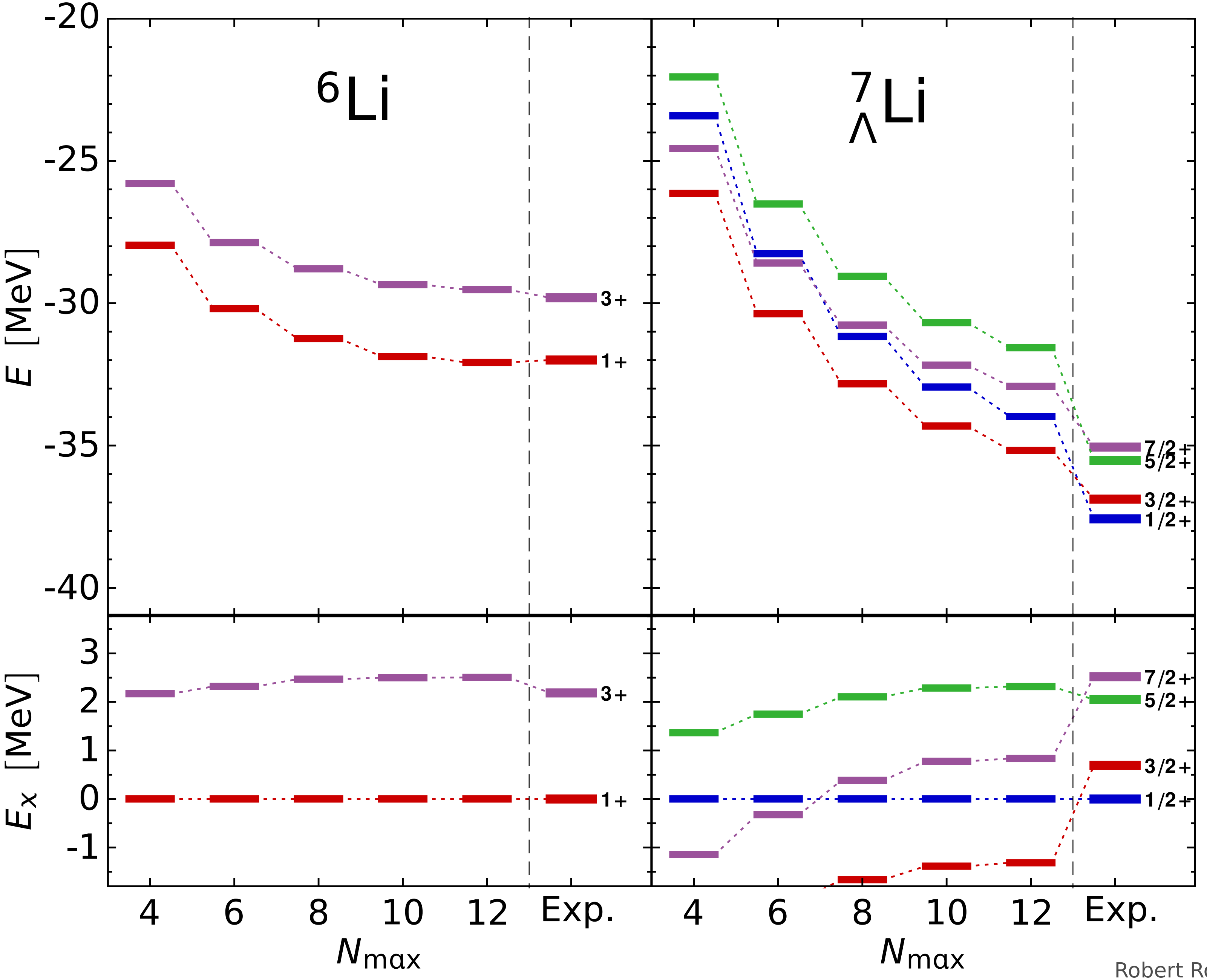

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Jülich'04
Haidenbauer et al.
scatt. & hypertriton

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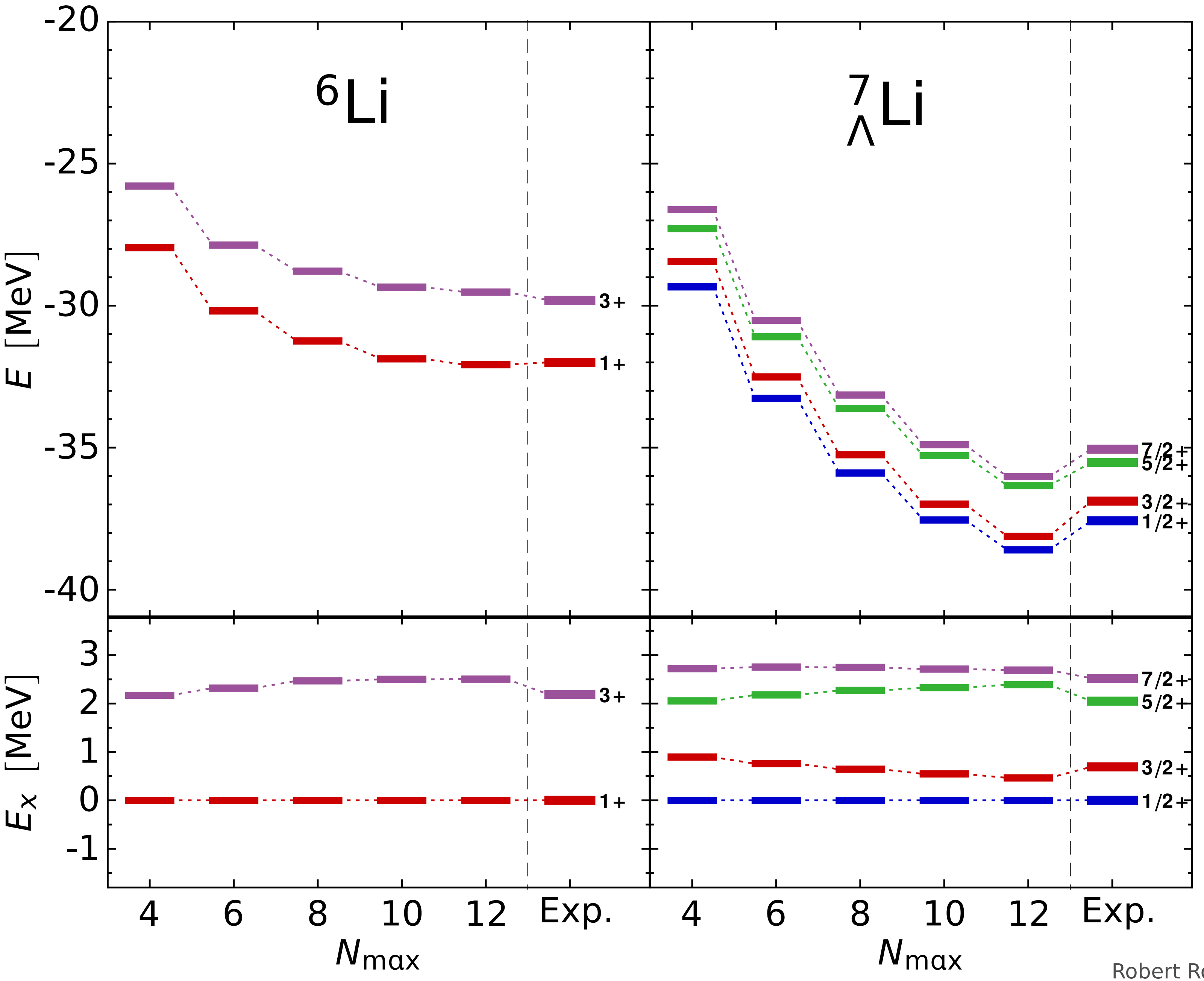

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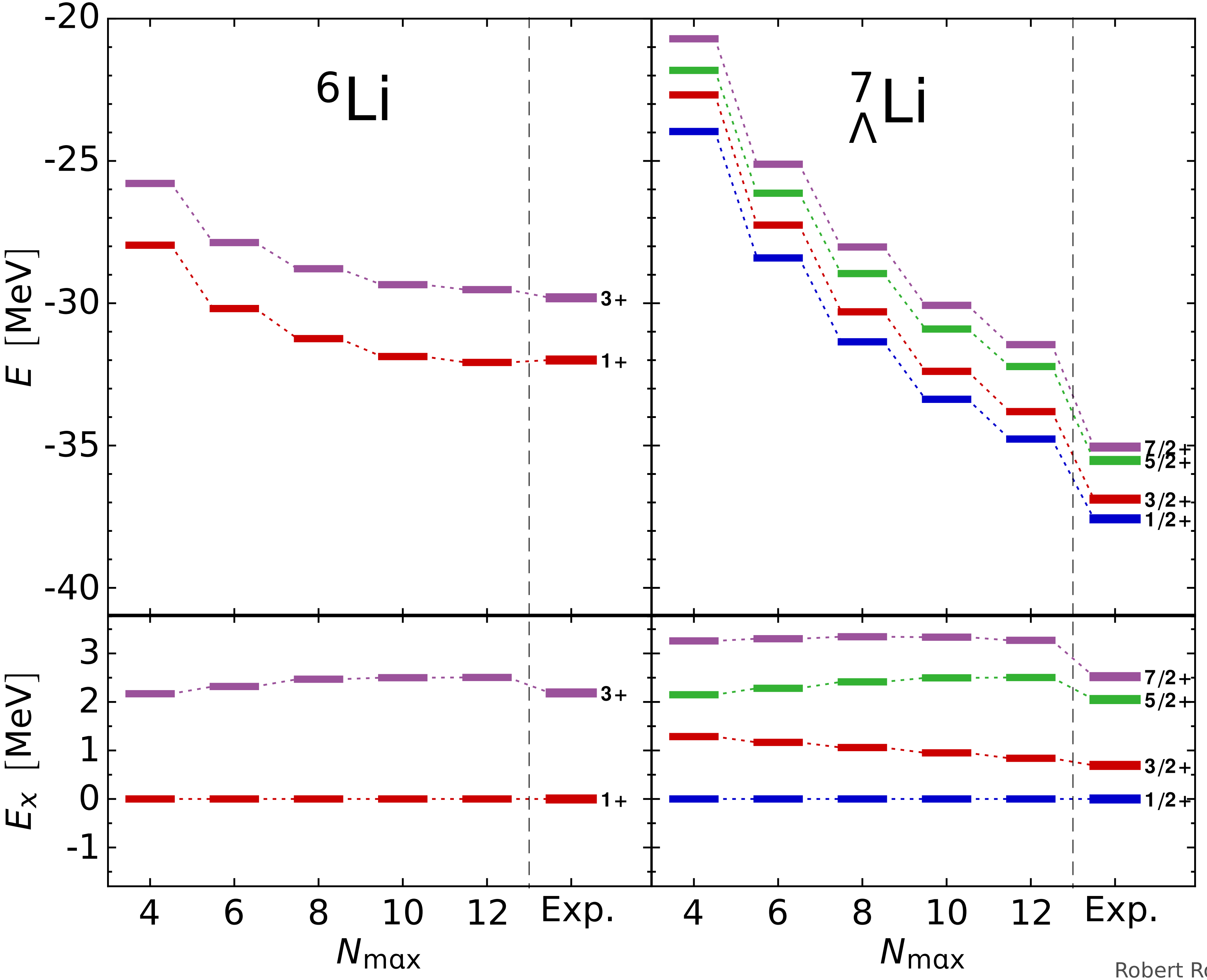

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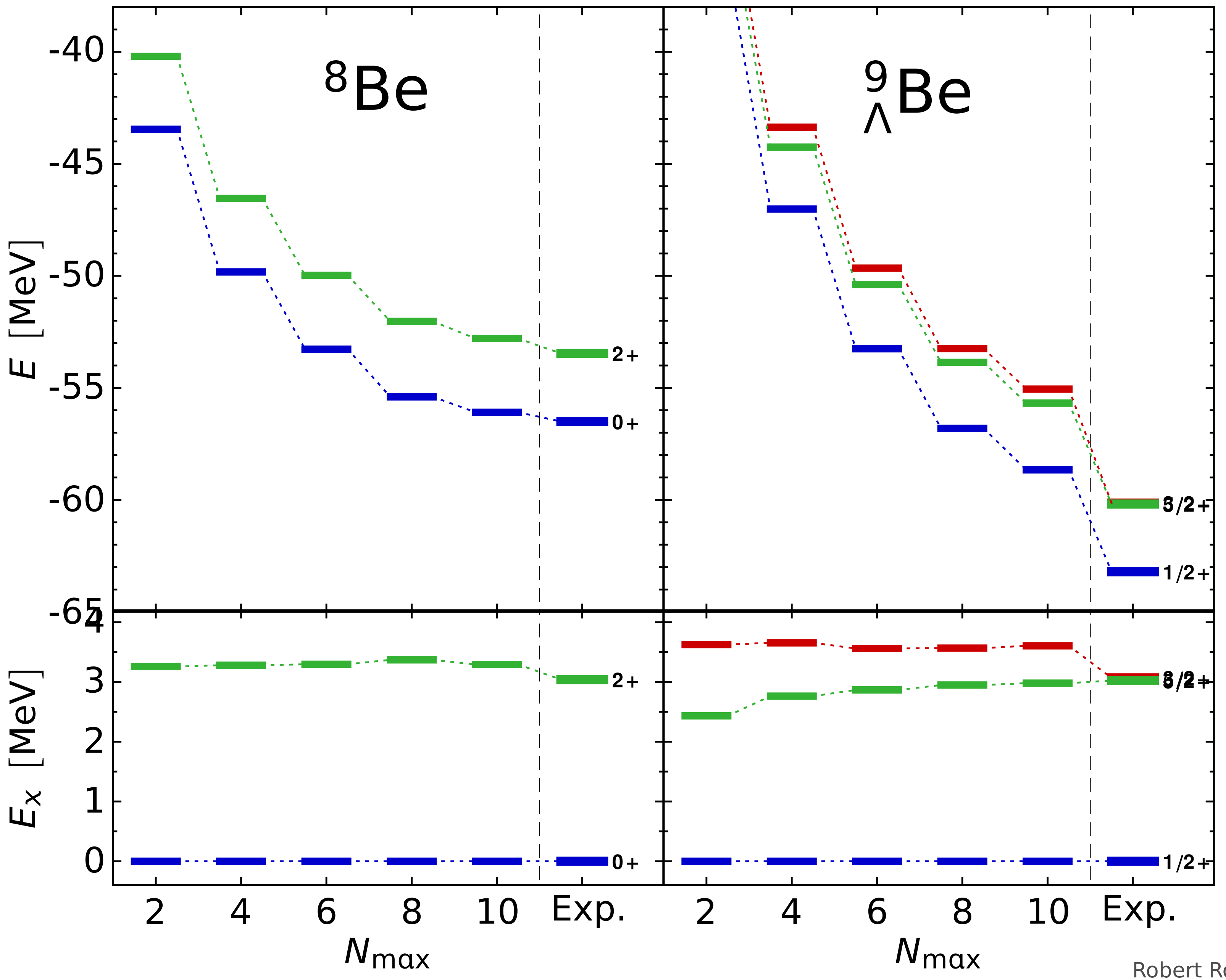
Application: $^{9}_{\Lambda}$Be



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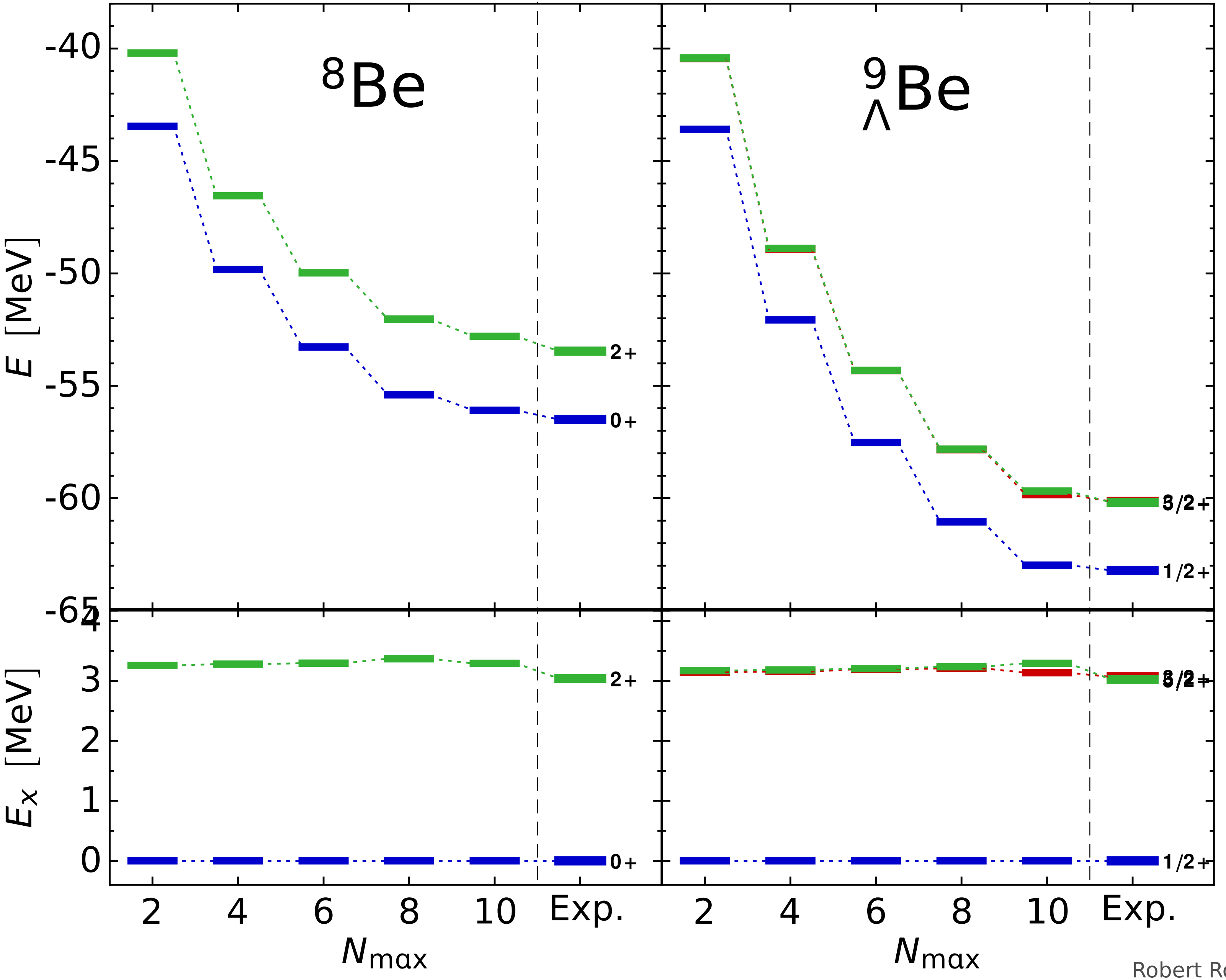

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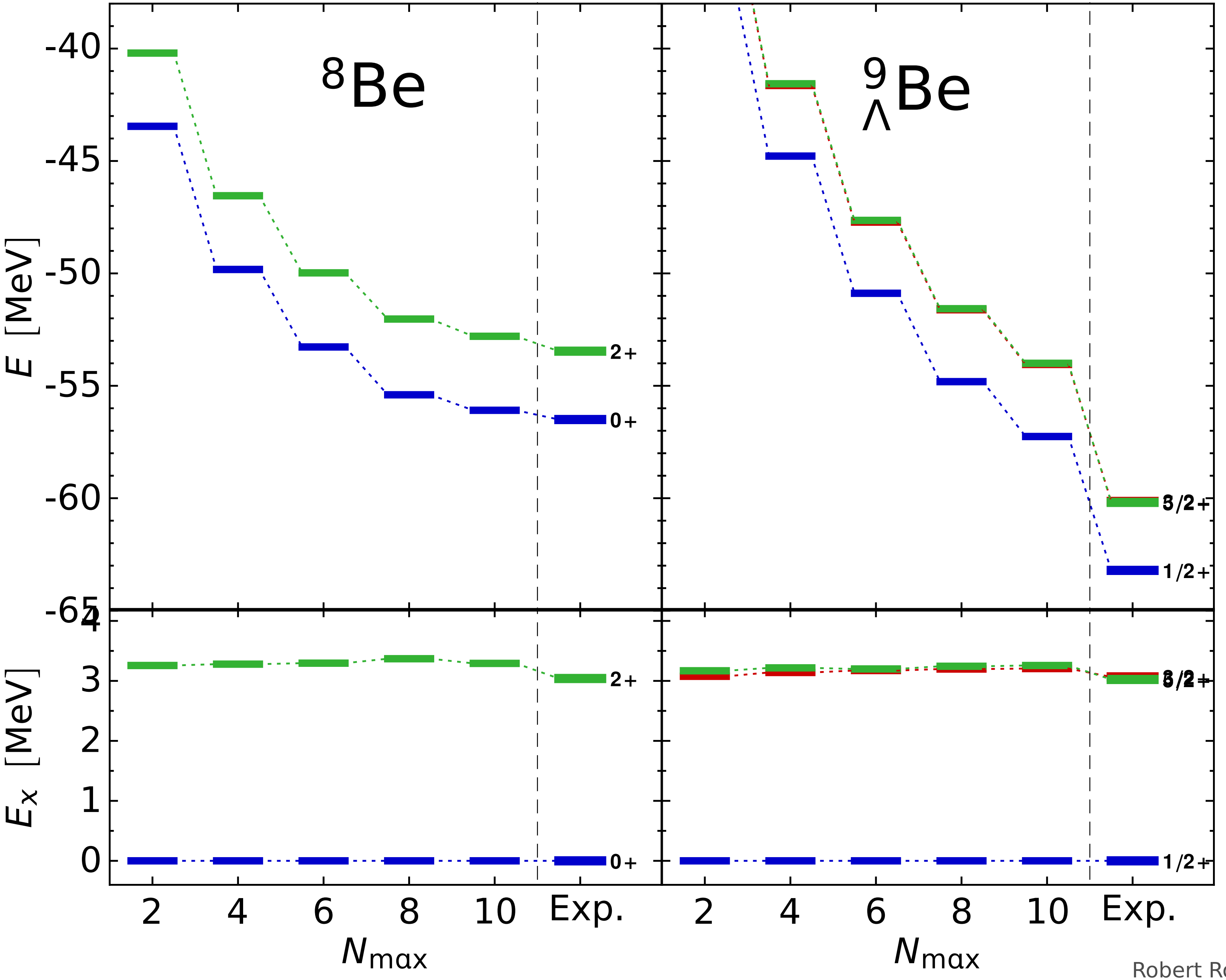

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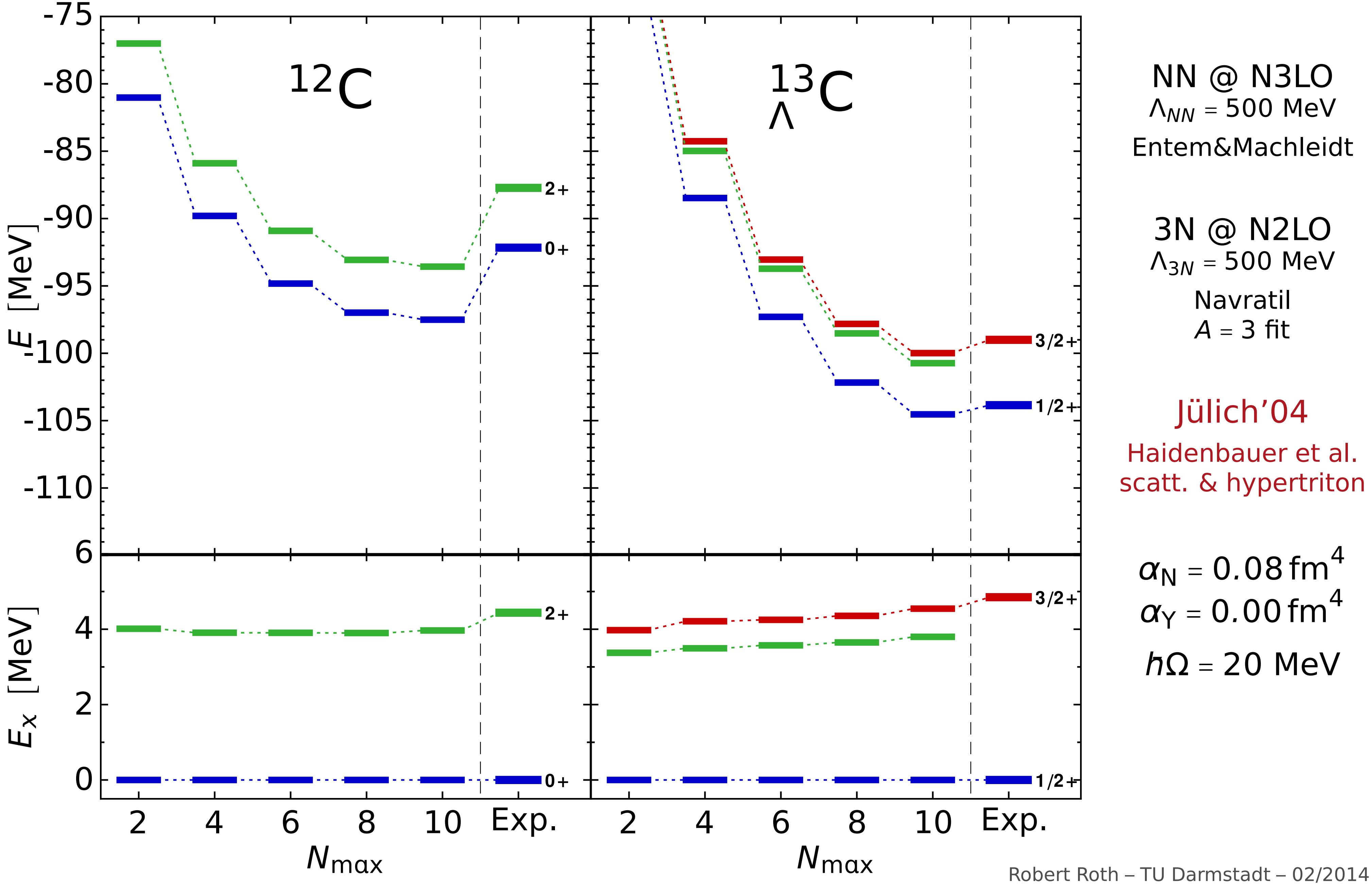

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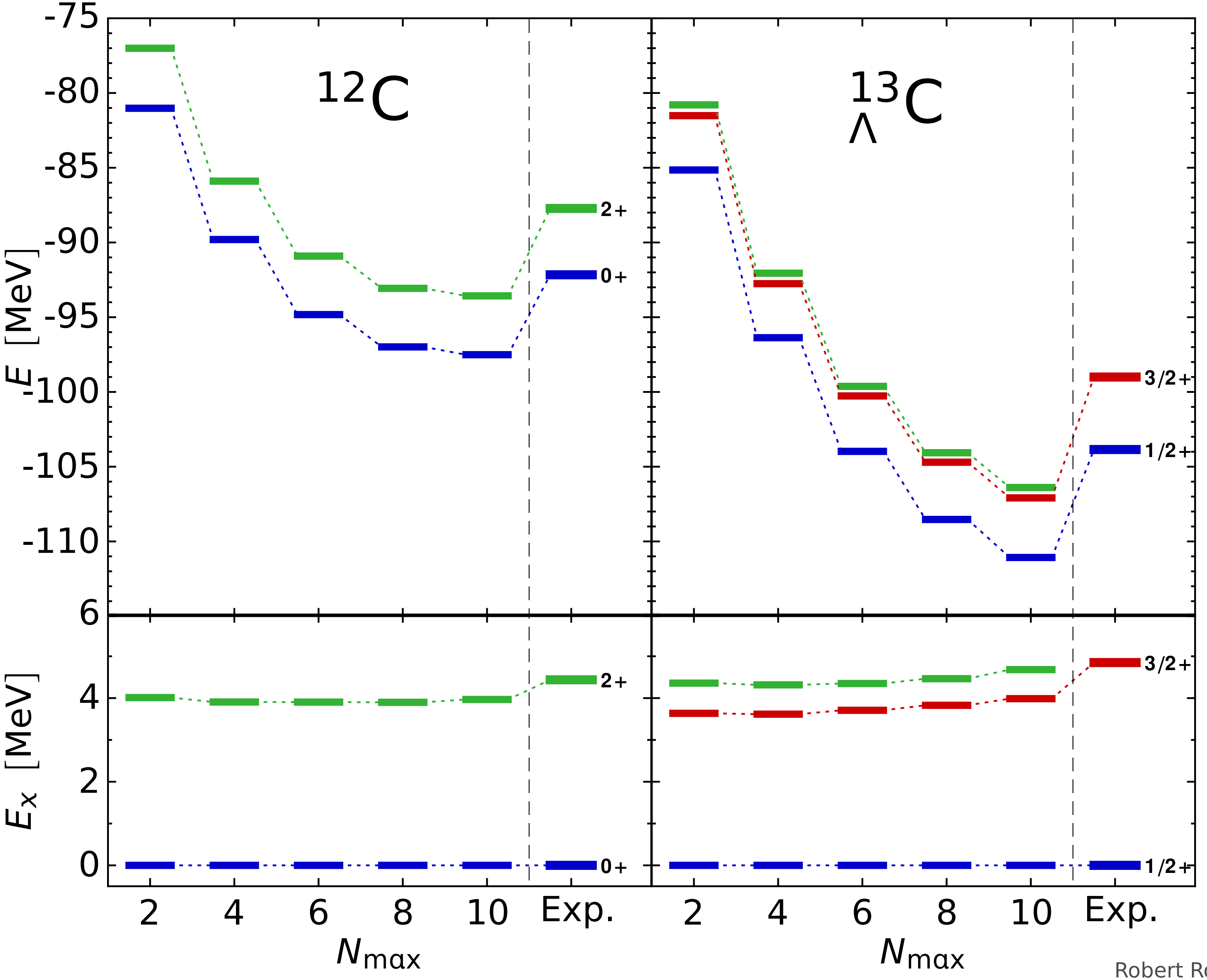

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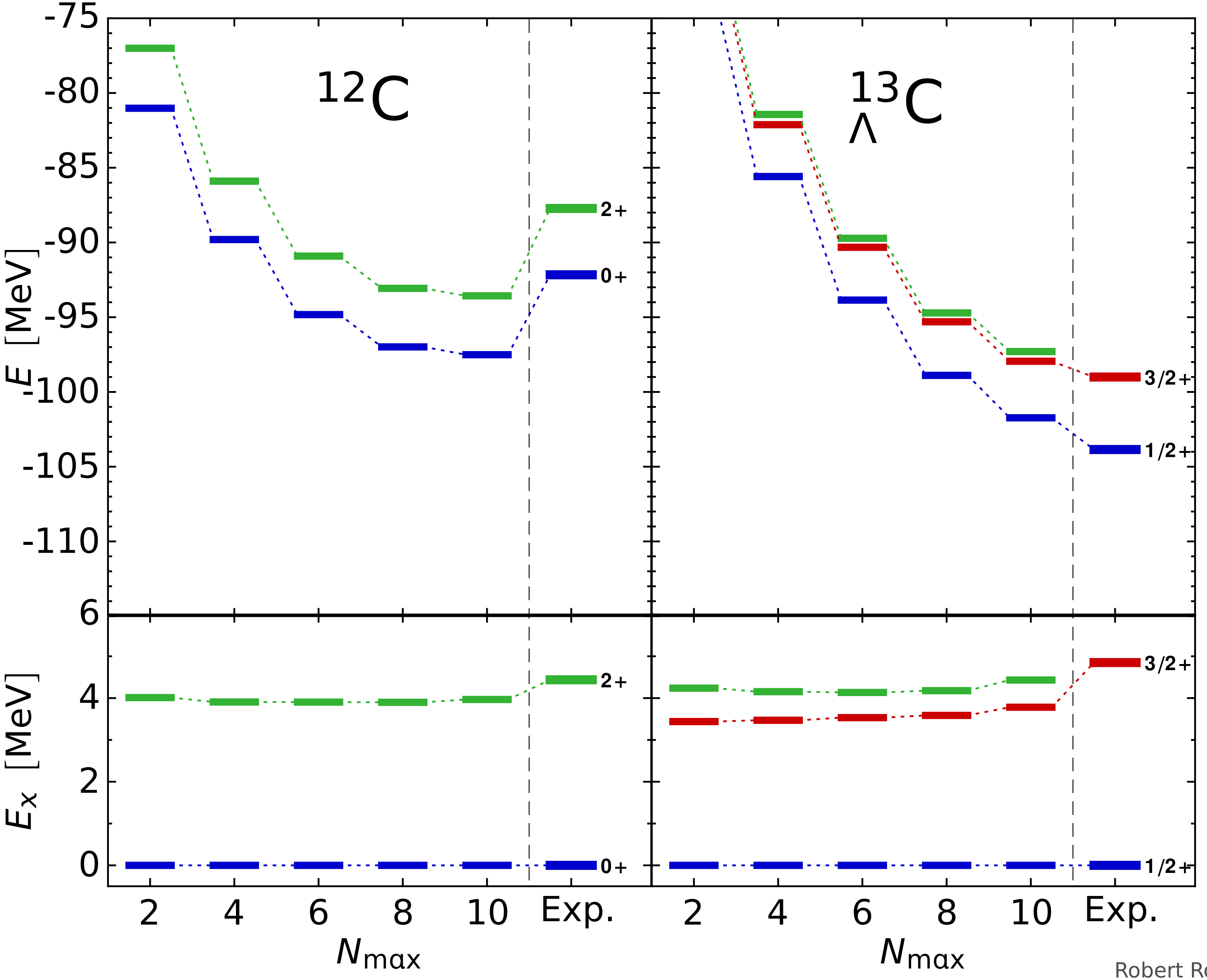

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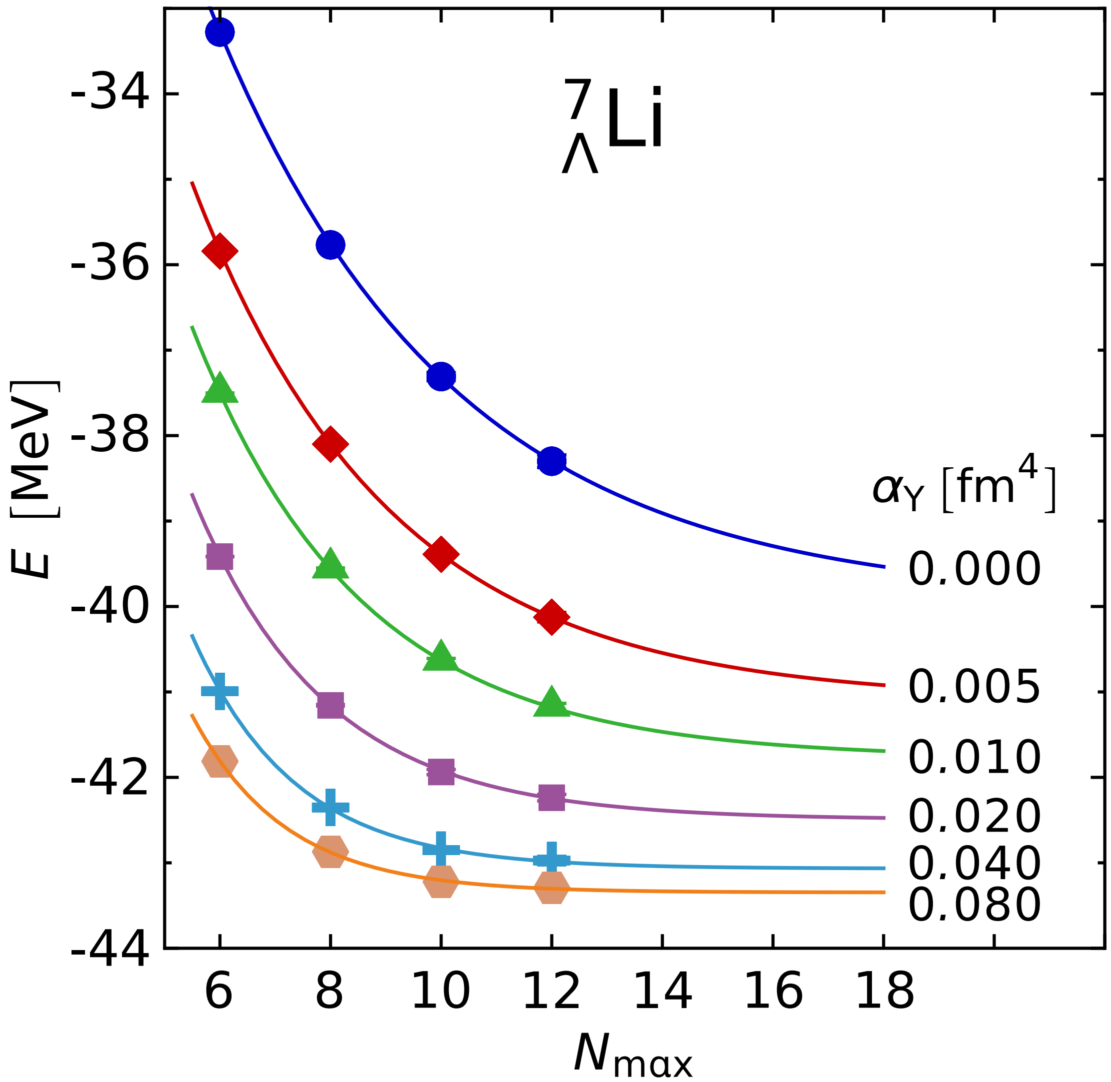
SRG Evolution of YN Channels



- SRG evolution of YN channels **improves convergence** as expected
- significant α_Y dependence indicates **SRG-induced YNN interactions**

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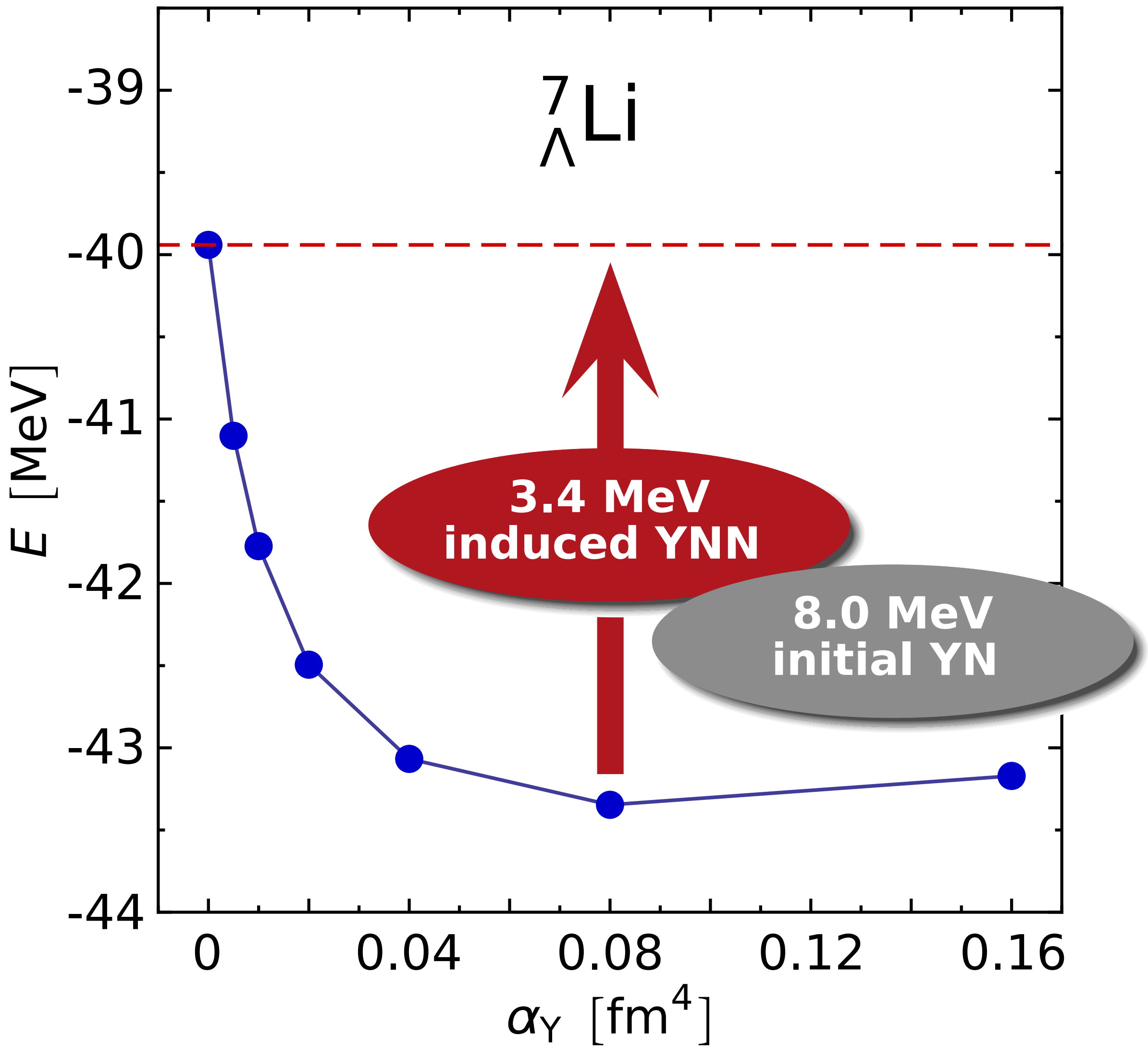

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Ab Initio Hypernuclear Structure

- ab initio hypernuclear structure in the IT-NCSM now possible for **all single-Λ p-shell hypernuclei**

- LO chiral YN interactions provide spectra that **agree with experiment** within cutoff uncertainties

- hypernuclear structure sets **tight constraints on YN interaction**

- significant **SRG-induced YNN interactions**, implications for mean-field type models and the hyperon puzzle ?

- **NLO chiral YN interactions** are expected to reduce cutoff dependence, but fit is difficult...
  (13 instead of 5 LECs in S/SD-waves assuming $SU(3)_f$ and neglecting P-waves; fit to 36 data)

- **lots of applications** are waiting...

Perturbation Theory — Ab Initio ?

with

Alexander Tichai, Christina Stumpf, Joachim Langhammer

Many-Body Perturbation Theory

- **low-order many-body perturbation theory** is a cheap and simple tool to access nuclear observables
- wouldn't it be great if low-order MBPT would **qualify as ab initio approach ?**
- problem: **convergence behavior** of perturbation series unclear
  - how to quantify uncertainties?
  - which factors influence the order-by-order convergence?
  - how to restore or accelerate the convergence?
- strategy: study convergence behavior with **explicit high-order calculations**

Explicit High-Order MBPT

- **partitioning**: definition of unperturbed basis $|\Phi_n\rangle$

$$H(\lambda) = H_0 + \lambda W \qquad\qquad H_0 |\Phi_n\rangle = \epsilon_n |\Phi_n\rangle$$

- **power-series ansatz** for energy and eigenstates

$$E_n(\lambda) = \sum_{p=0}^{\infty} \lambda^p \, E_n^{(p)} \qquad\qquad |\Psi_n(\lambda)\rangle = \sum_{p=0}^{\infty} \lambda^p \, |\Psi_n^{(p)}\rangle$$

- **recursive relations** for energy $E_n^{(p)}$ and states $|\Psi_n^{(p)}\rangle = \sum_m C_{n,m}^{(p)} |\Phi_m\rangle$

$$E_n^{(p)} = \sum_m \langle\Phi_n| W |\Phi_m\rangle \, C_{n,m}^{(p-1)}$$

$$C_{n,m}^{(p)} = \frac{1}{\epsilon_n - \epsilon_m} \left(\sum_{m'} \langle\Phi_m| W |\Phi_{m'}\rangle \, C_{n,m'}^{(p-1)} - \sum_{j=1}^{p} E_n^{(j)} \, C_{n,m}^{(p-j)} \right)$$

- easy to evaluate to 'arbitrary' order with NCSM technology...

Summation and Resummation

- **partial sum**: starting point for convergence study

$$E_{\text{sum}}(p) = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \dots \lambda^p E^{(p)}\Big|_{\lambda=1}$$

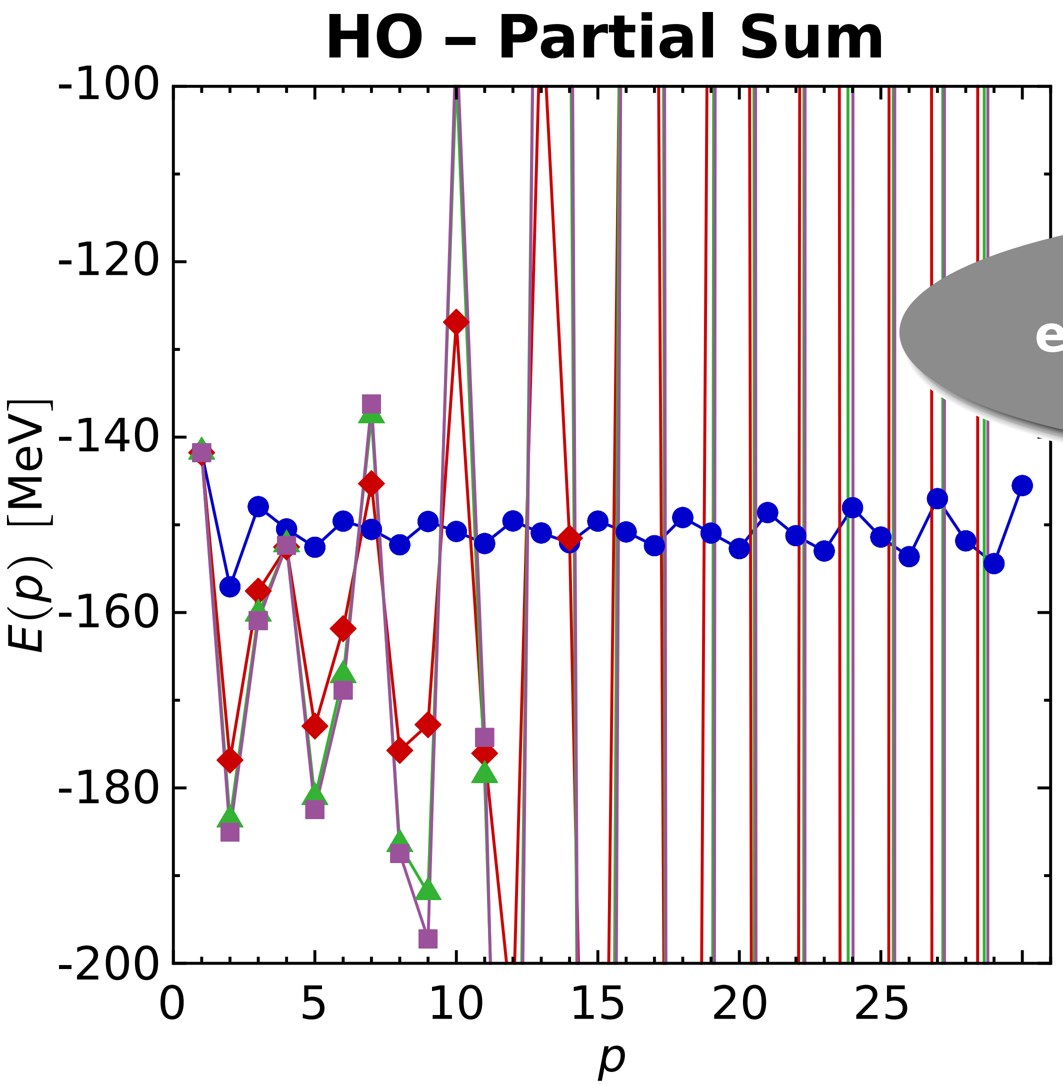
- **Padé approximant**: map power series of order p to a quotient of polynomials of orders M and N

$$E_{\text{Padé}}(M/N) = \frac{A^{(0)} + \lambda A^{(1)} + \lambda^2 A^{(2)} + \dots \lambda^M A^{(M)}}{B^{(0)} + \lambda B^{(1)} + \lambda^2 B^{(2)} + \dots \lambda^N B^{(N)}}\Bigg|_{\lambda=1}$$

$$= E_{\text{sum}}(M+N) + \mathcal{O}(M+N+1)$$

  - focus on Padé main sequence: $E_{\text{Padé}}(M/M)$ and $E_{\text{Padé}}(M/M-1)$
  - powerful convergence theory for special power series (e.g. Stieltjes)...
  - additional sequence transformations on top of Padé can further accelerate convergence (Shanks, Levin-Weniger)...

^{16}O: MBPT Convergence



partial sum exhibits exponential oscillatory divergence

e_{max} = 2 e_{max} = 4 e_{max} = 6 e_{max} = 8

NN_{only} , $\alpha = 0.08\,\mathrm{fm}^4$, $\hbar\Omega = 20$ MeV , 2p2h truncated

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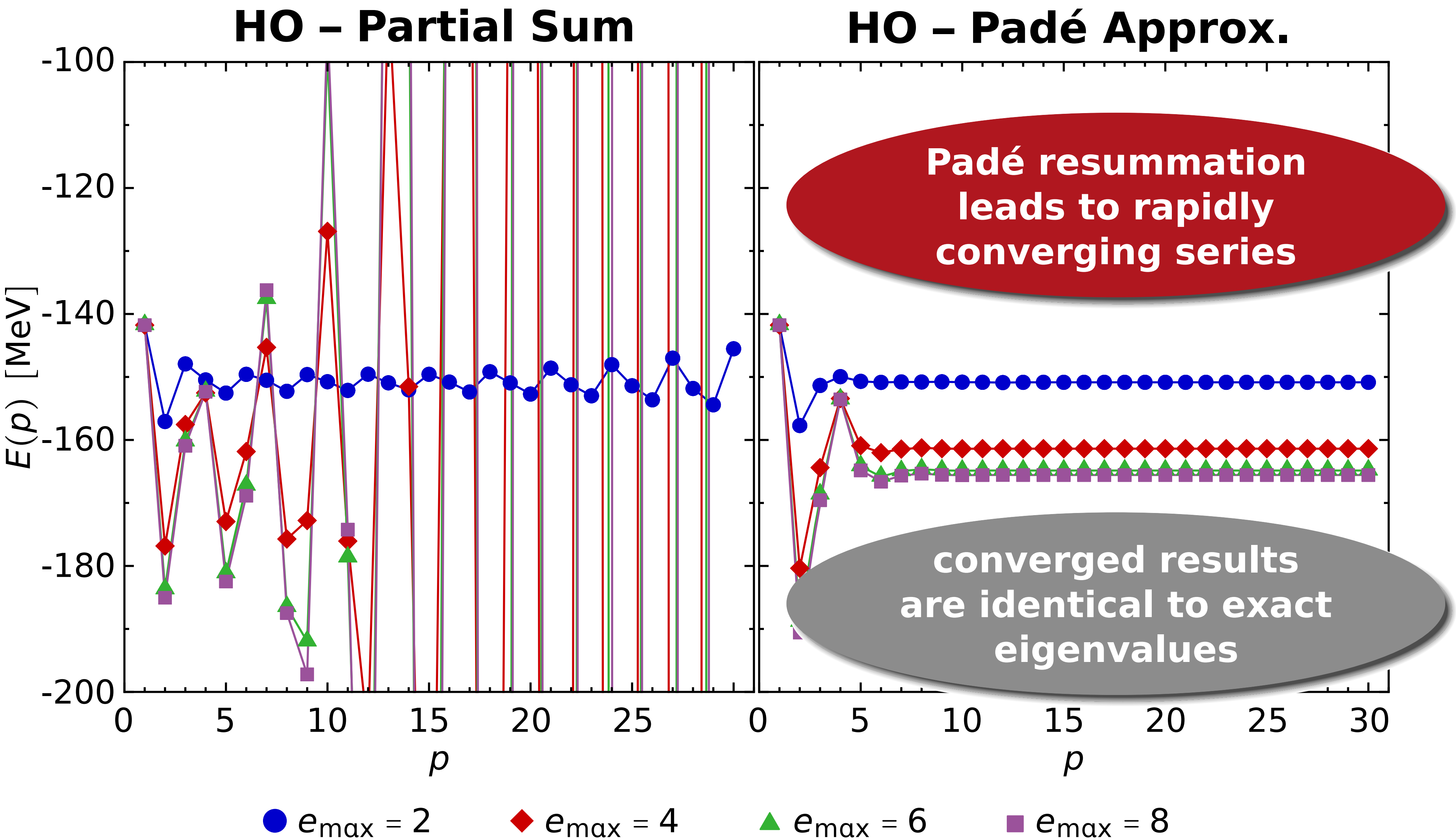

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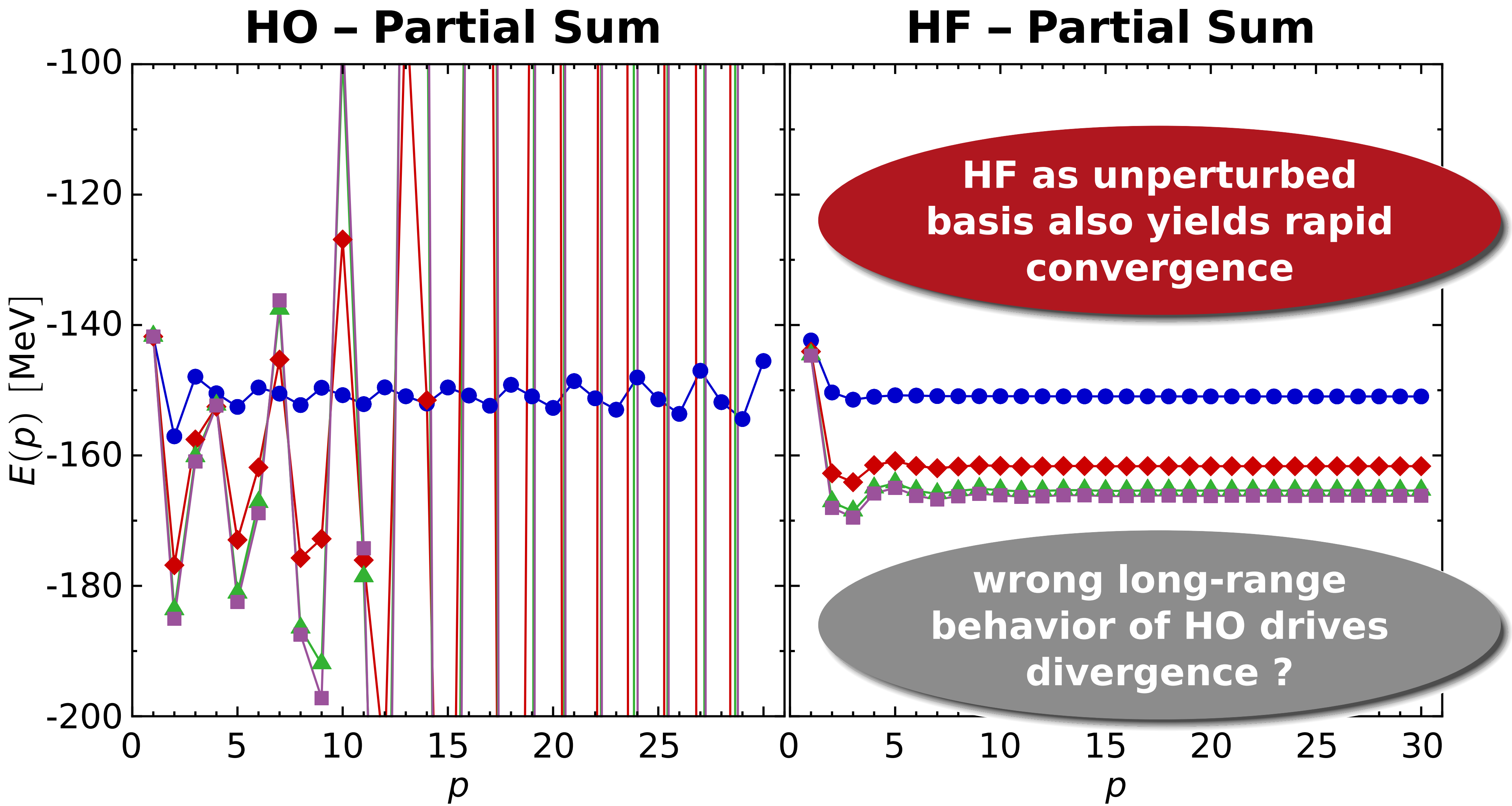

$e_{max} = 2$ $e_{max} = 4$ $e_{max} = 6$ $e_{max} = 8$

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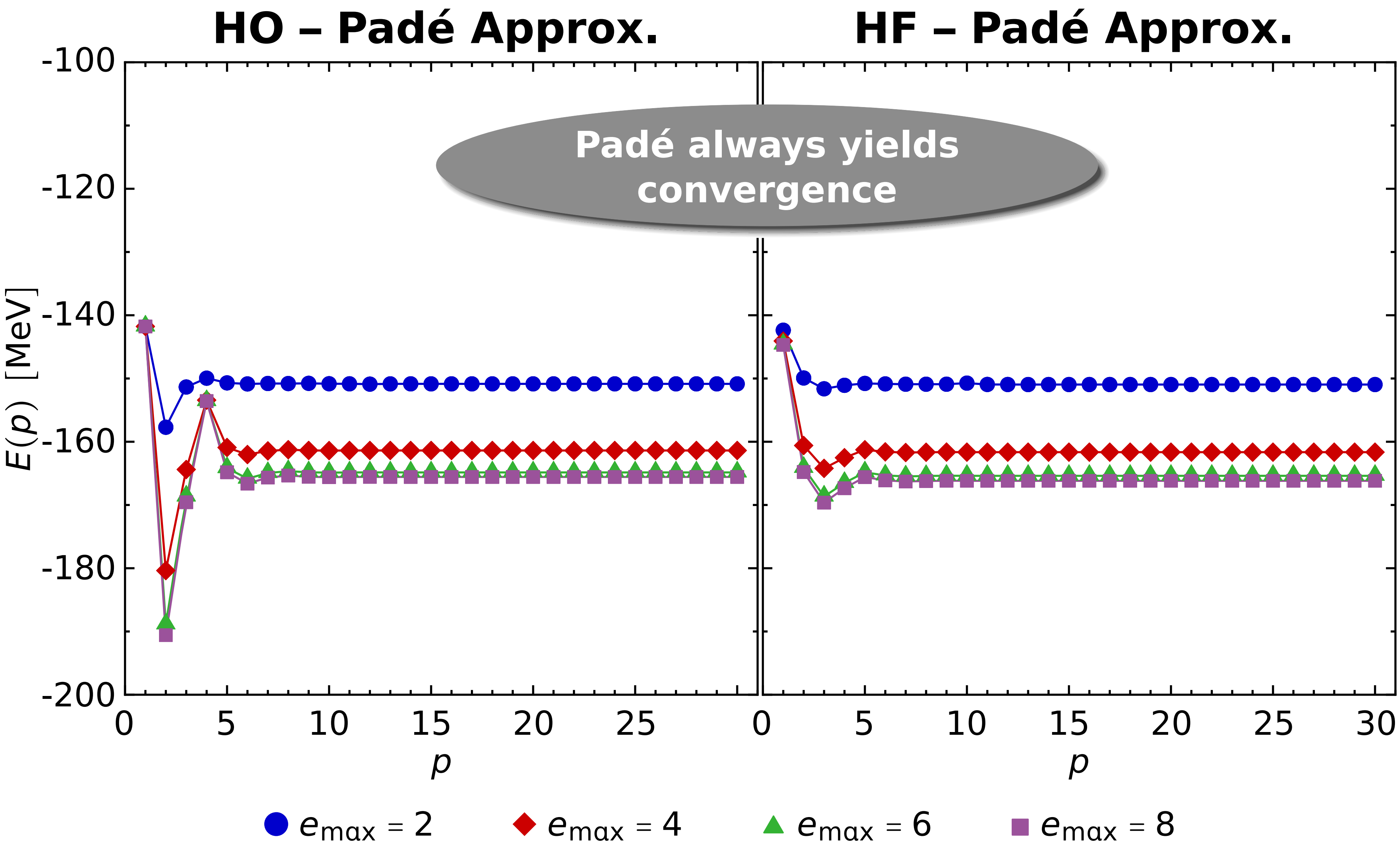

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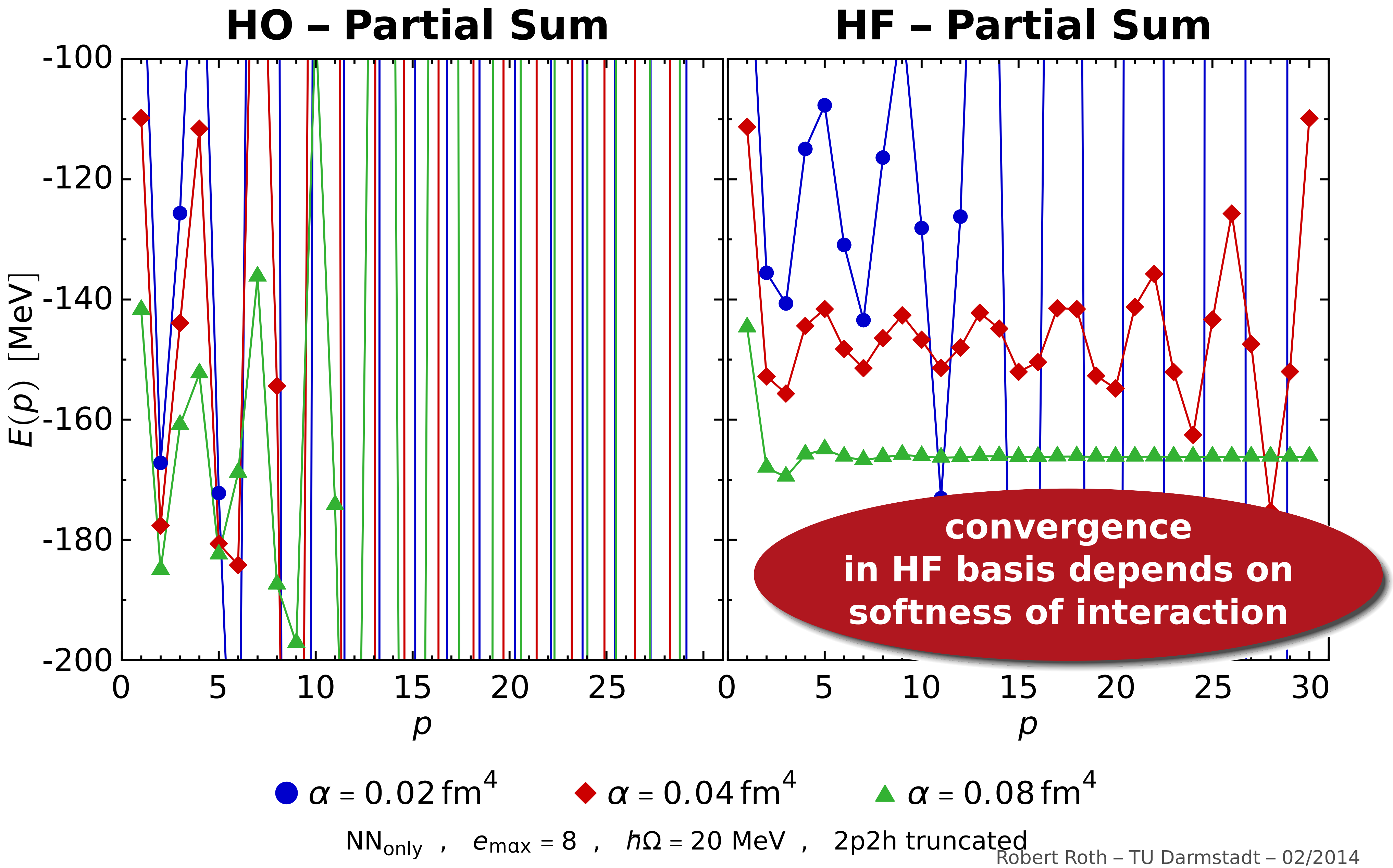

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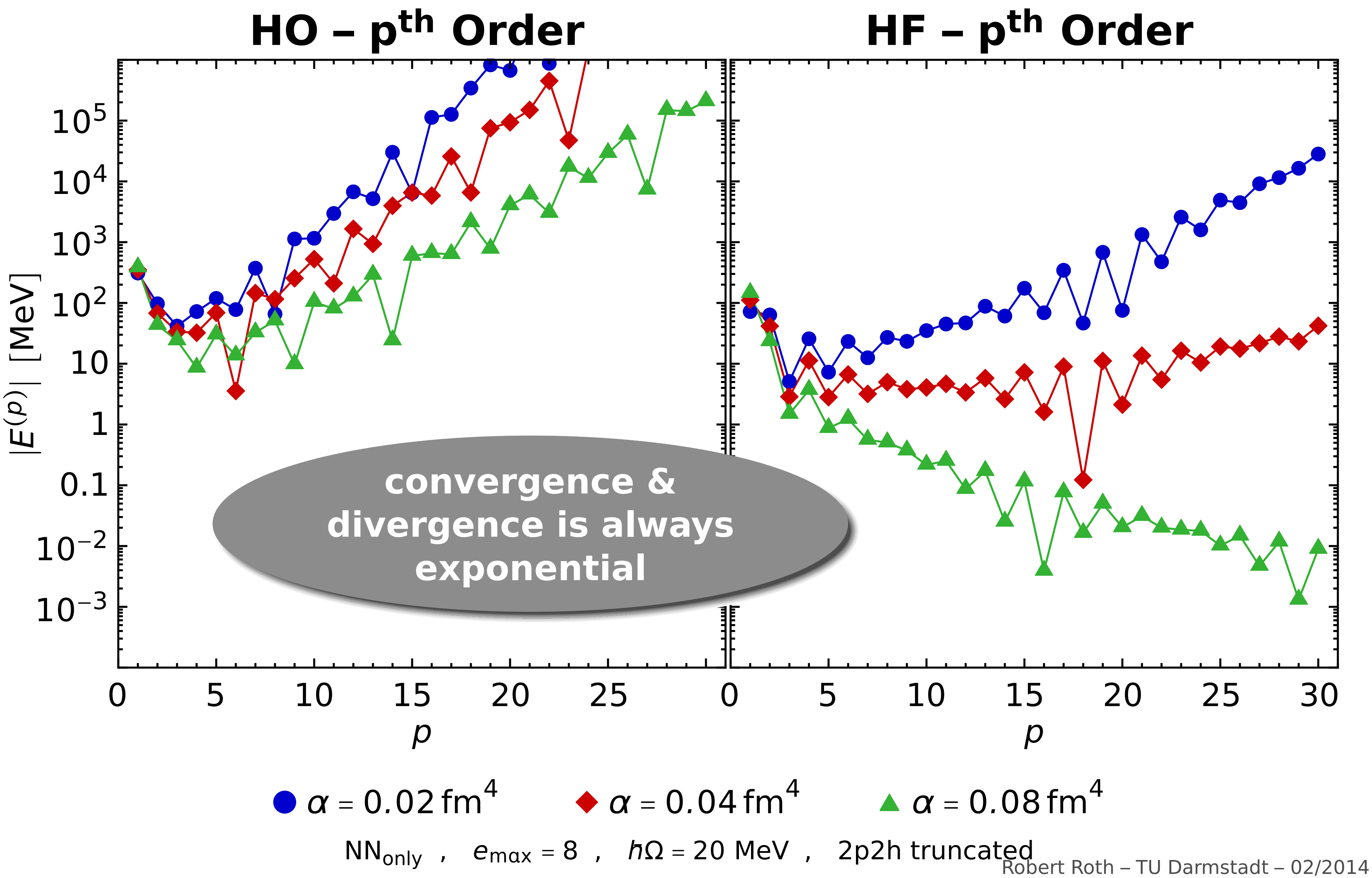

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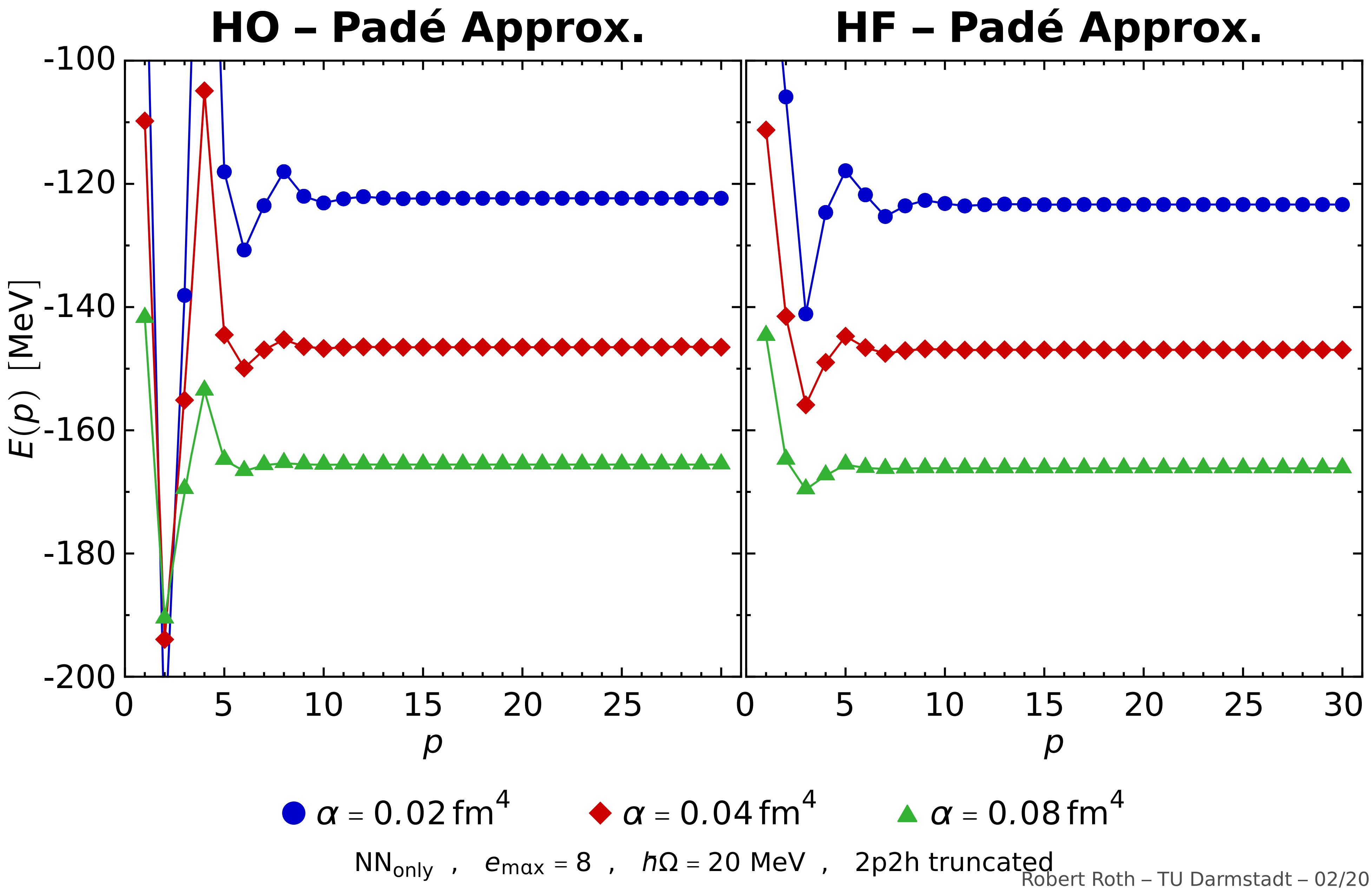
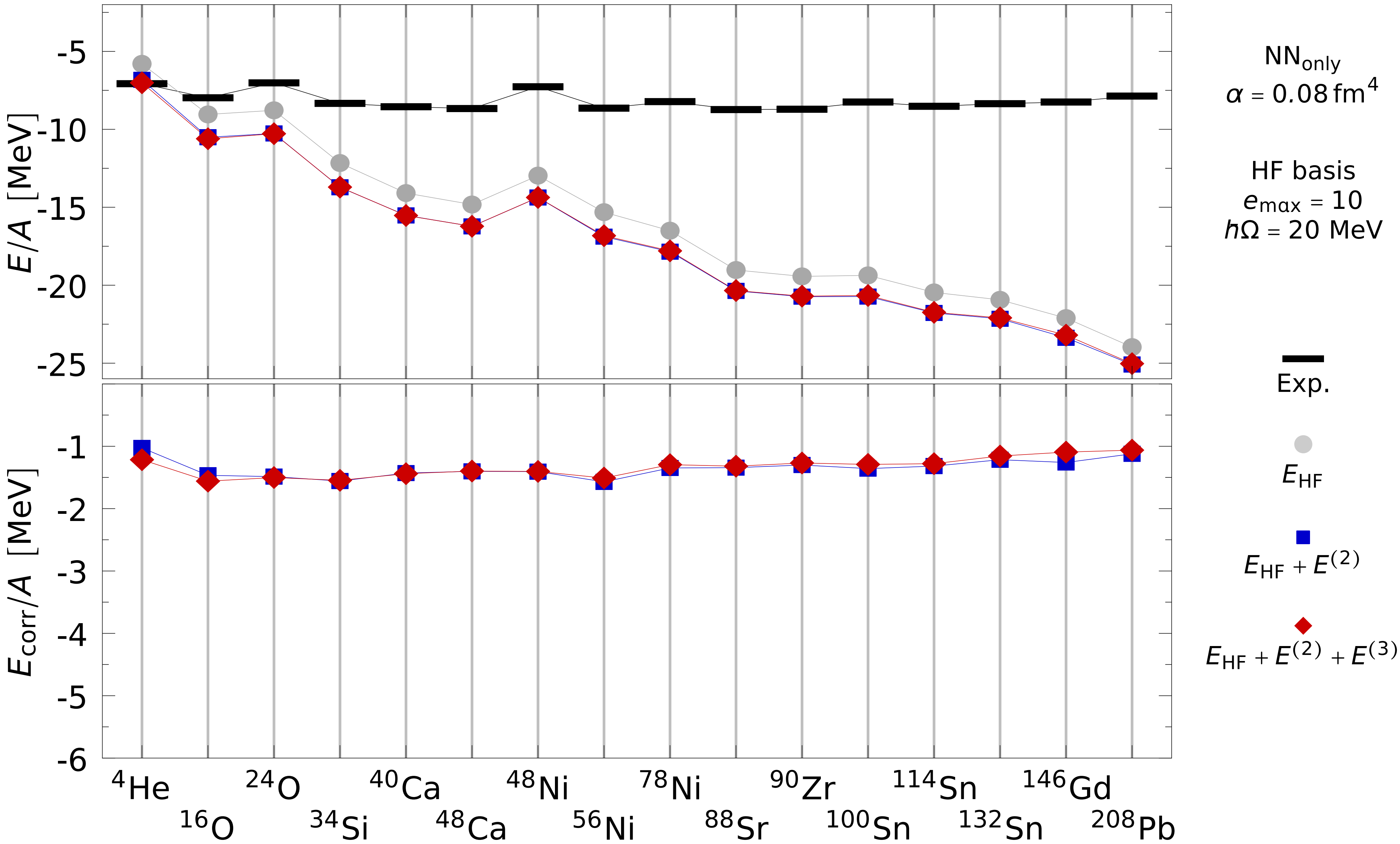


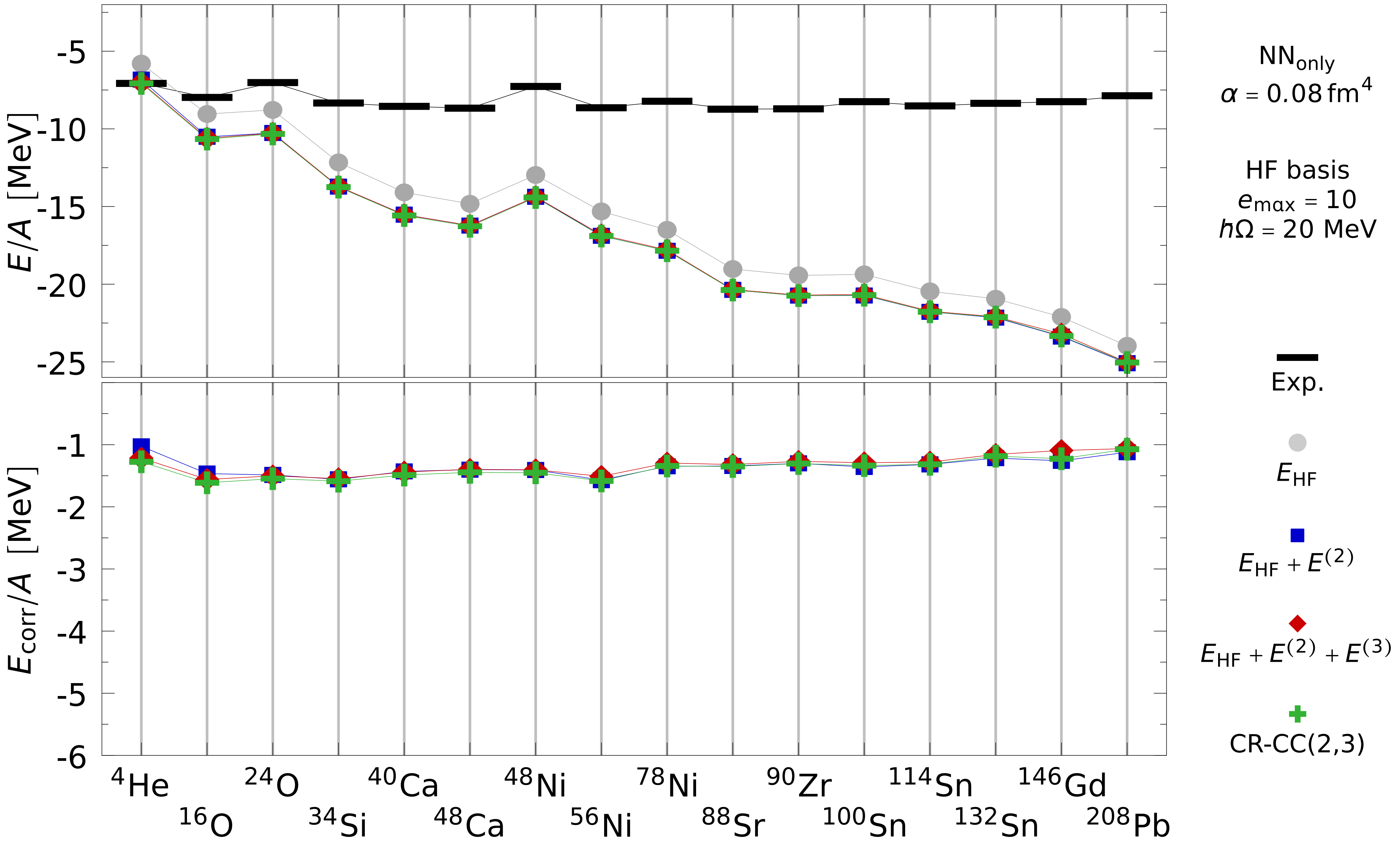
MBPT Convergence Heuristics

- in many cases partial sums **do not converge**, but there are systematic exceptions
- factors causing the non-convergence
  - **unperturbed basis** (partitioning) is the primary factor
  - **softness of the interaction** is a secondary factor
  - **many-body truncation** also has some influence
- **Padé resummation** robustly provides convergence at intermediate orders and agrees with exact diagonalization
- **can we rely on low-order MBPT ?**

Low-Order MBPT



Low-Order MBPT vs. Coupled-Cluster



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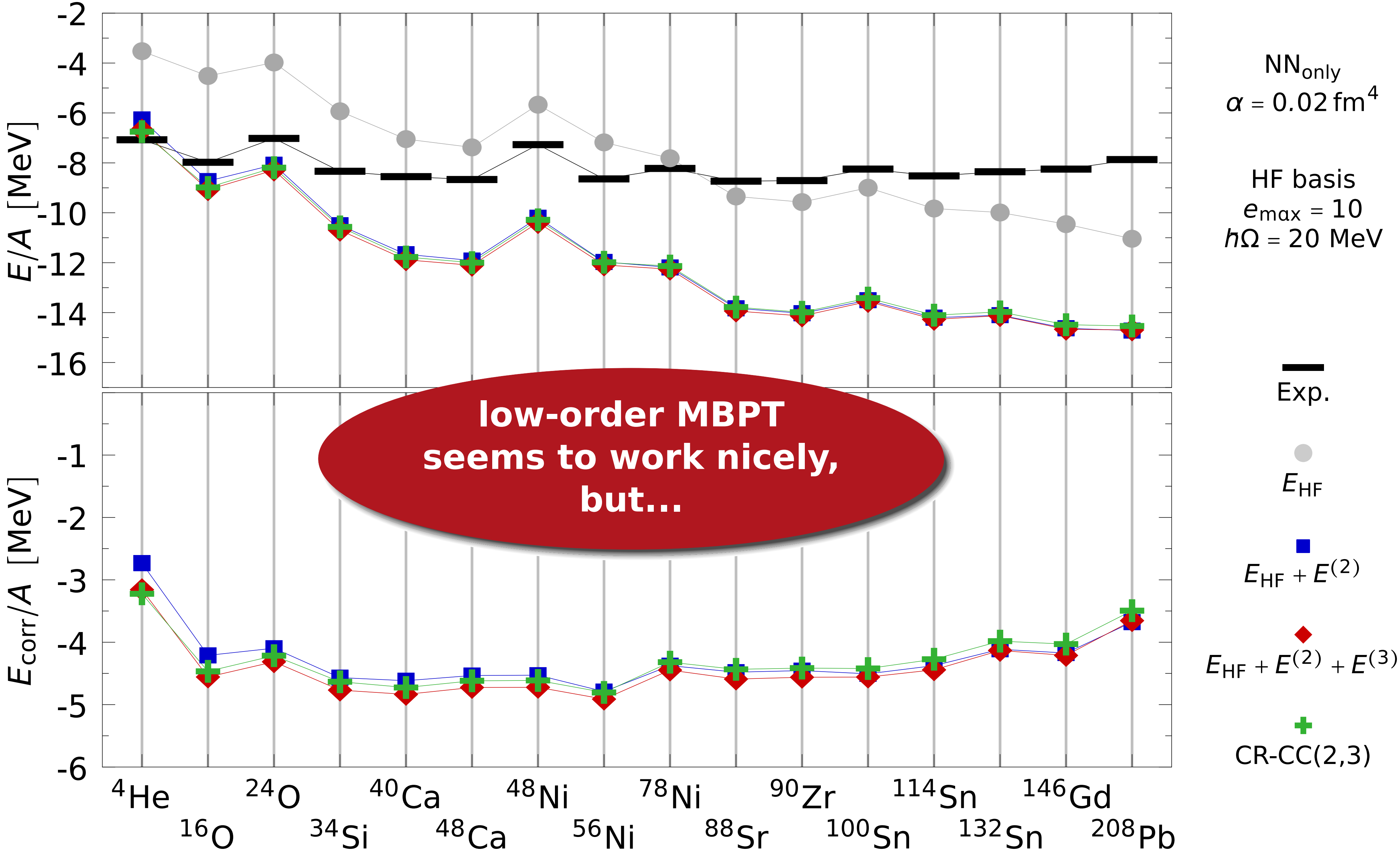
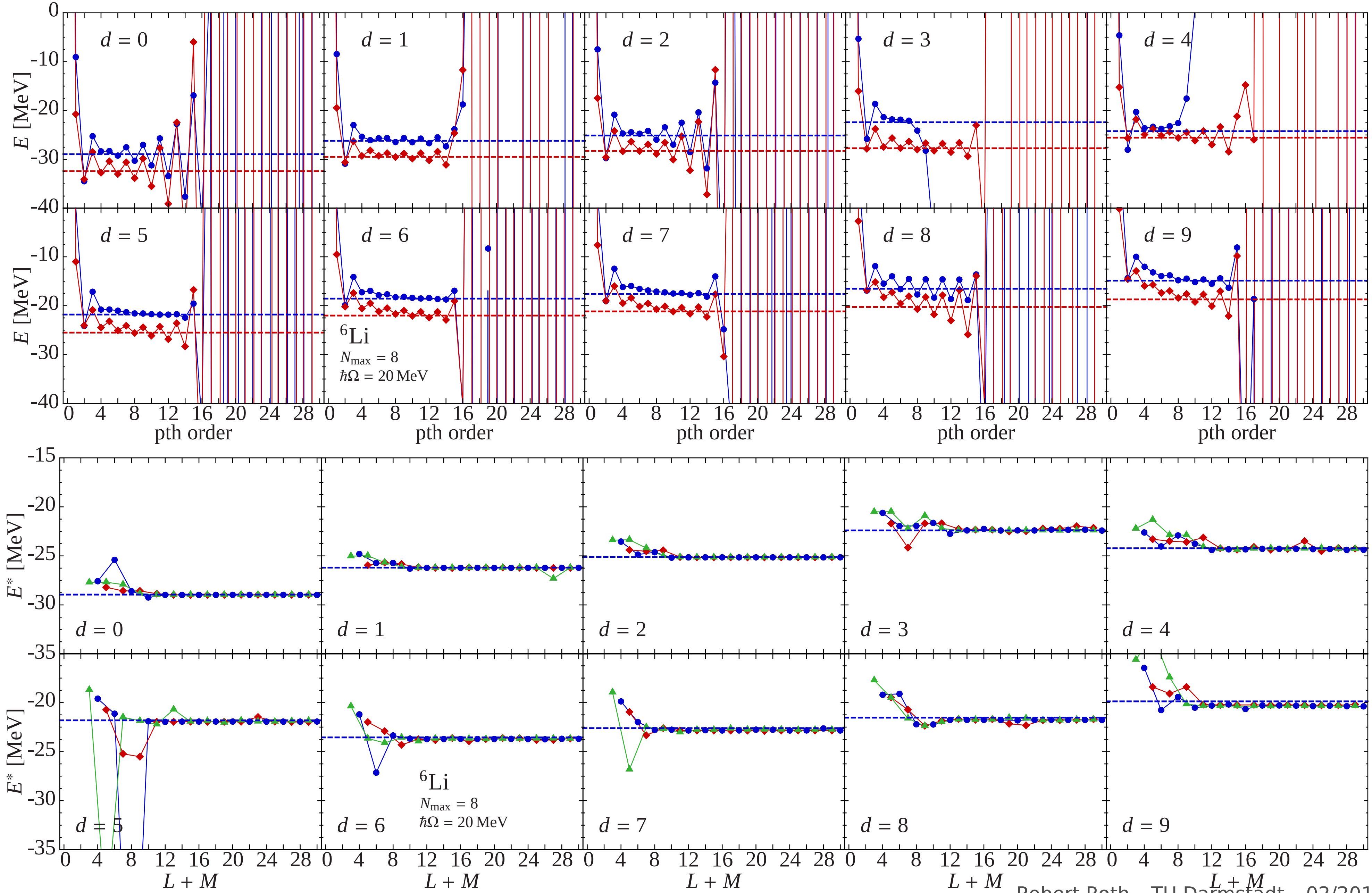


low-order MBPT seems to work nicely, but...

Perspectives: Degenerate MBPT

PRC 86, 054315 (2012), PLB 683, 272 (2010)



Epilogue

- **thanks to my group & my collaborators**
  - S. Binder, J. Braun, A. Calci, S. Fischer, E. Gebrerufael, H. Spiess, J. Langhammer, S. Schulz, C. Stumpf, A. Tichai, R. Trippel, R. Wirth, K. Vobig
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    Iowa State University, USA
  - S. Quaglioni, G. Hupin
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert
    Ohio State University, USA
  - P. Papakonstantinou
    IBS/RISP, Korea
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

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DFG
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