Ab Initio Spectroscopy of Open-Shell Medium-Mass Nuclei: Merging NCSM and In-Medium SRG

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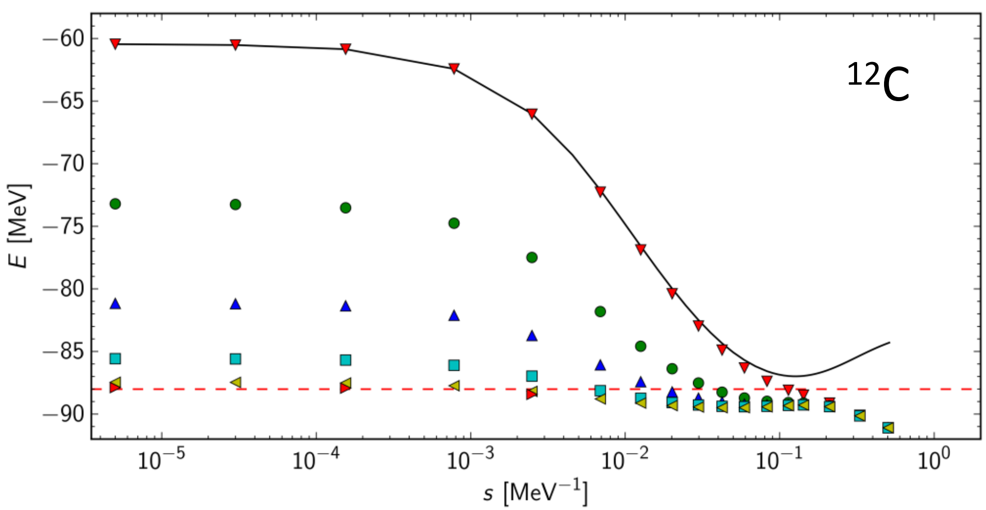

Motivation

Why should we merge NCSM and IM-SRG?

NCSM

- limited to light nuclei
- factorial growth of model space
- computationally demanding
- difficult to obtain model-space convergence

+ exact method
+ easy access to excited states
+ spectroscopy for free
+ no limitation to even nuclei

IM-SRG

+ easy access to heavy nuclei
+ soft computational scaling with *A*
+ computationally very efficient
+ decoupling in *A*-body space

- not exact method
- only for ground state
- spectroscopy not straight-forward
- spherical formulation limits to even nuclei

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Overview

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- No-Core Shell Model (NCSM)
- In-Medium Similarity Renormalization Group (IM-SRG)
- Novel Approach: NCSM+IM-SRG
- Results
  - Flow of Ground-State Energy
  - Flow of Excitation Energies
  - Spectra
- Summary and Outlook

Barrett, Vary, Navratil, ...

one of the most powerful
universal exact ab initio methods
for the p- and lower sd-shell

- construct matrix representation of Hamiltonian using **basis of HO Slater determinants** truncated w.r.t. HO excitation quanta N_{max}
- solve **large-scale eigenvalue problem** for a few smallest eigenvalues
- range of applicability limited by **factorial growth** of basis with N_{max} & A
- adaptive **importance-truncation** extends the range of NCSM by reducing the model space to physically relevant states

In-Medium Similarity Renormalization Group
Basics

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Tsukiyama, Bogner, Schwenk, Hergert,..

use flow eqn. for
normal-ordered Hamiltonian to decouple
the **reference state** from excitations

- flow equation for Hamiltonian: $\frac{\mathrm{d}}{\mathrm{d}s} H(s) = [\eta(s), H(s)]$ with flow parameter *s*
- *H* in normal order w.r.t. to a given reference state $|\Psi\rangle$
  [Kutzelnigg, Mukherjee]

$$H(s) = E(s) + \sum f^{\circ}_{\circ}(s)\tilde{a}^{\circ}_{\circ} + \frac{1}{4}\sum \Gamma^{\circ\circ}_{\circ\circ}(s)\tilde{a}^{\circ\circ}_{\circ\circ} + \frac{1}{36}\sum W^{\circ\circ\circ}_{\circ\circ\circ}(s)\tilde{a}^{\circ\circ\circ}_{\circ\circ\circ}$$

- Note: $\langle\Psi|H(s)|\Psi\rangle = E(s)$
- choose generator $\eta(s)$ to achieve desired behaviour:
  use the numerically stable Imaginary Time [Morris, Bogner]

Novel Approach: NCSM+IM-SRG
Procedure

- pick interaction and nucleus
- solve NCSM problem in small N_{max}=0
- take first 0^+ (often ground-state) as reference state

↓ compute density matrices and (multi-ref.) normal-ordered Hamiltonian

- solve (multi-ref.) IM-SRG flow equation
- spherical formulation limited to scalar densities for now

↓ extract evolved Hamiltonian in vacuum representation

↓ consistently evolve secondary operator H_{cm}

- NCSM calculation for ground-state energy
- NCSM calculation for excitation energies

Hamilton Matrix in *A*-Body Basis: Calculation Details

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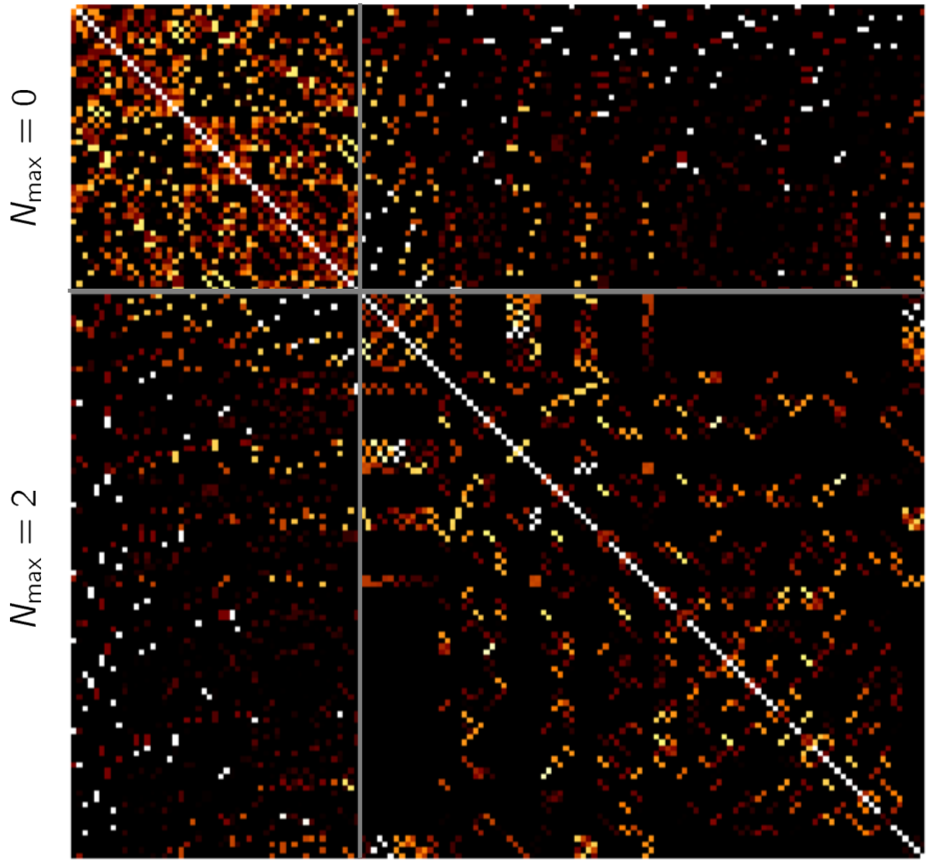
- standard chiral NN @ N^3LO from Entem and Machleidt
  + 3N @ N^2LO from Navratil
- reduced 3N cutoff $\Lambda_{3N} = 400\,\text{MeV}$
- free-space SRG $\alpha = 0.08\,\text{fm}^4$
- harmonic-oscillator parameter $\hbar\Omega = 20\,\text{MeV}$

- IM-SRG performed using **Imaginary Time**
- reference state is first 0^+ state in $N_{\text{max}}^{\text{ref}} = 0$

Novel Approach: NCSM+IM-SRG
Hamilton Matrix in *A*-Body Basis: ^{12}C

$s = 0.00$



N_{max}=0
Slater determinants

N_{max}=2
Slater determinants

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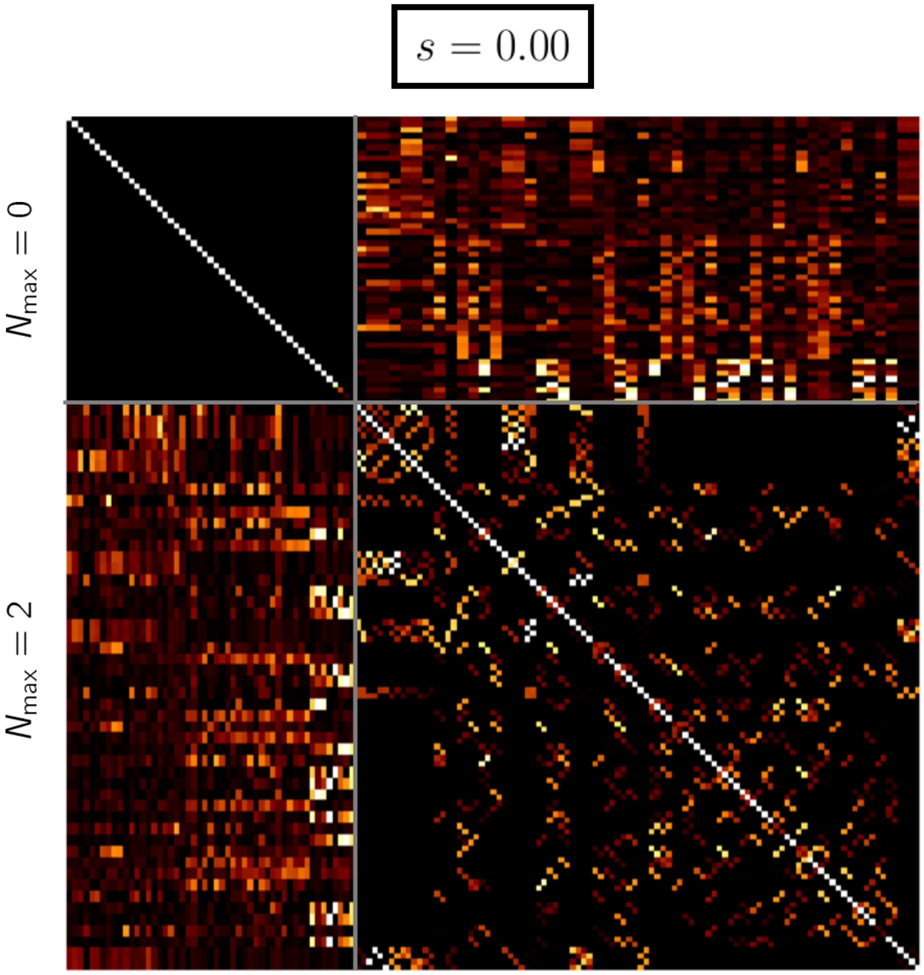

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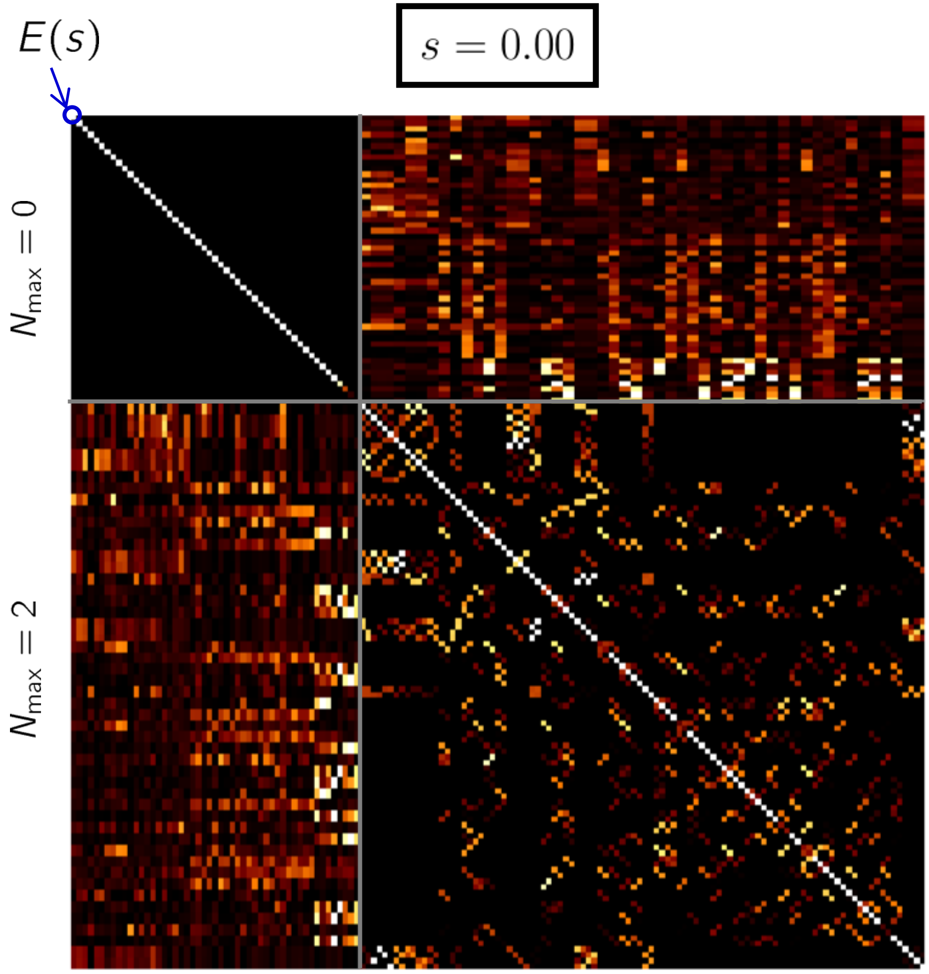

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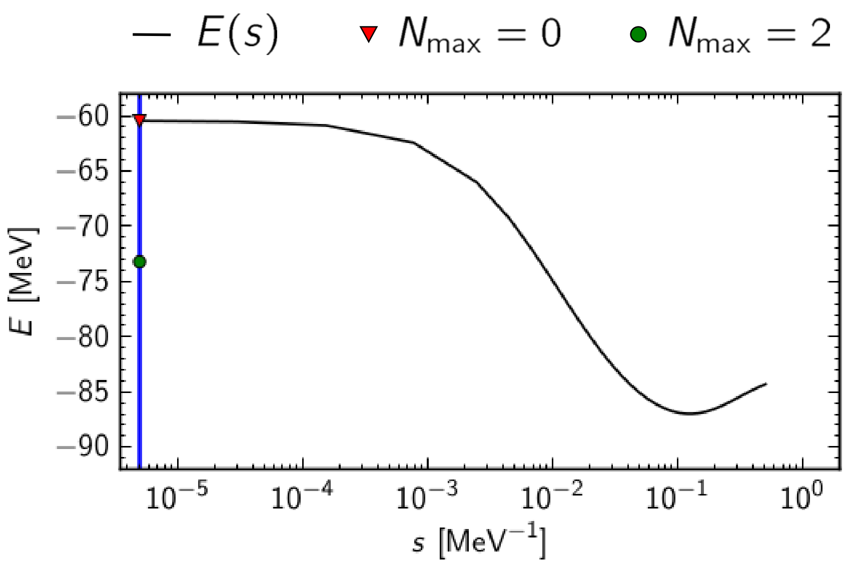

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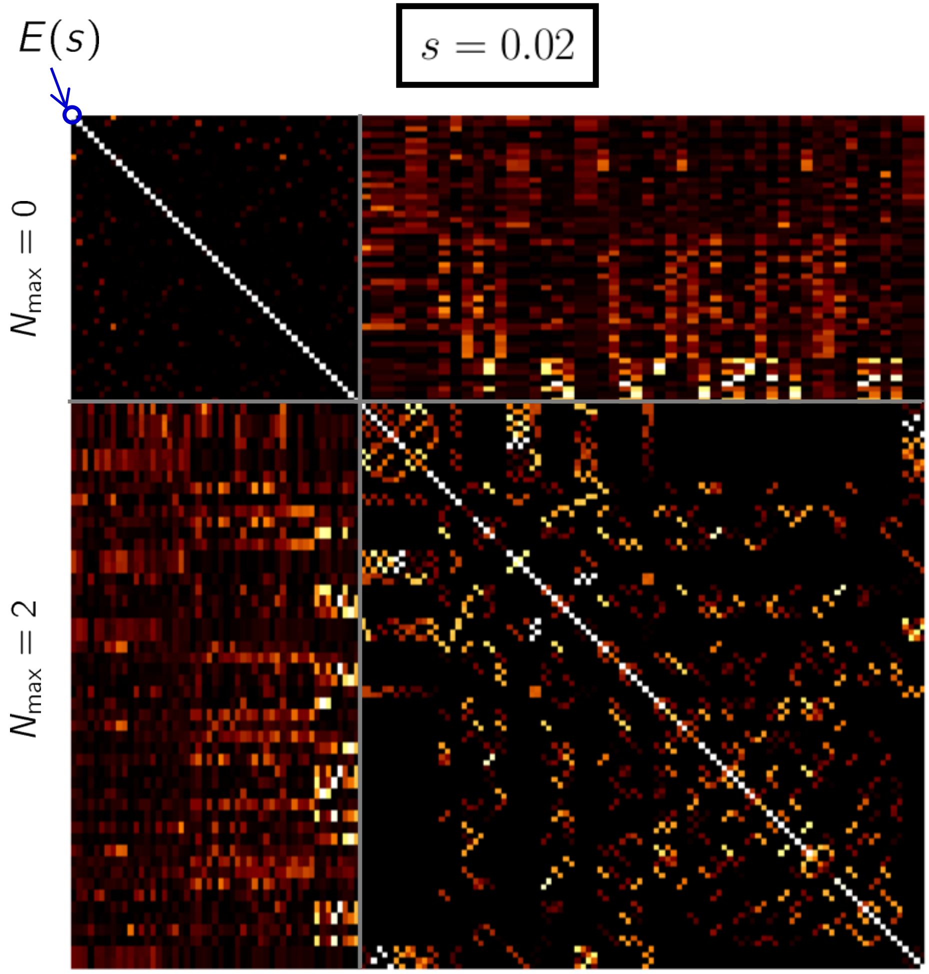

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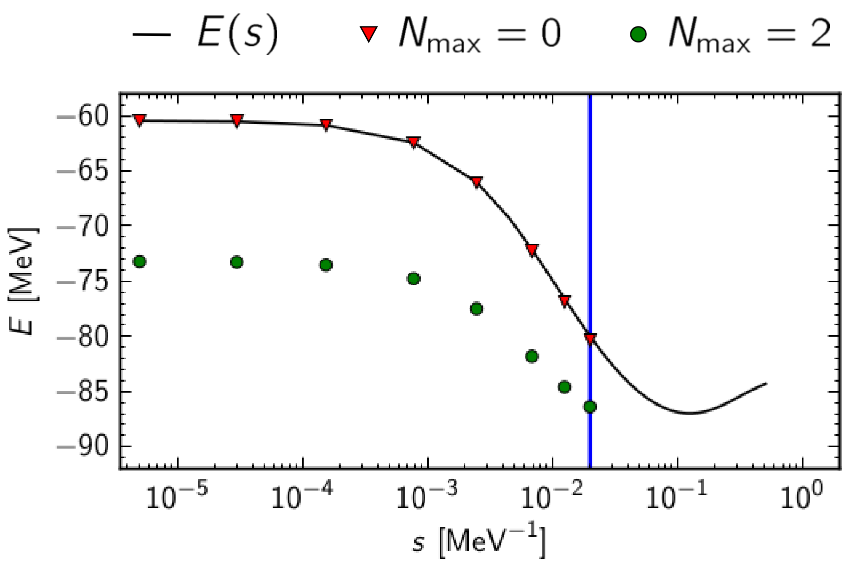

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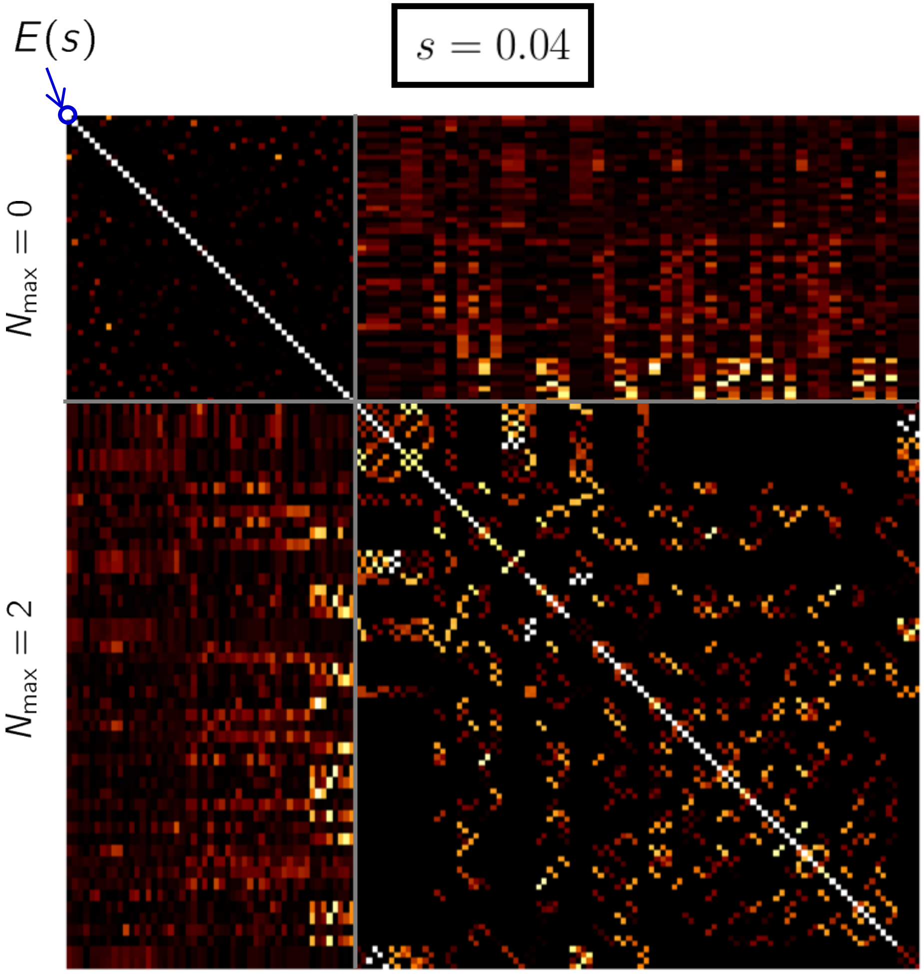

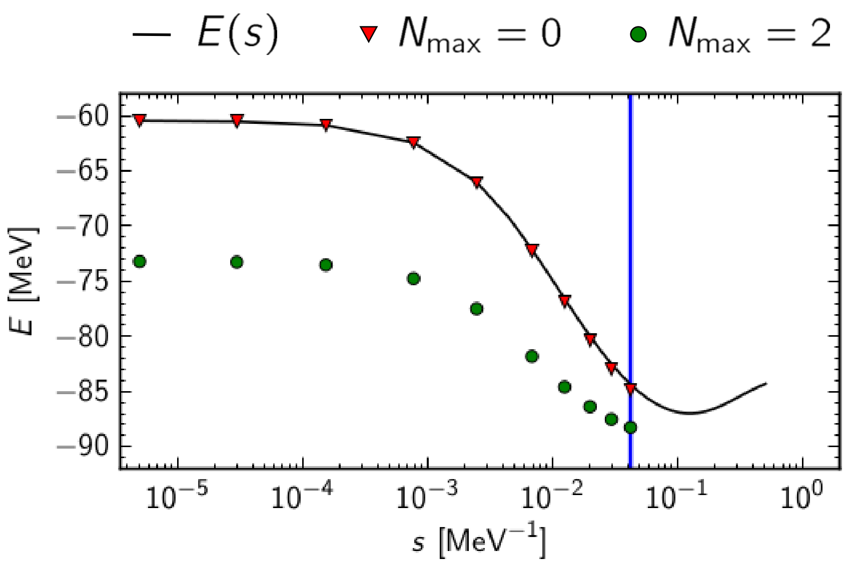

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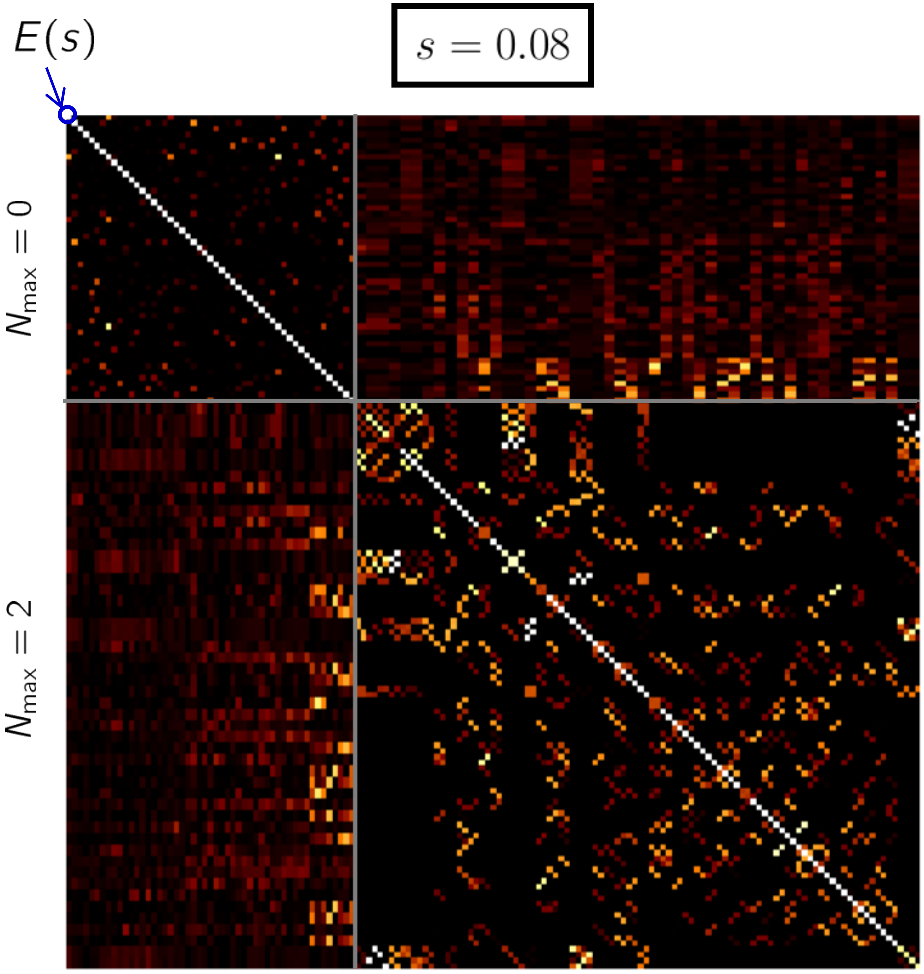

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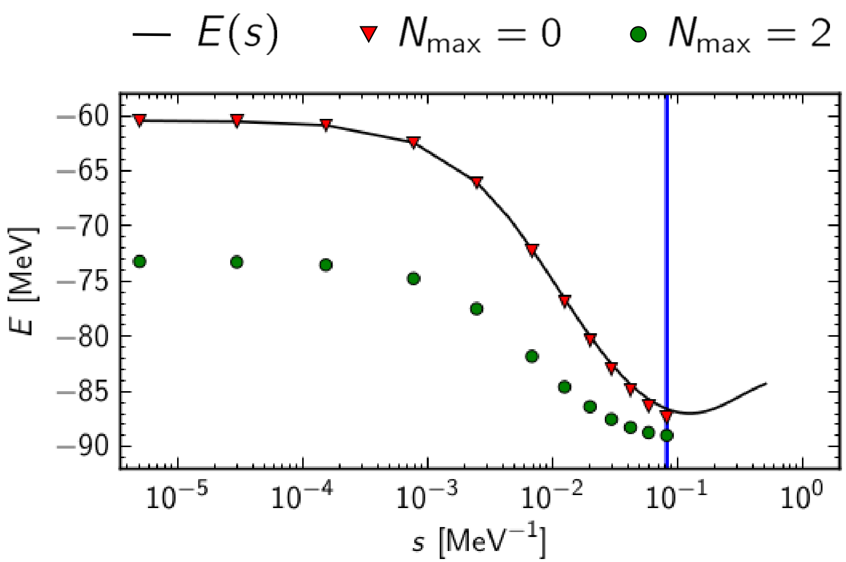

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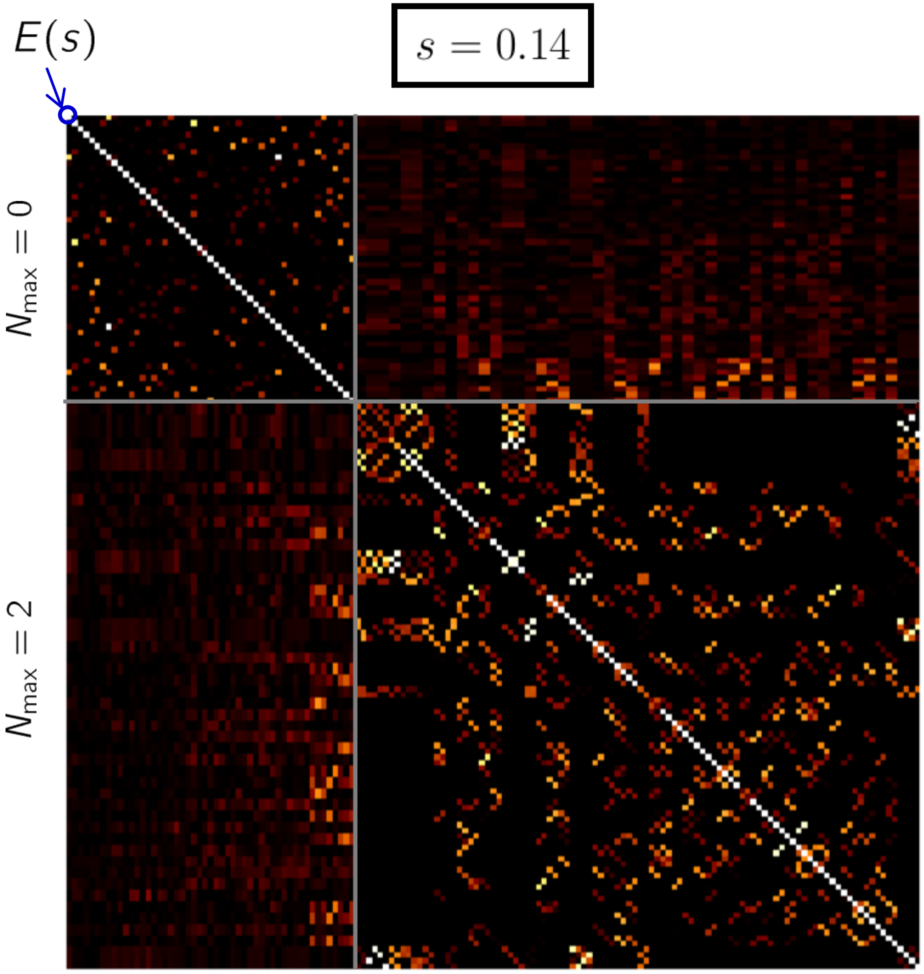

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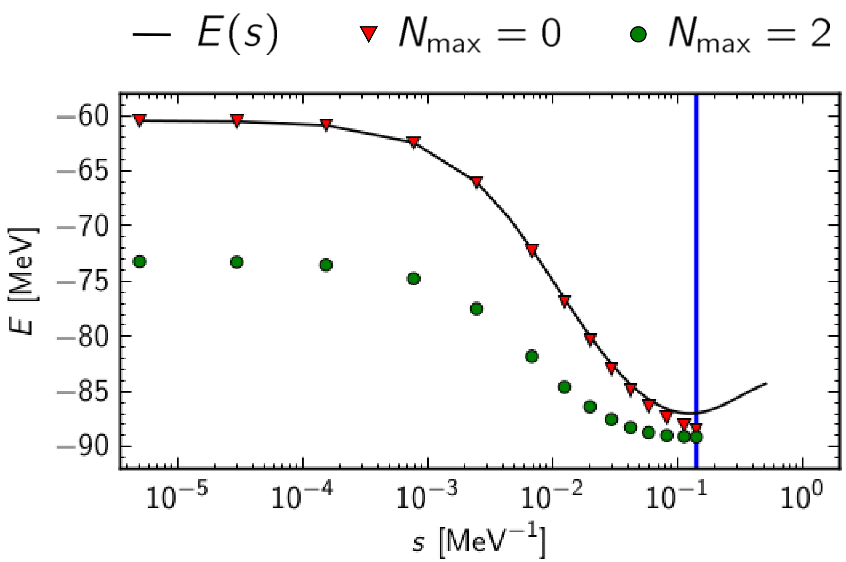

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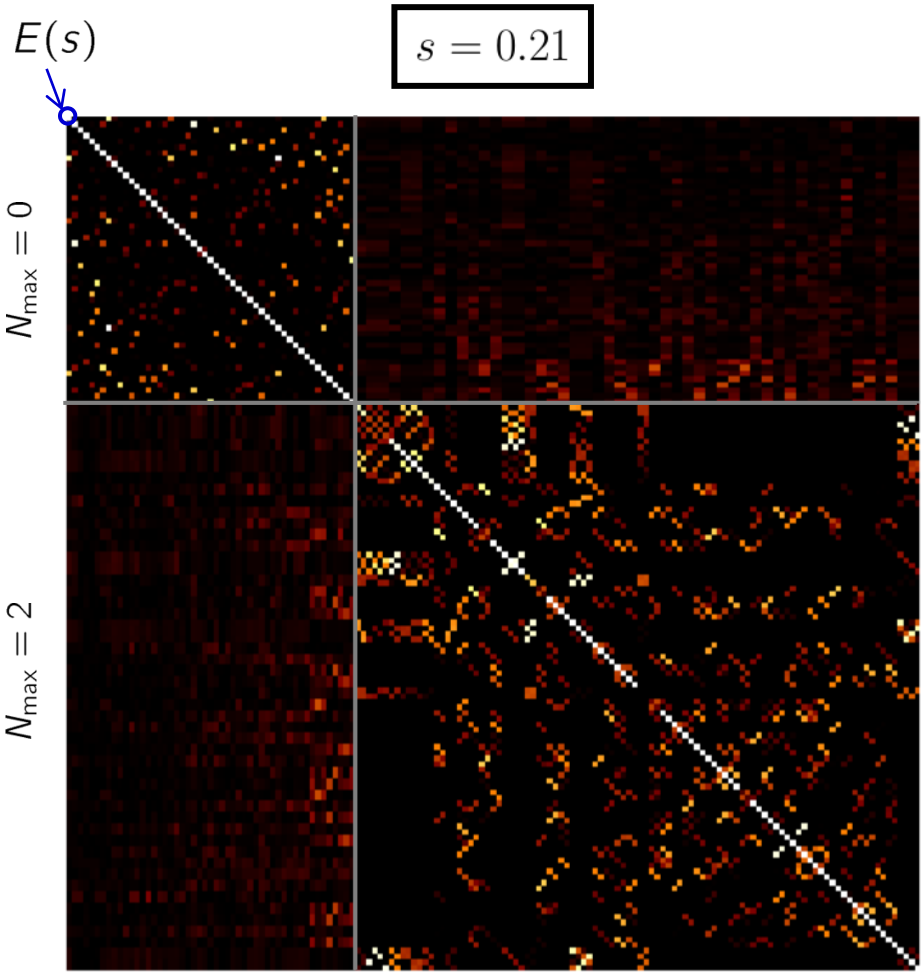

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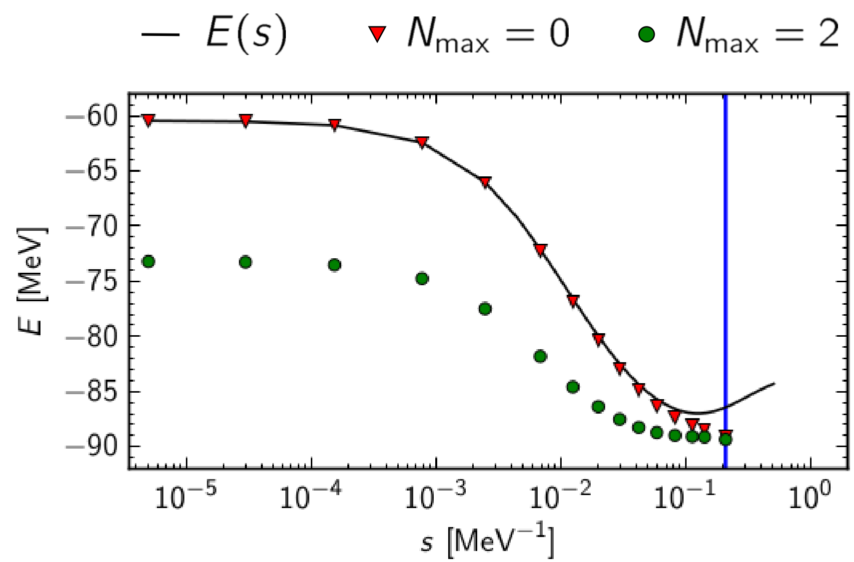

Novel Approach: NCSM+IM-SRG

Hamilton Matrix in *A*-Body Basis: ^{12}C

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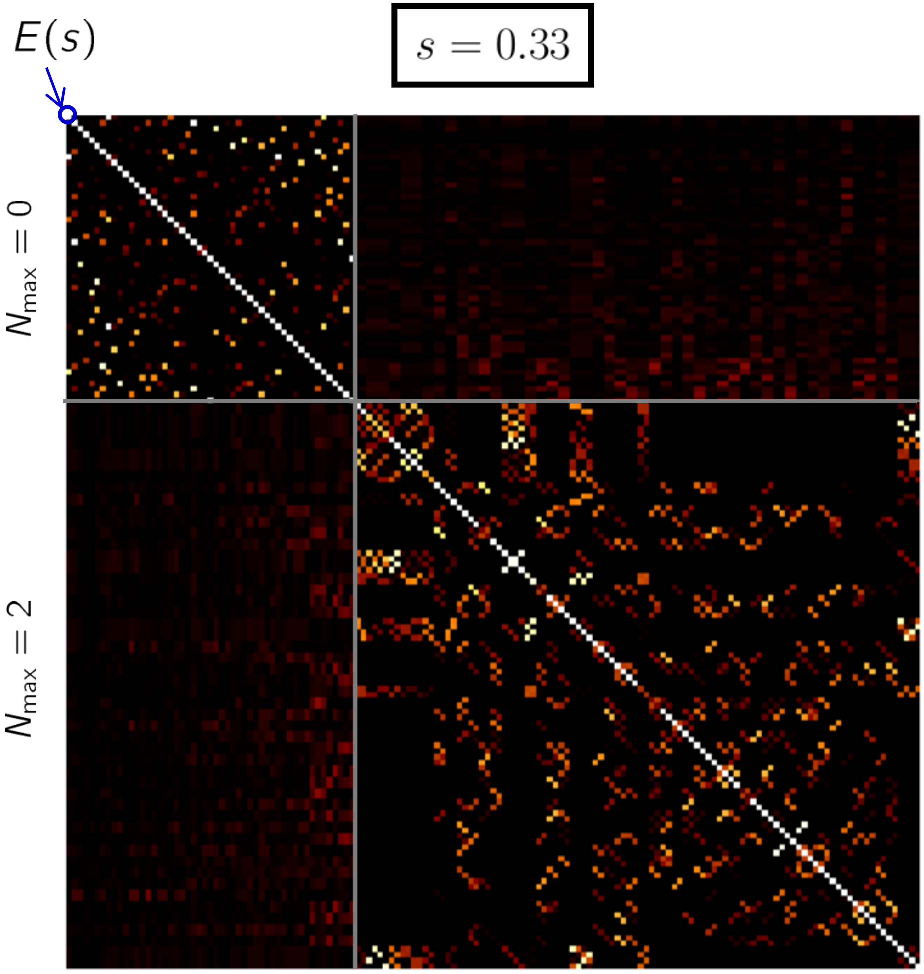
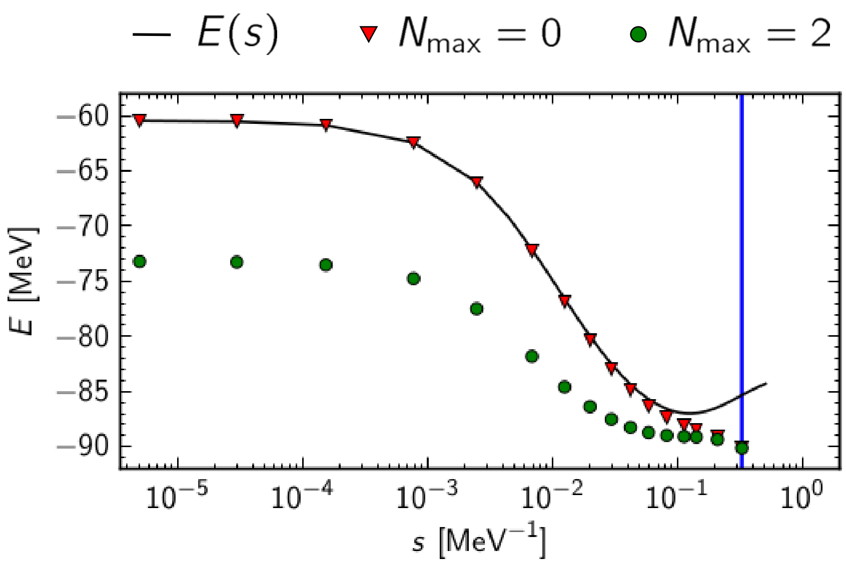
$s = 0.33$



N_{max}=0 **eigenstates**

N_{max}=2 Slater determinants



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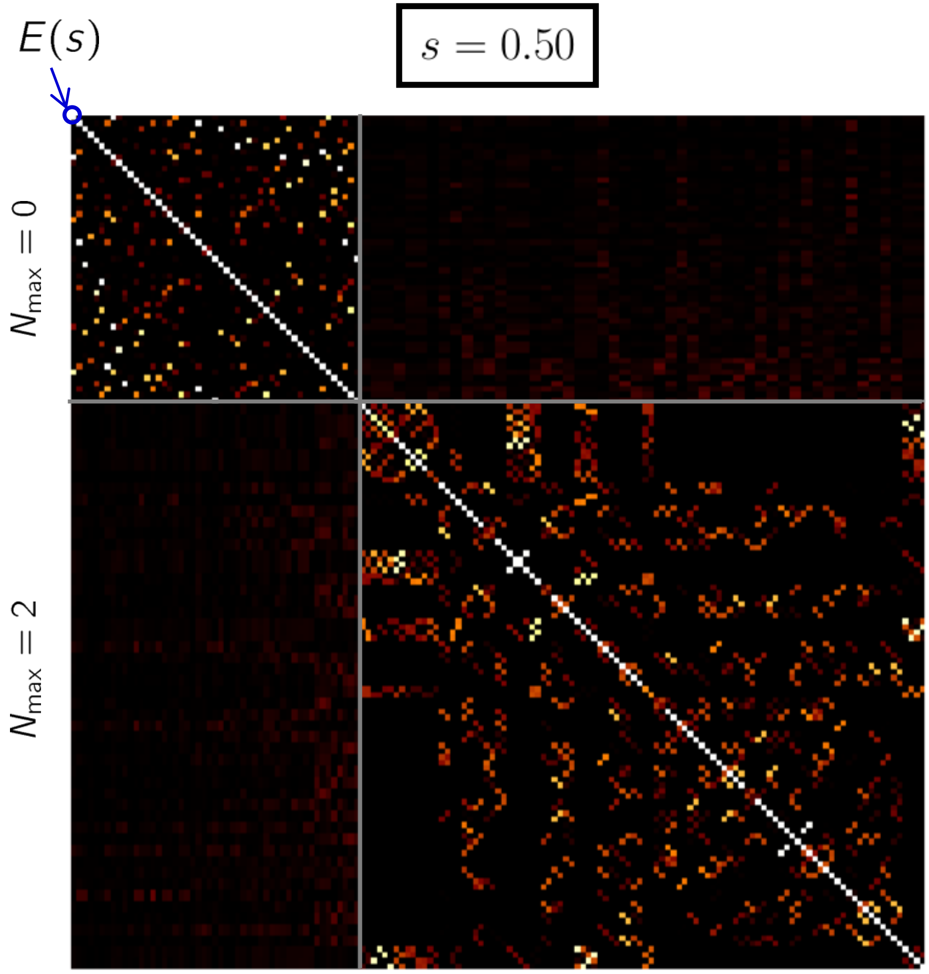

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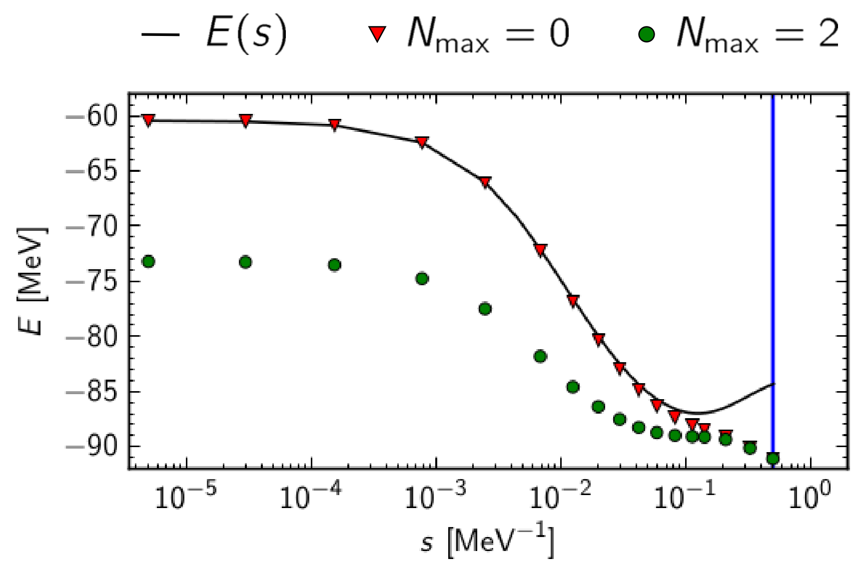
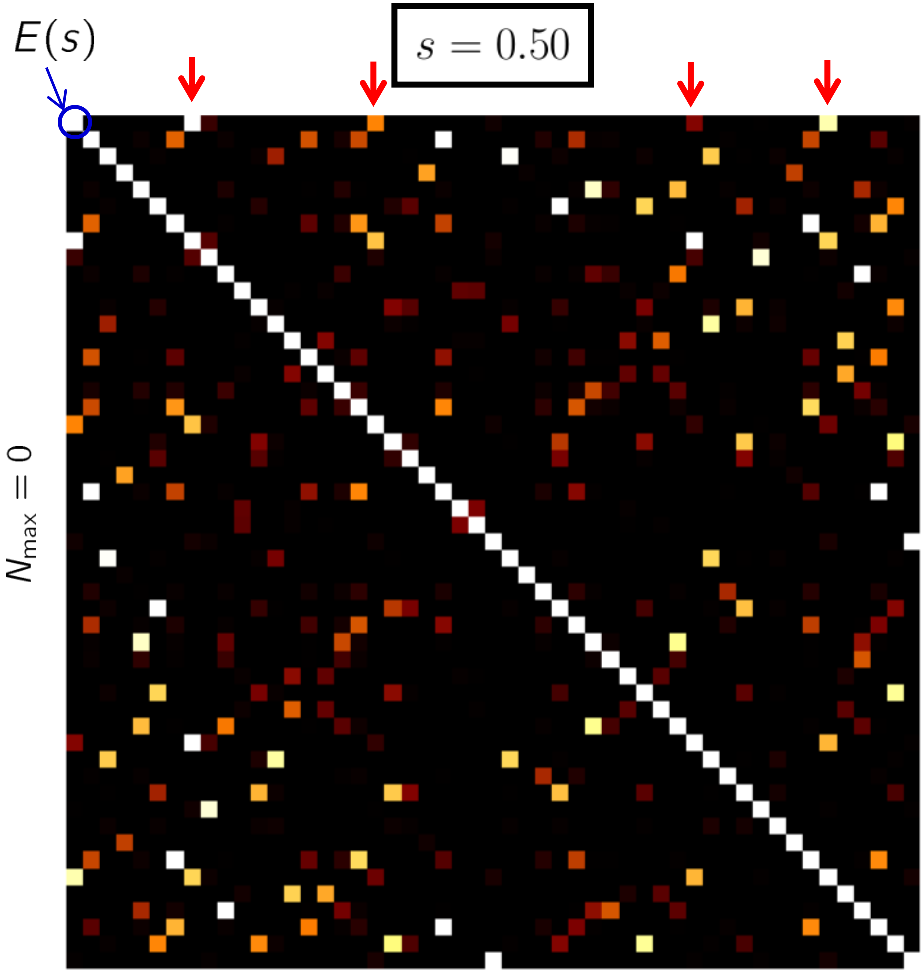


for large enough flow parameter eigenvalues in N_{max}=0 and N_{max}=2 equal

IM-SRG decouples reference state (not only) from N_{max} =2 space

--> why differ *E*(s) and N_{max}=0 eigenvalue?

Hamilton Matrix in *A*-Body Basis: ^{12}C



N_{max}=0 eigenstates

← first basis state = reference state

- reference state couples to N_{max}=0 eigenstates
- E(s) and N_{max}=0 eigenvalue cannot be identical

diagonalization of evolved Hamiltonian necessary

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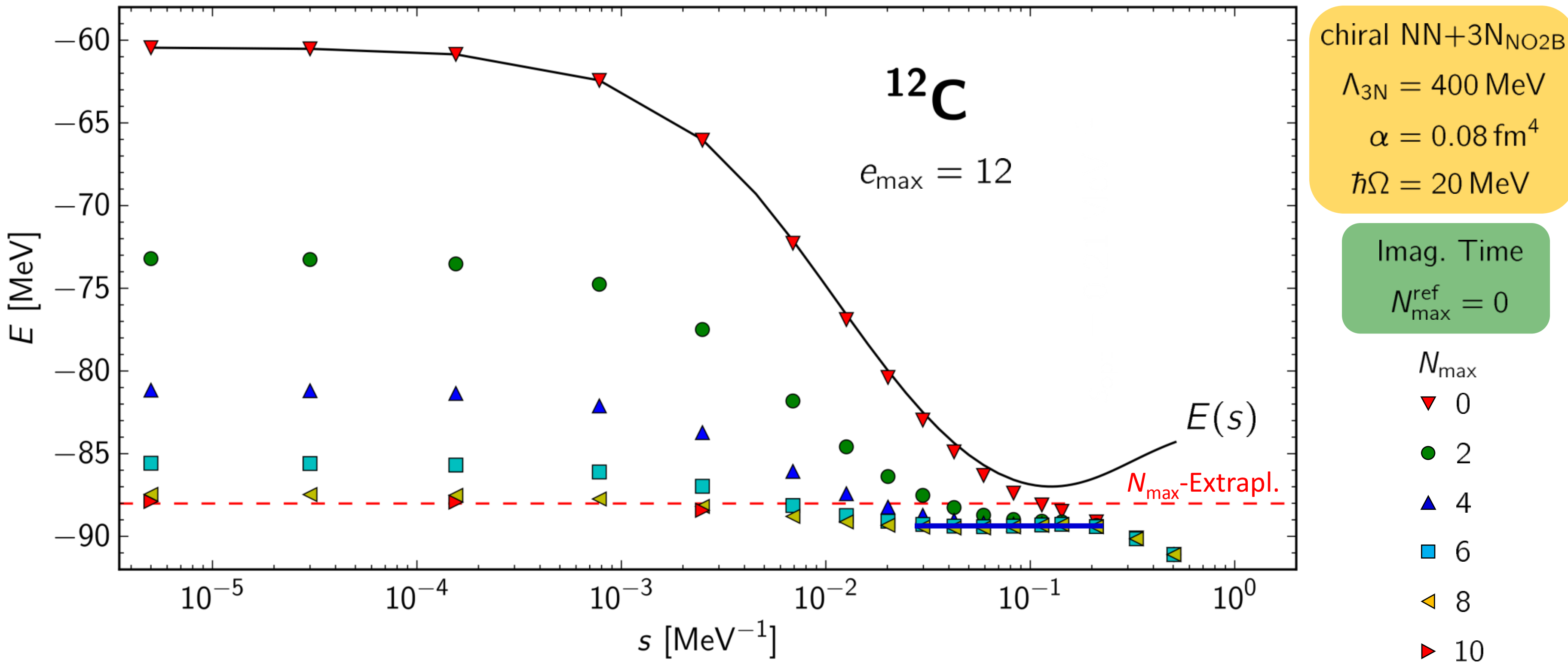
Results

Flow of Ground-State Energy



- $E(s)$ does not converge and has a minimum
- drastically enhanced model-space convergence for NCSM+IM-SRG
- induced many-body contribution 1.5 MeV less than 2 %

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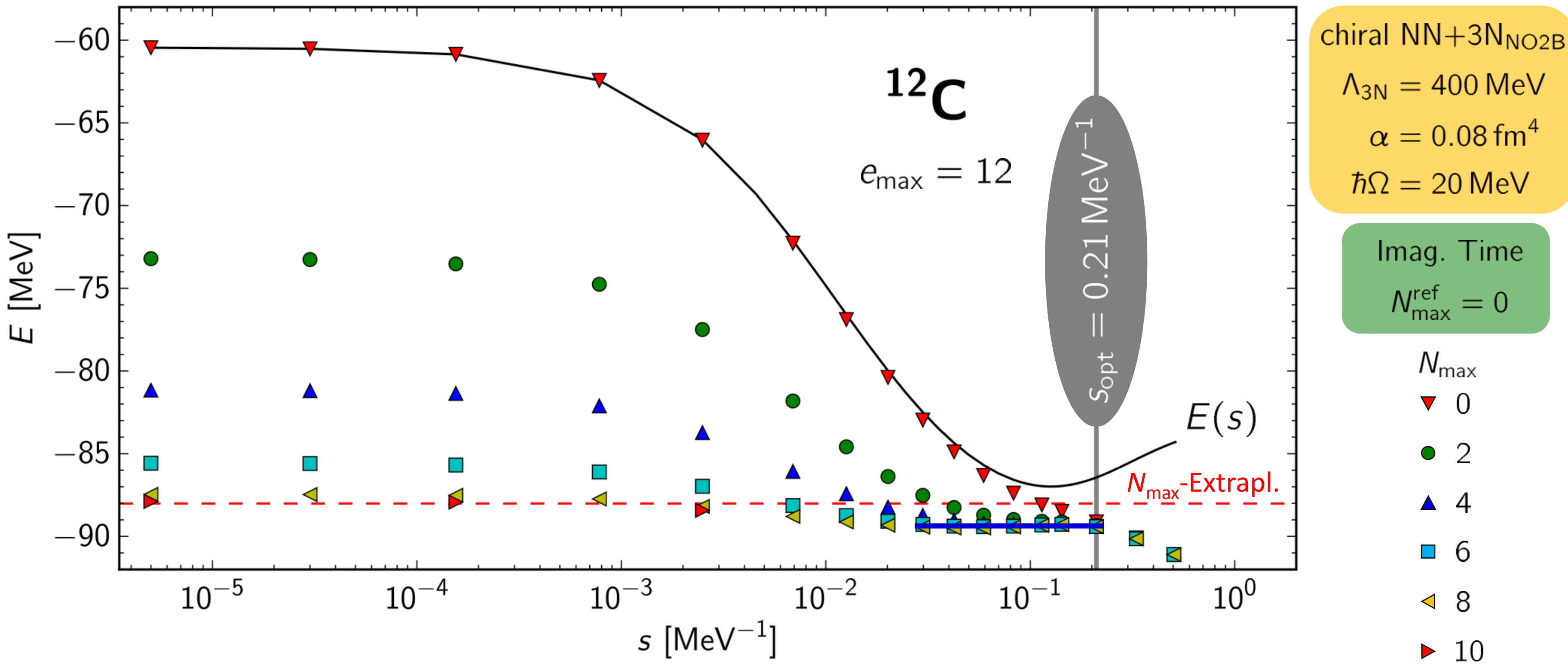

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- choice of s_{opt}: best N_{max} convergence and end of plateau region

Flow of Ground-State Energy

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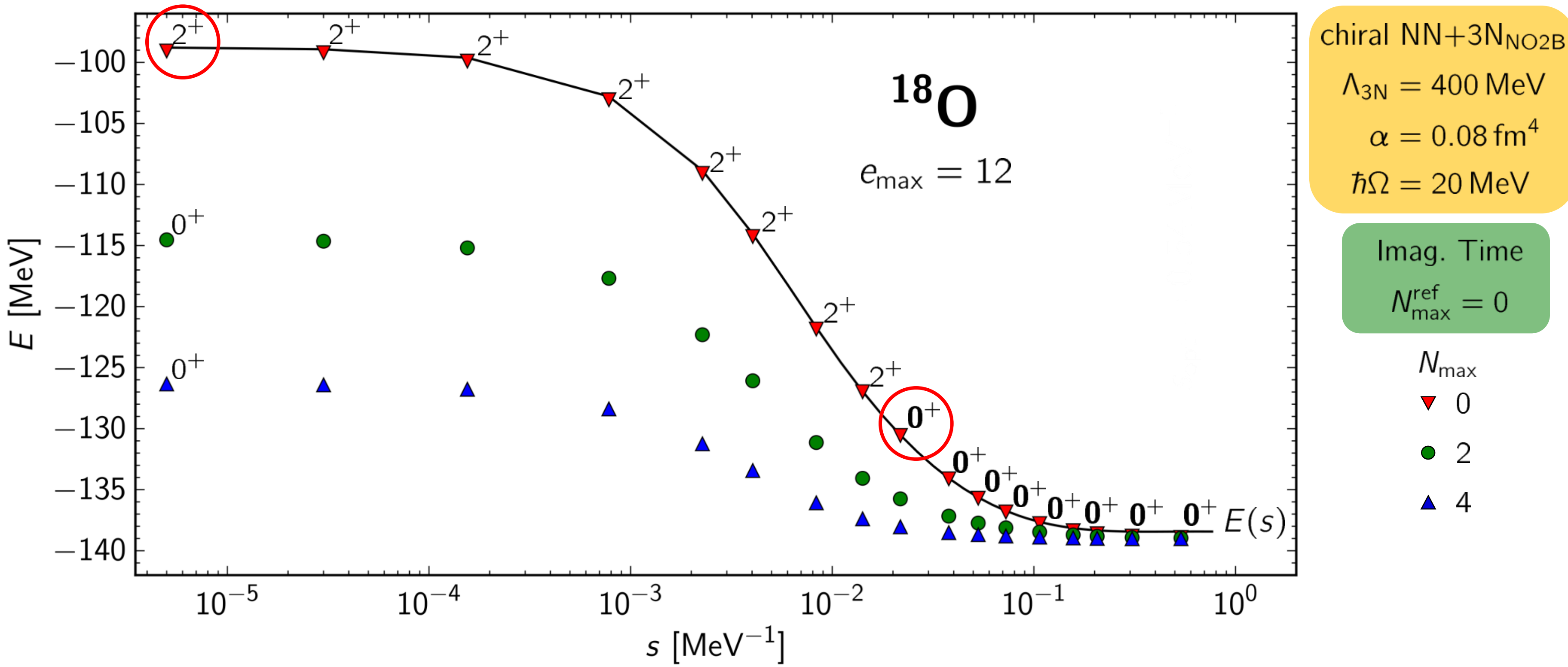

- initial Hamiltonian in N_{max}=0 wrongly predicts **2^+ ground state**, corrected in N_{max}=2
- reference state is **first 0^+** state in N_{max}=0 (**not** the ground state here)
- IM-SRG transforms more information into N_{max}=0
  - ground state correctly reproduced
  - feature: **level crossing** between 2^+ and 0^+

Flow of Ground-State Energy

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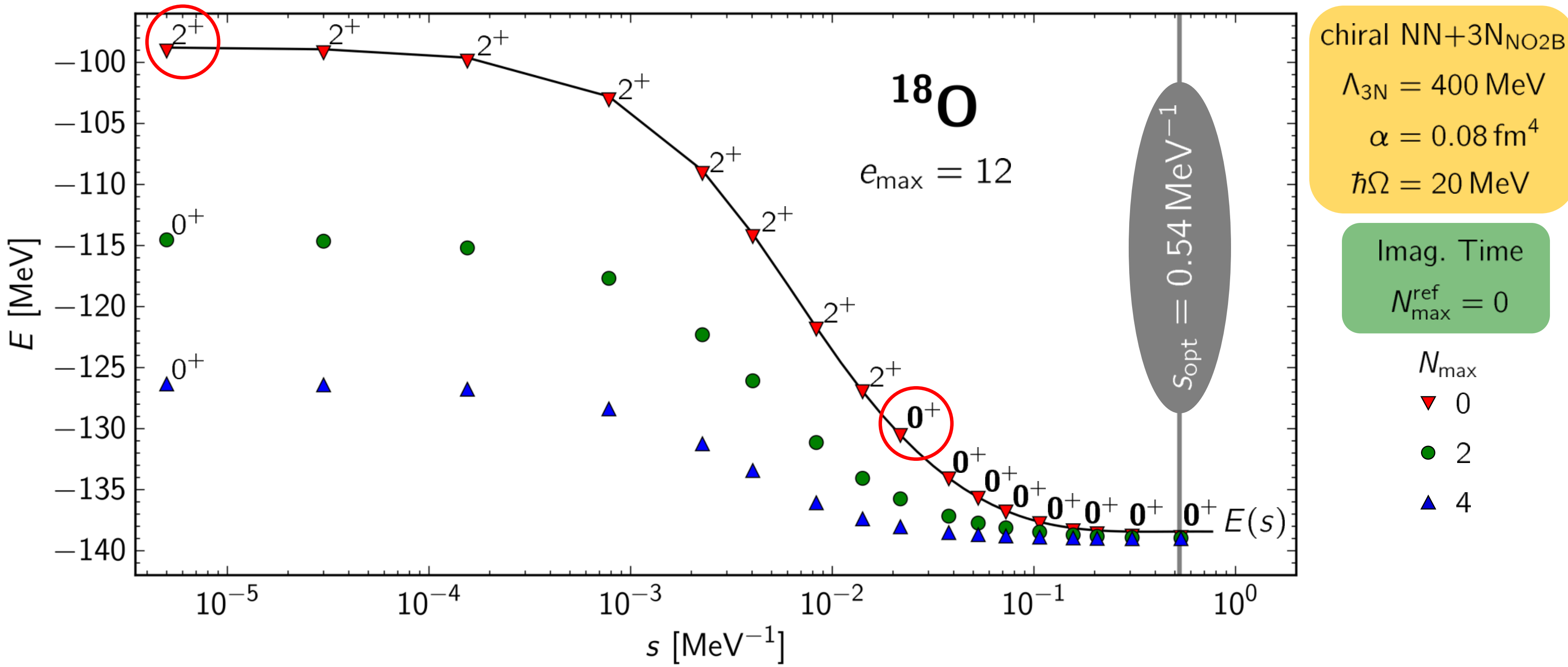

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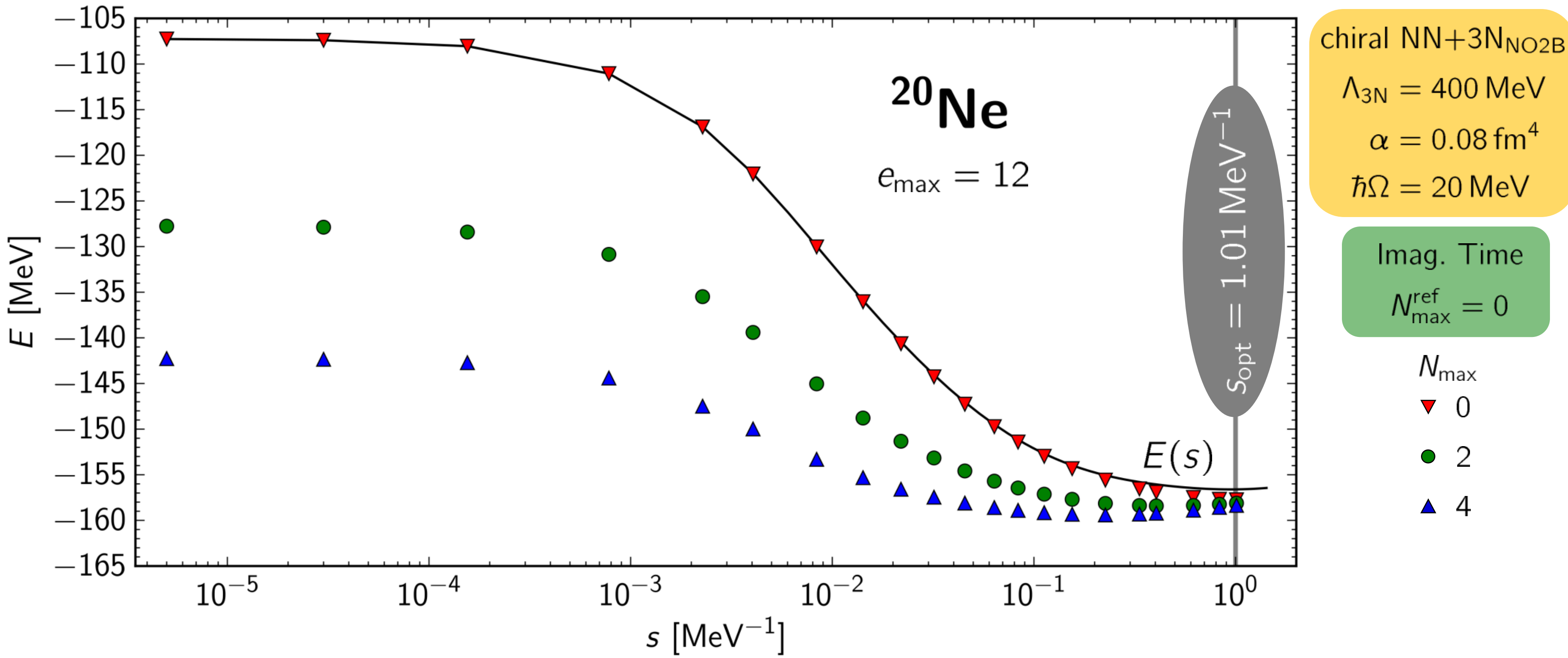

Results

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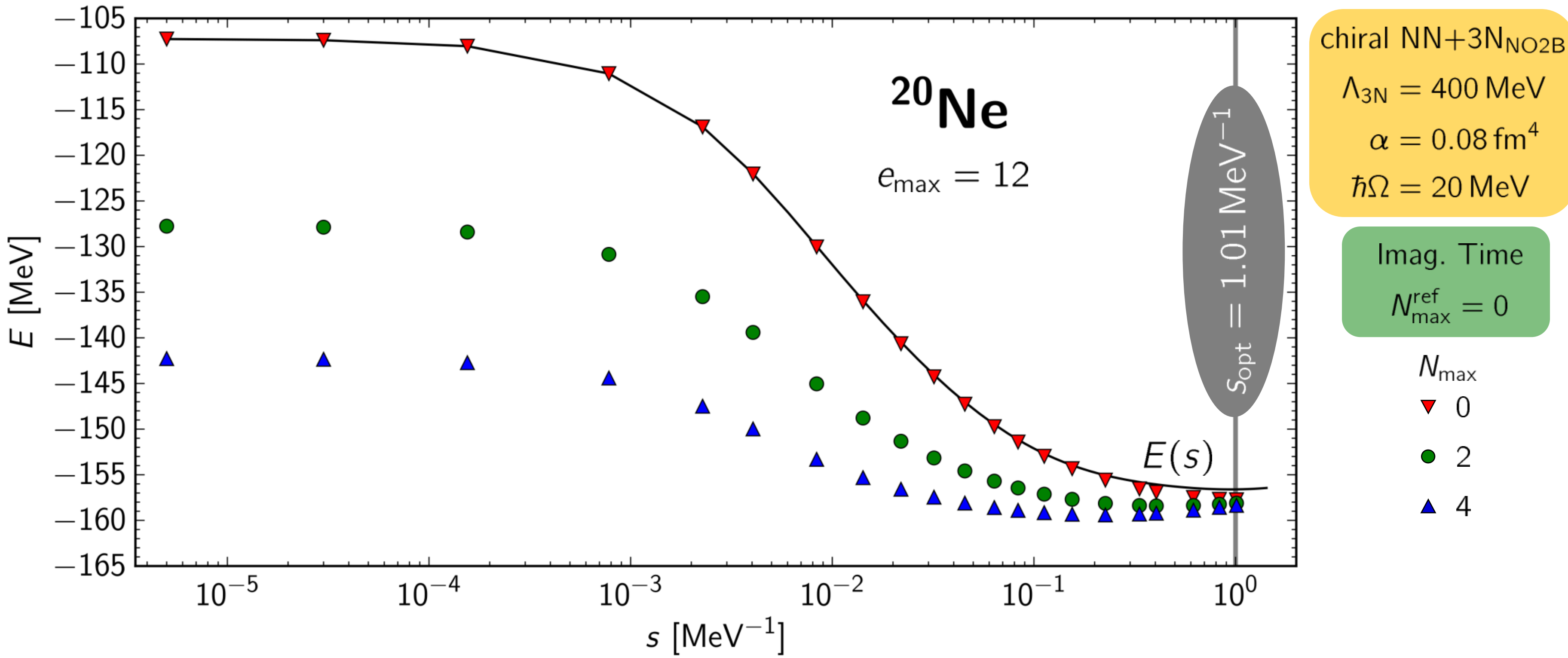

analyze effect of e_{max} truncation on ground-state energy

Flow of Ground-State Energy – e_{max} Convergence

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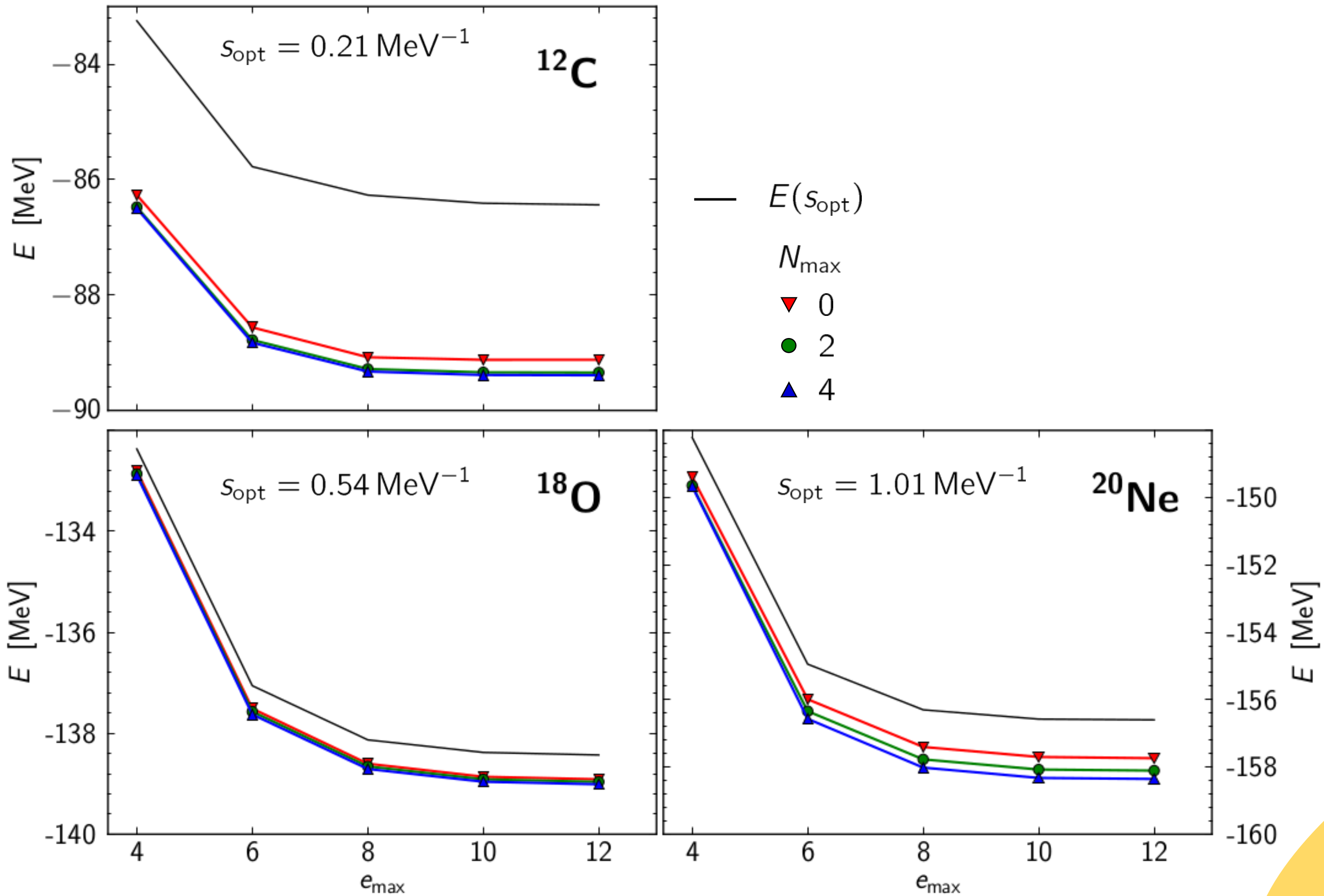


chiral NN+3N$_{NO2B}$

$\Lambda_{3N} = 400$ MeV

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

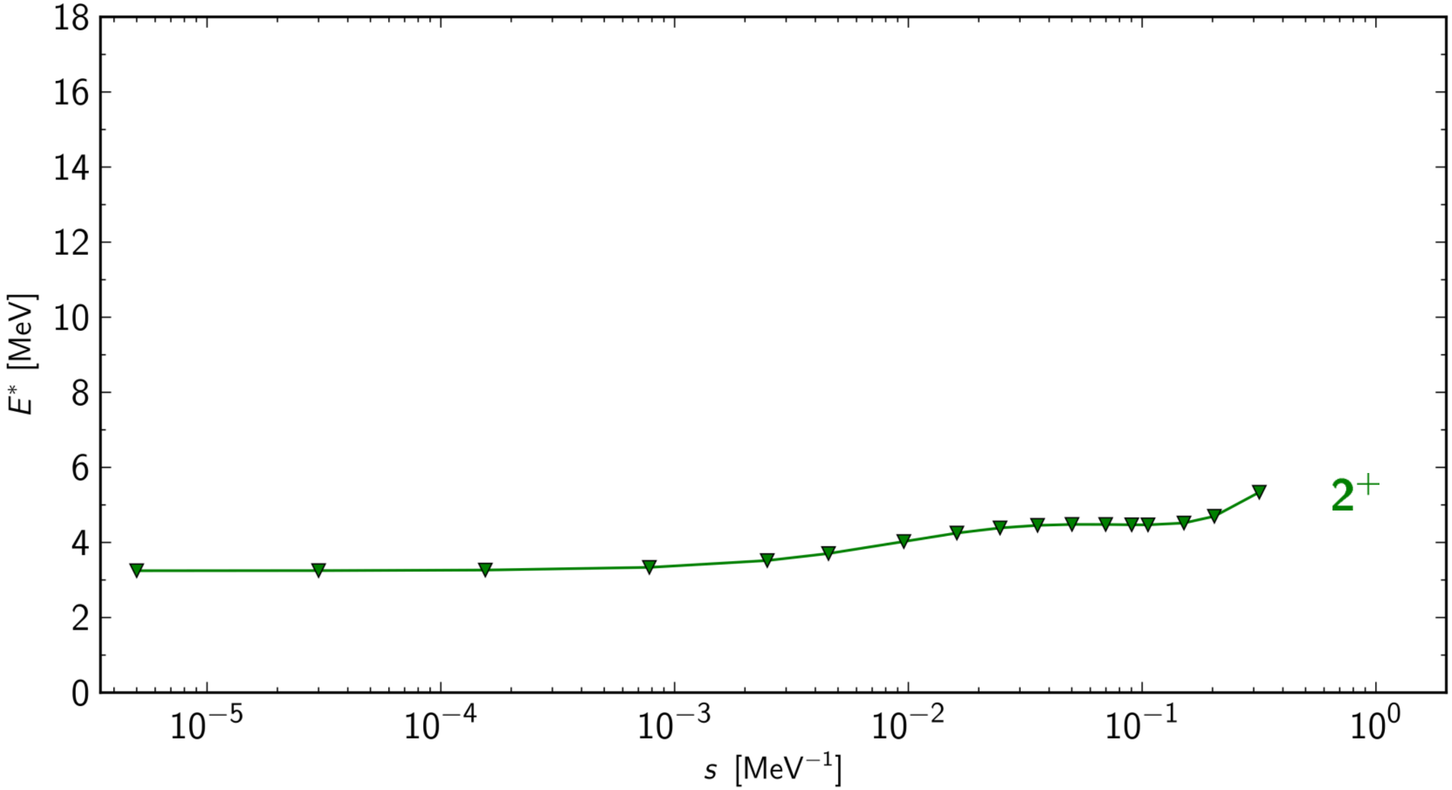
$\hbar\Omega = 20$ MeV

Imag. Time

$N_{max}^{ref} = 0$

e_{max}=12 sufficient

Flow of Excitation Energies



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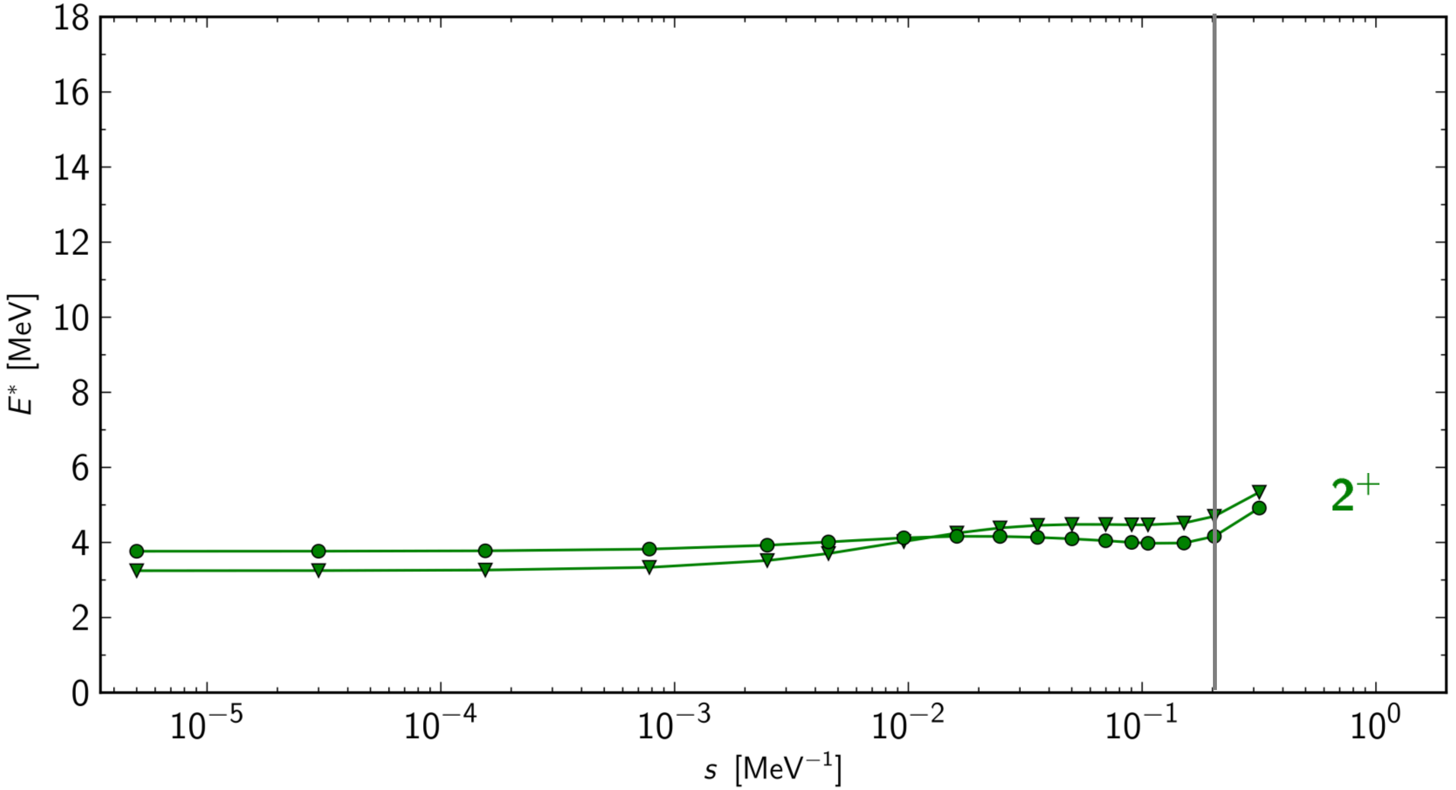
^{12}C
$e_{\max} = 12$
$\lambda_{\text{Hcm}} = 1$

$N_{\max}$
▽ 0
○ 2
△ 4
□ 6

- E^* of 2^+ increases abruptly at the end due kink in ground-state energy

Results
Flow of Excitation Energies



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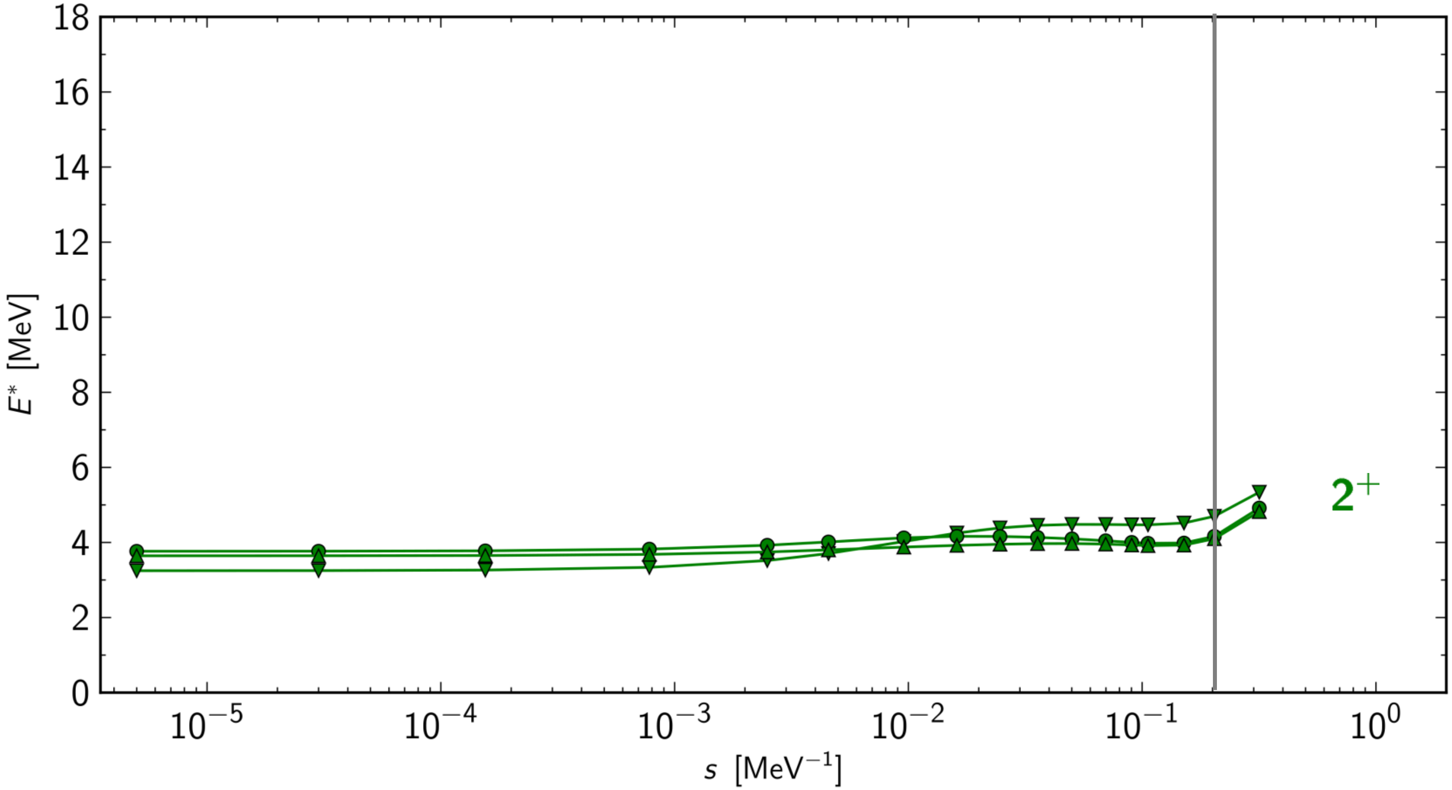
- new feature: E^* converges **monotonically from above** for evolved Hamiltonian (**variational principle** for **excitation energies**!)

Flow of Excitation Energies



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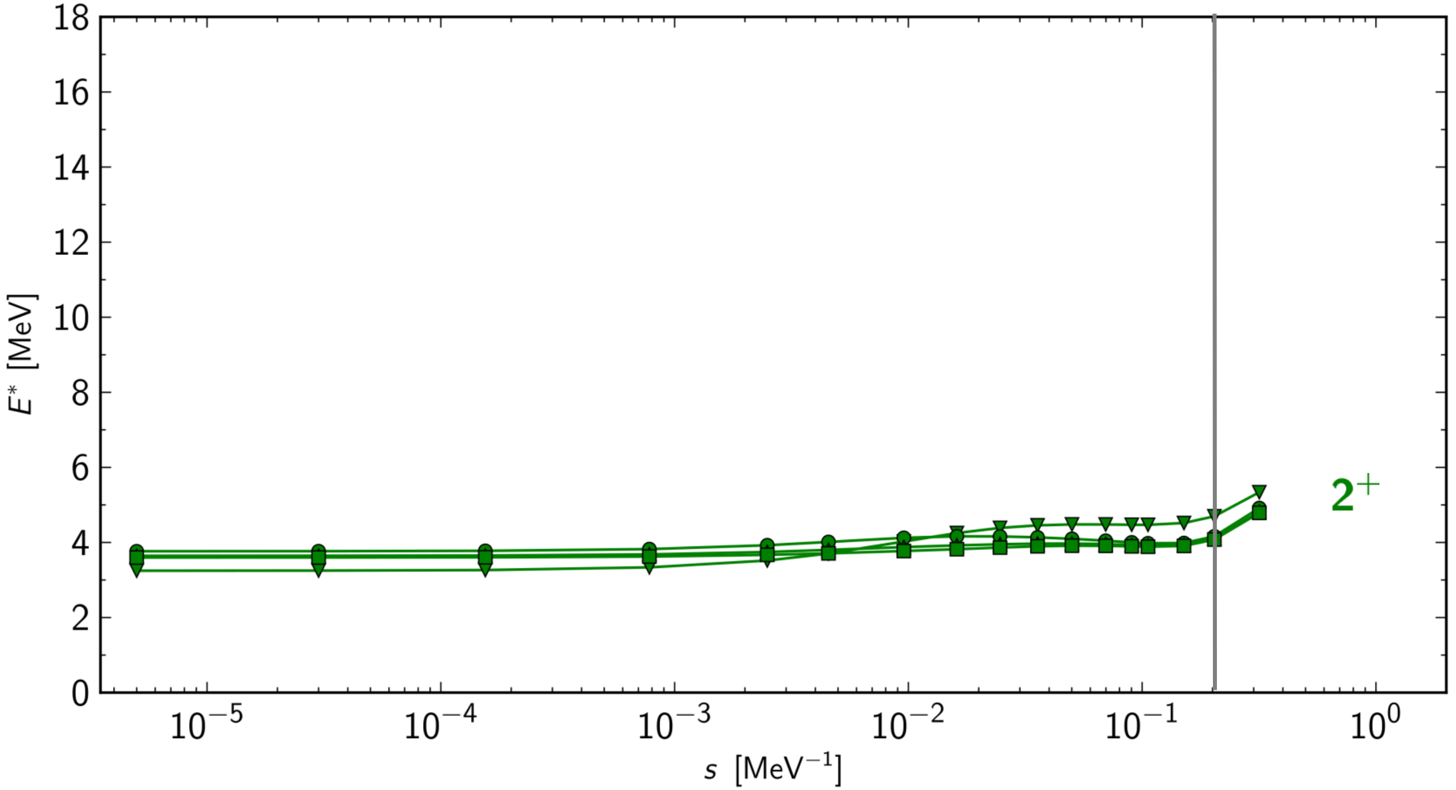

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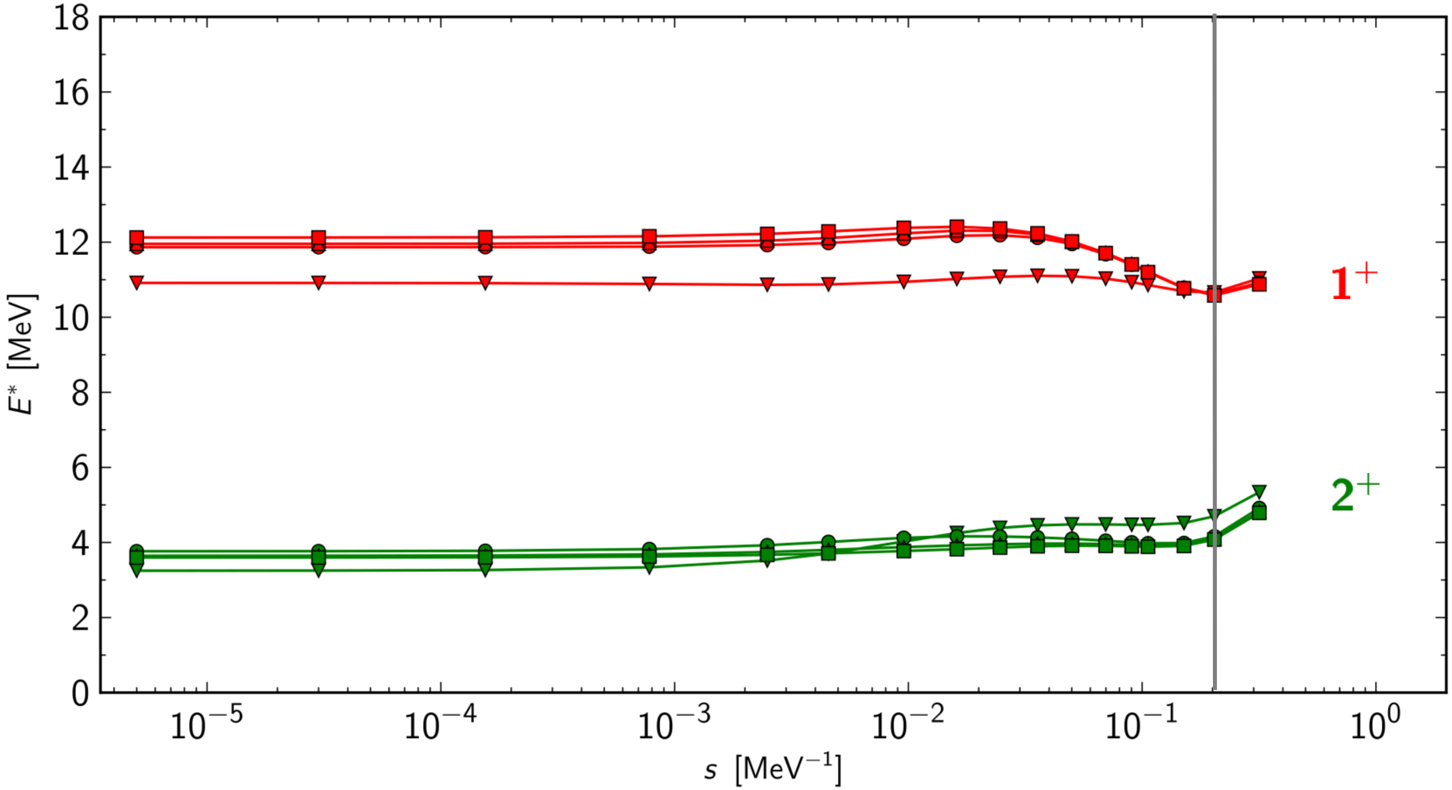

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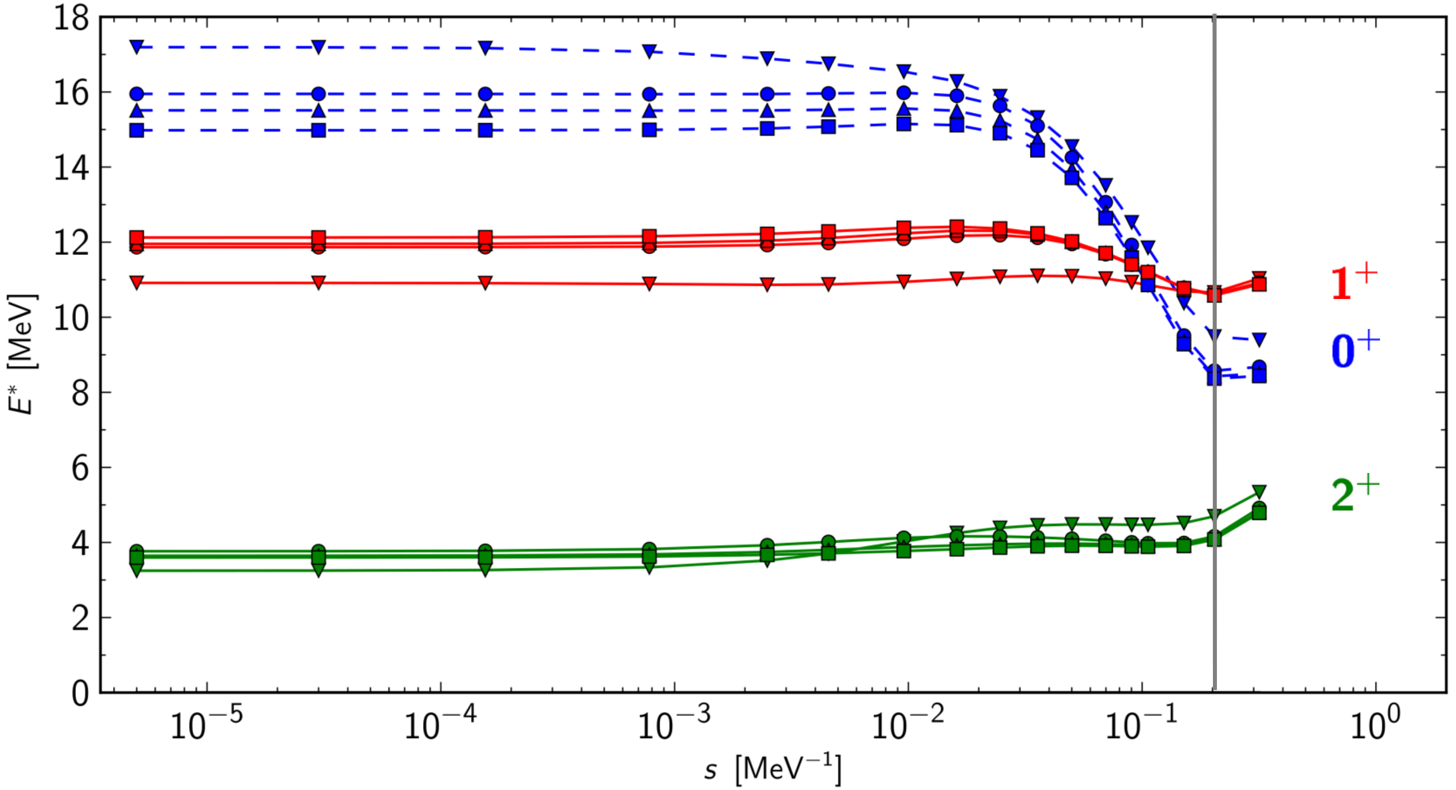

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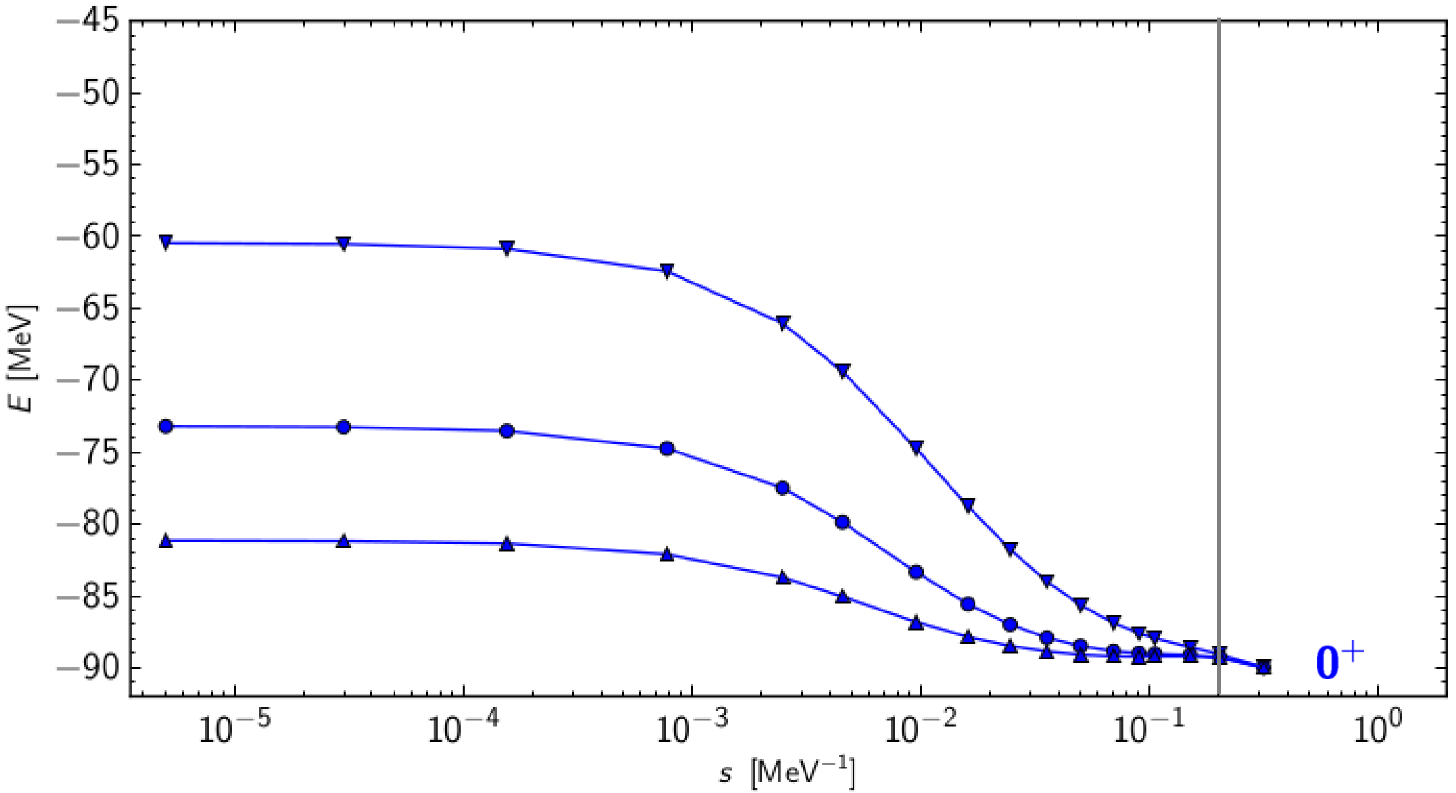
- **Hoyle state**? --> very sensitive to flow parameter --> needs further investigation

Flow of Excitation Energies – On Absolute Scale



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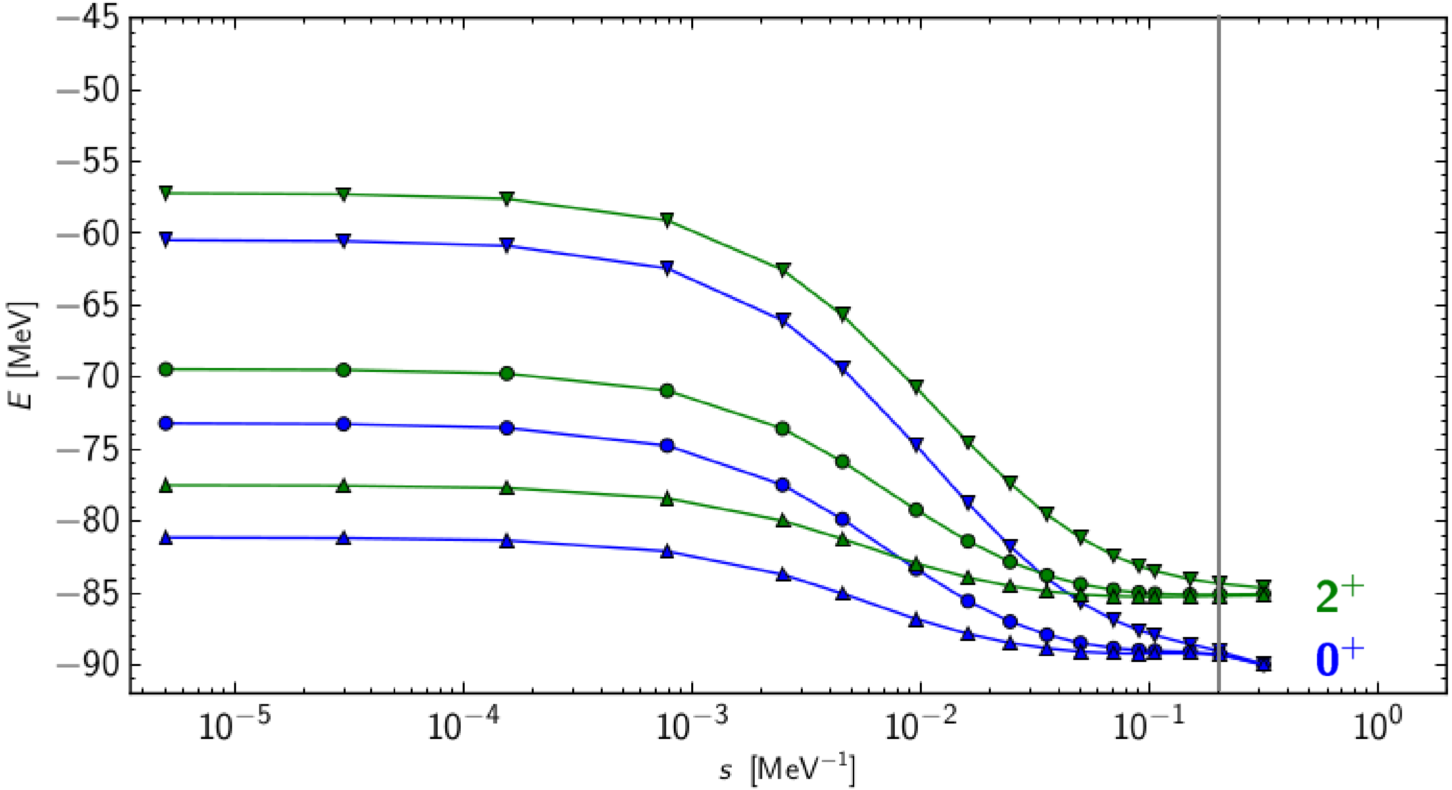

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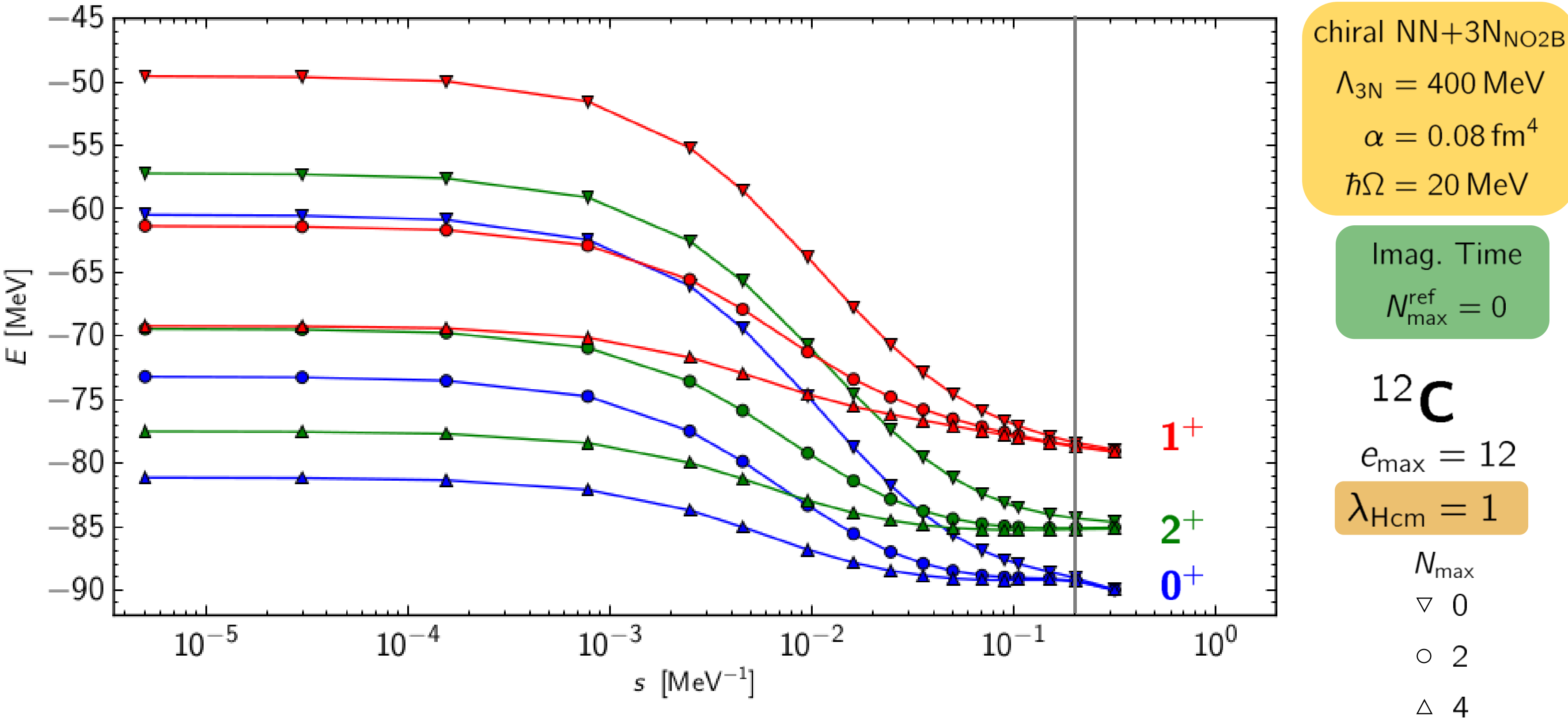
Flow of Excitation Energies – On Absolute Scale



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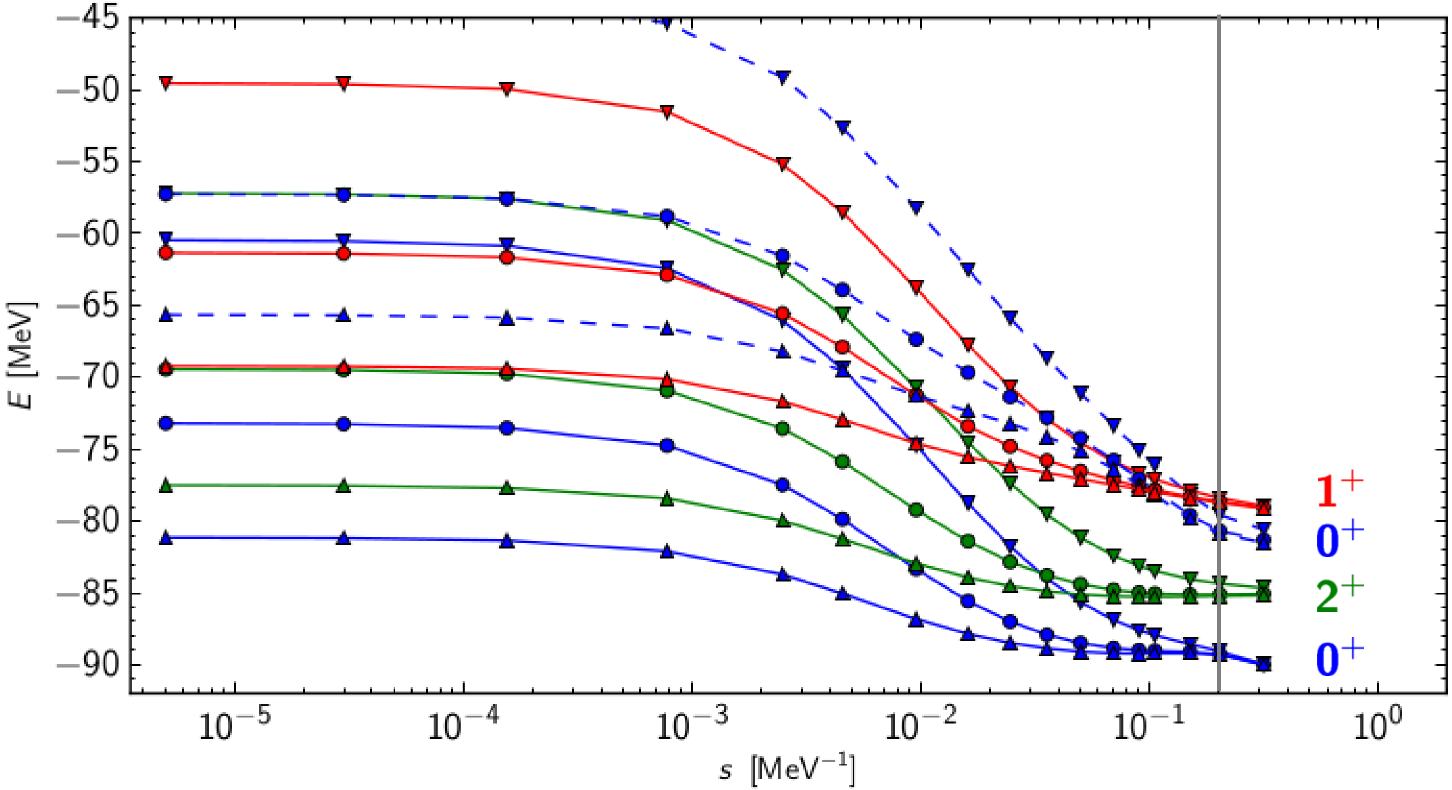

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$\lambda_{Hcm} = 1$

N_{max}

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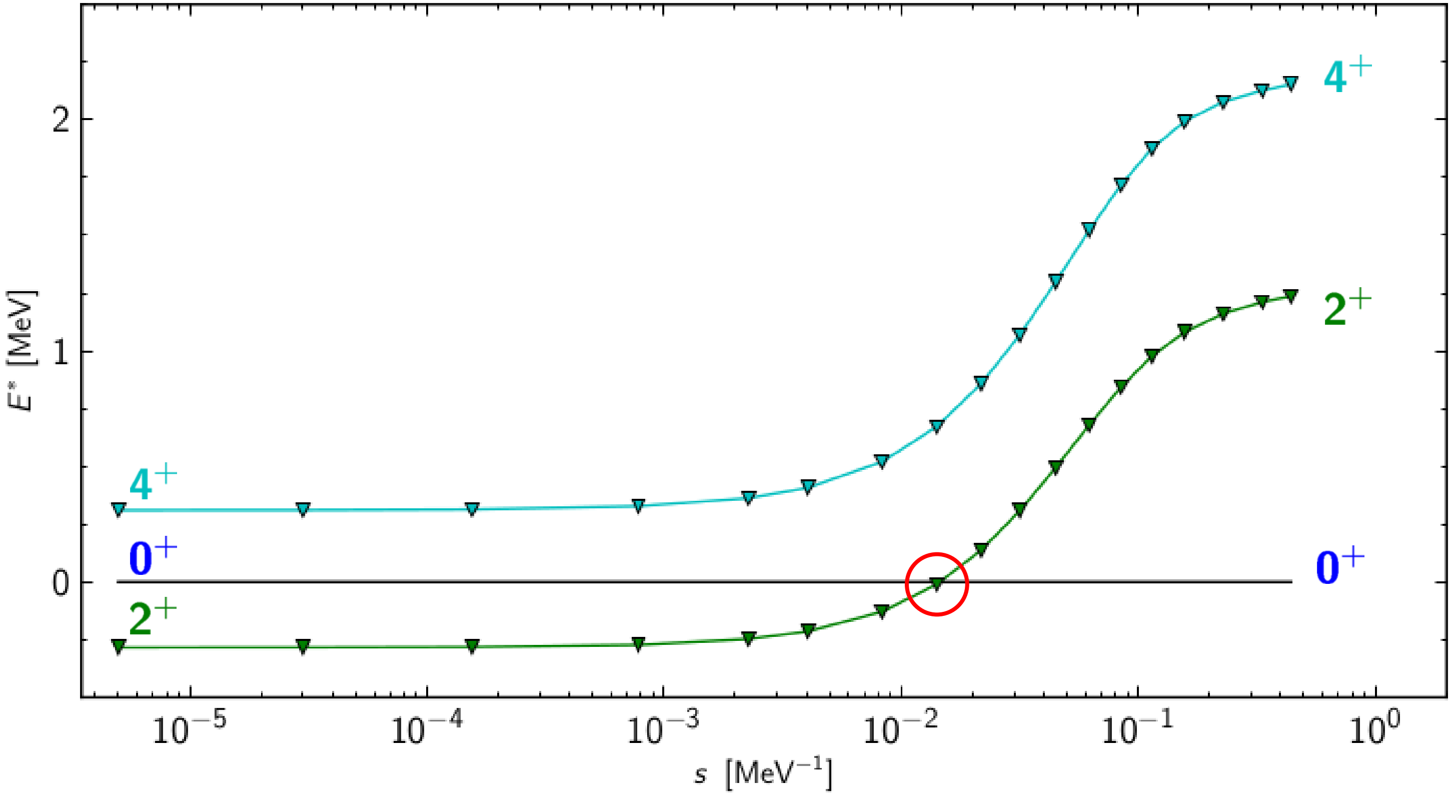
○ 2

△ 4

- 2^+ perfectly converged on absolute scale
- induced many-body contribution different for each state

Flow of Excitation Energies – Relative to 0^+



chiral NN+$3N_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08\ \mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

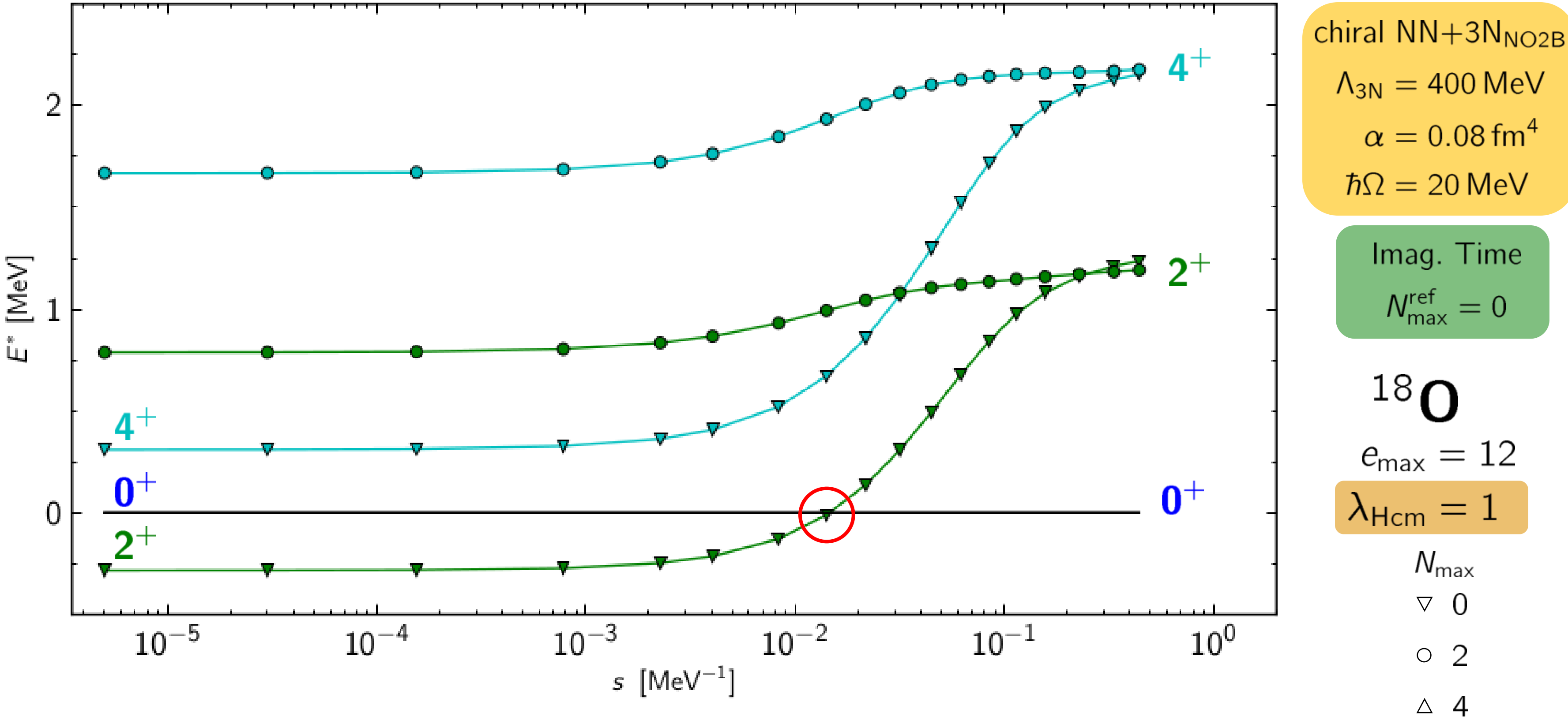
Imag. Time
$N_{max}^{ref} = 0$

^{18}O
$e_{max} = 12$
$\lambda_{Hcm} = 1$

N_{max}
▽ 0
○ 2
△ 4

- initial Hamiltonian does not reproduce the right ground-state in N_{max}=0, but far enough evolved Hamiltonian does

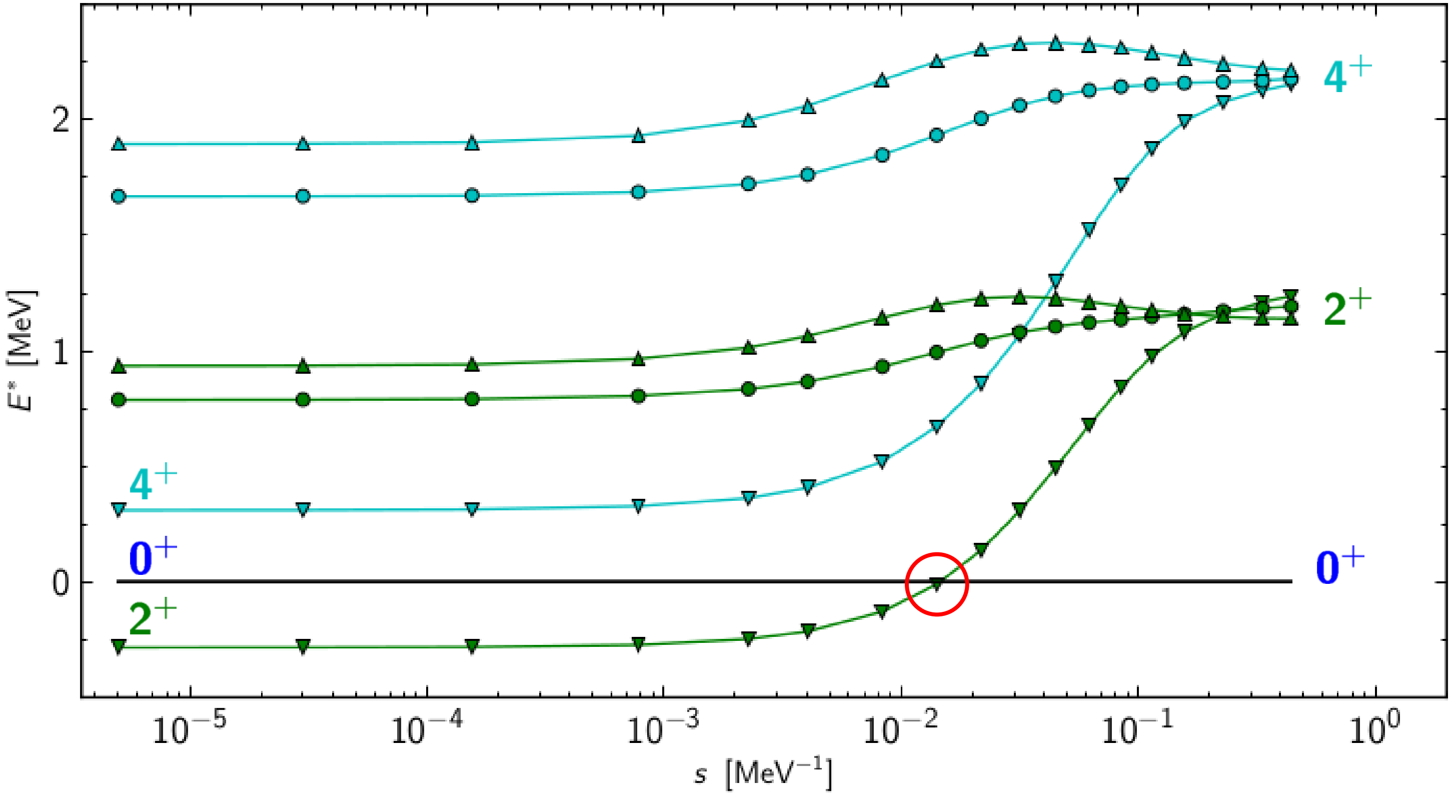
Flow of Excitation Energies – Relative to 0^+



- initial Hamiltonian does not reproduce the right ground-state in N_{max}=0, but far enough evolved Hamiltonian does

Results

Flow of Excitation Energies – Relative to 0^+



chiral NN+3N$_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08$ fm^4
$\hbar\Omega = 20$ MeV

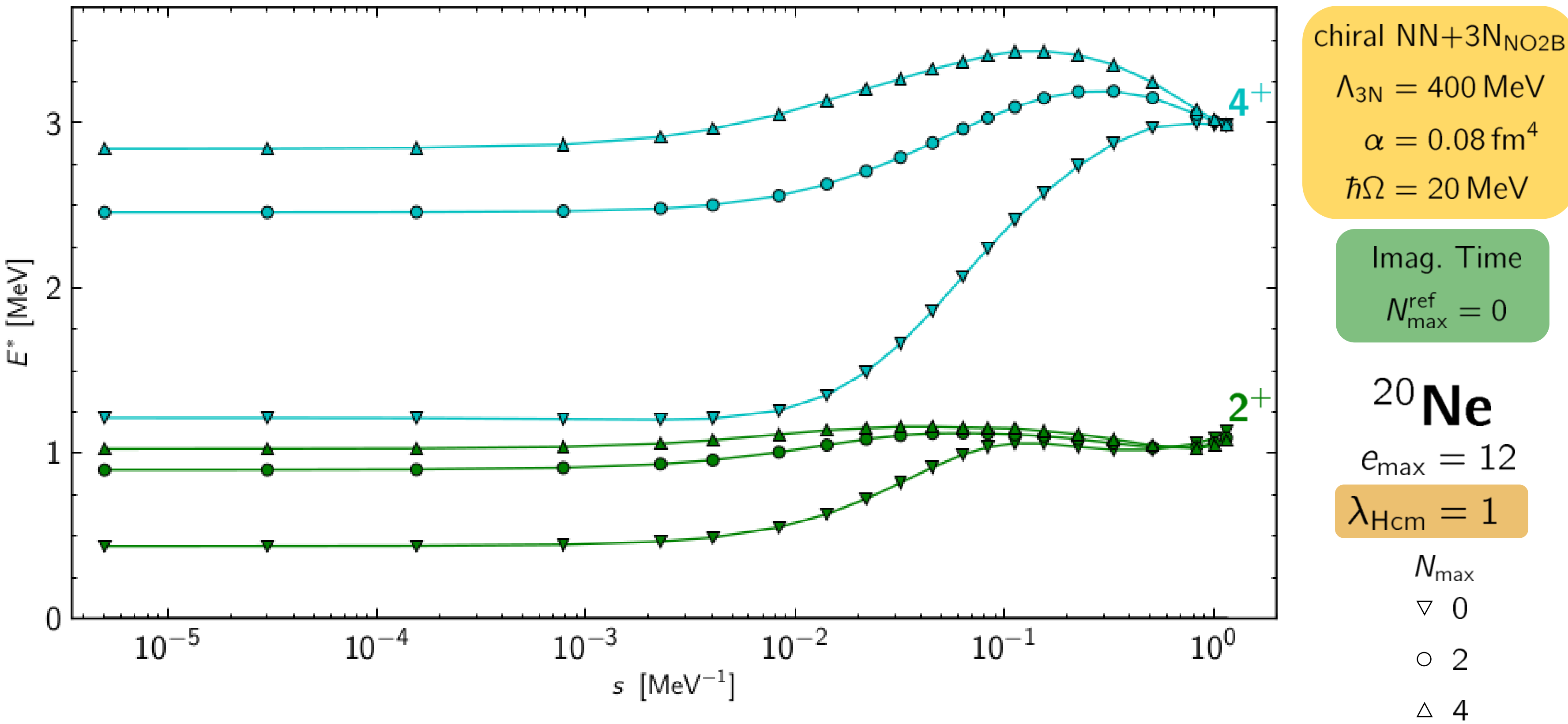
Imag. Time
$N^{ref}_{max} = 0$

^{18}O
$e_{max} = 12$
$\lambda_{Hcm} = 1$

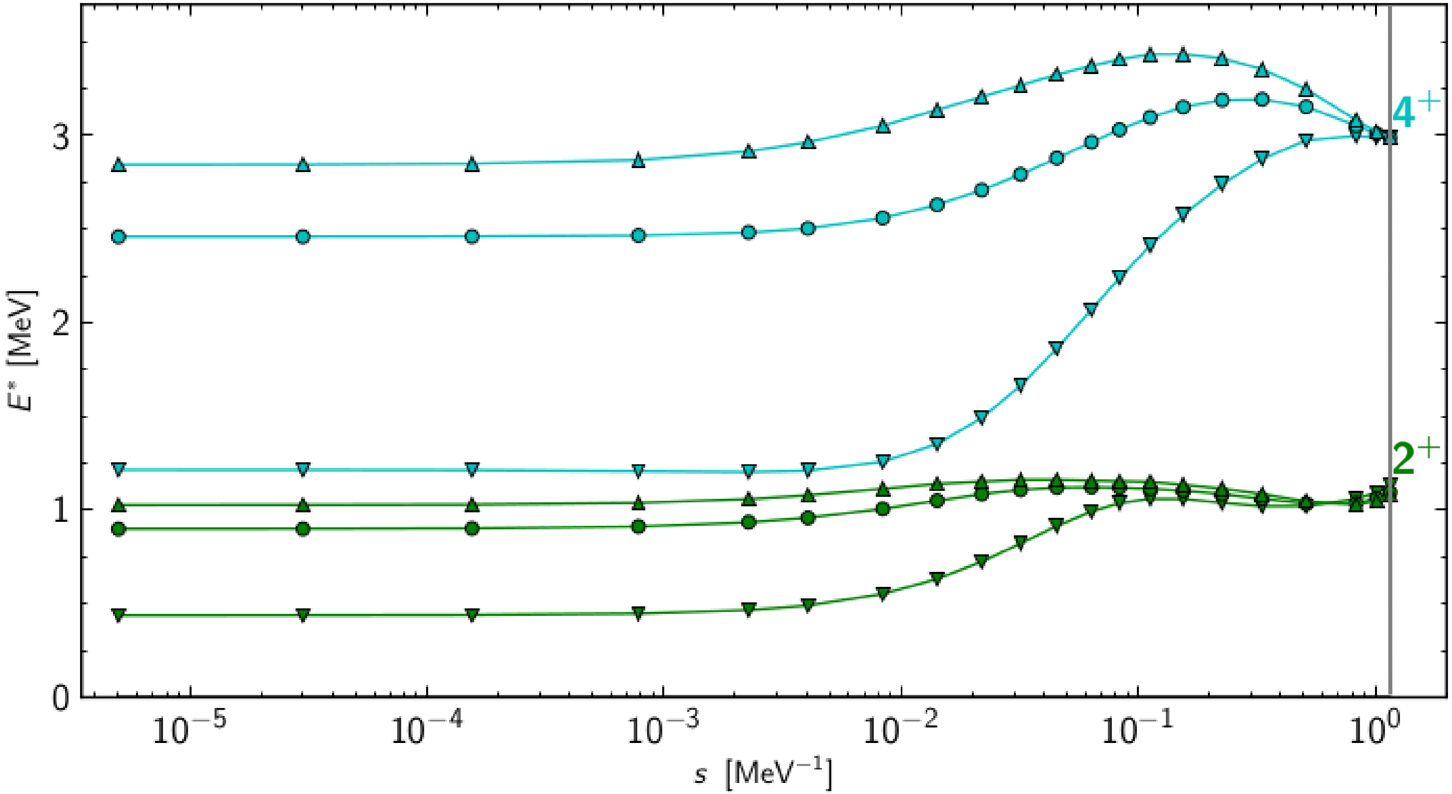
N_{max}
▽ 0
○ 2
△ 4

- initial Hamiltonian does not reproduce the right ground-state in N_{max}=0, but far enough evolved Hamiltonian does
- again nice monotonical convergence from above for 2^+
- seems **not** the case for 4^+ (should go to larger value of flow parameter)

Flow of Excitation Energies



Flow of Excitation Energies



chiral NN+3N$_{\text{NO2B}}$

$\Lambda_{3N} = 400$ MeV

$\alpha = 0.08$ fm^4

$\hbar\Omega = 20$ MeV

Imag. Time

$N_{max}^{ref} = 0$

^{20}**Ne**

$e_{max} = 12$

$\lambda_{Hcm} = 1$

N_{max}

▽ 0

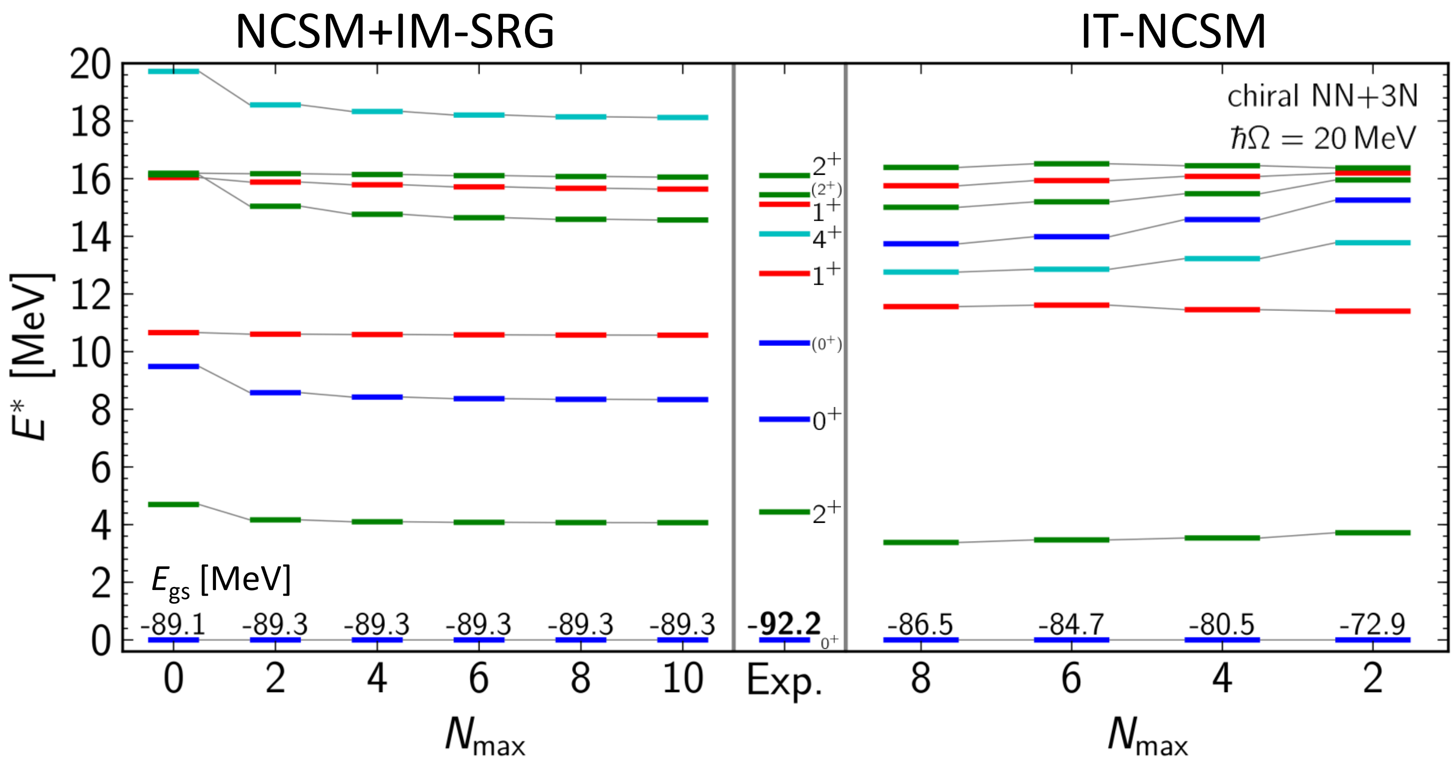
○ 2

△ 4

analyze E^*
as function of N_{max}
at s_{opt}

Results

Spectra



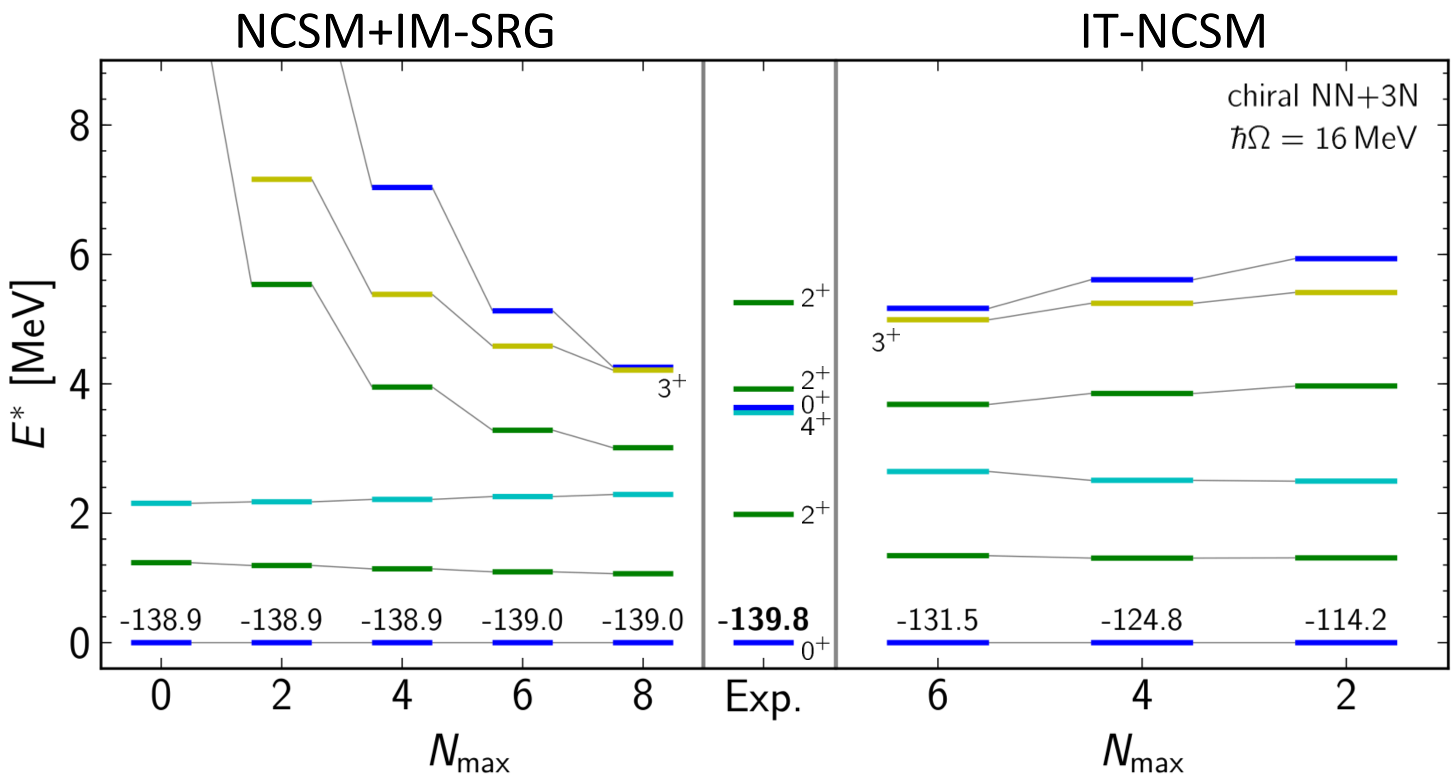
chiral NN+3N$_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08\ \mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

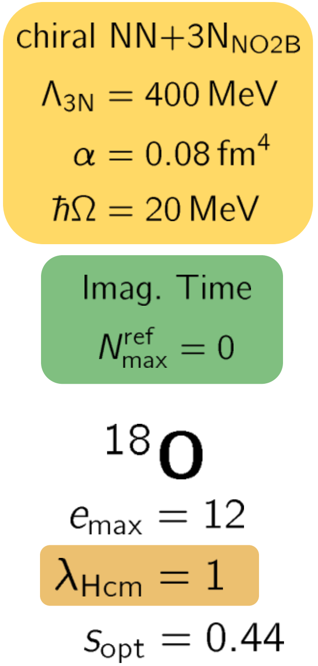
Imag. Time
$N^{ref}_{max} = 0$

^{12}C
$e_{max} = 12$
$\lambda_{Hcm} = 1$
$s_{opt} = 0.20$

- IT-NCSM calculated using **complete** 3N interaction
- difference between NCSM+IM-SRG and IT-NCSM: **induced many body** and **NO2B**
- NCSM+IM-SRG can easily access larger model spaces since NO2B approximation
- IT-NCSM ground-state energies not converged yet

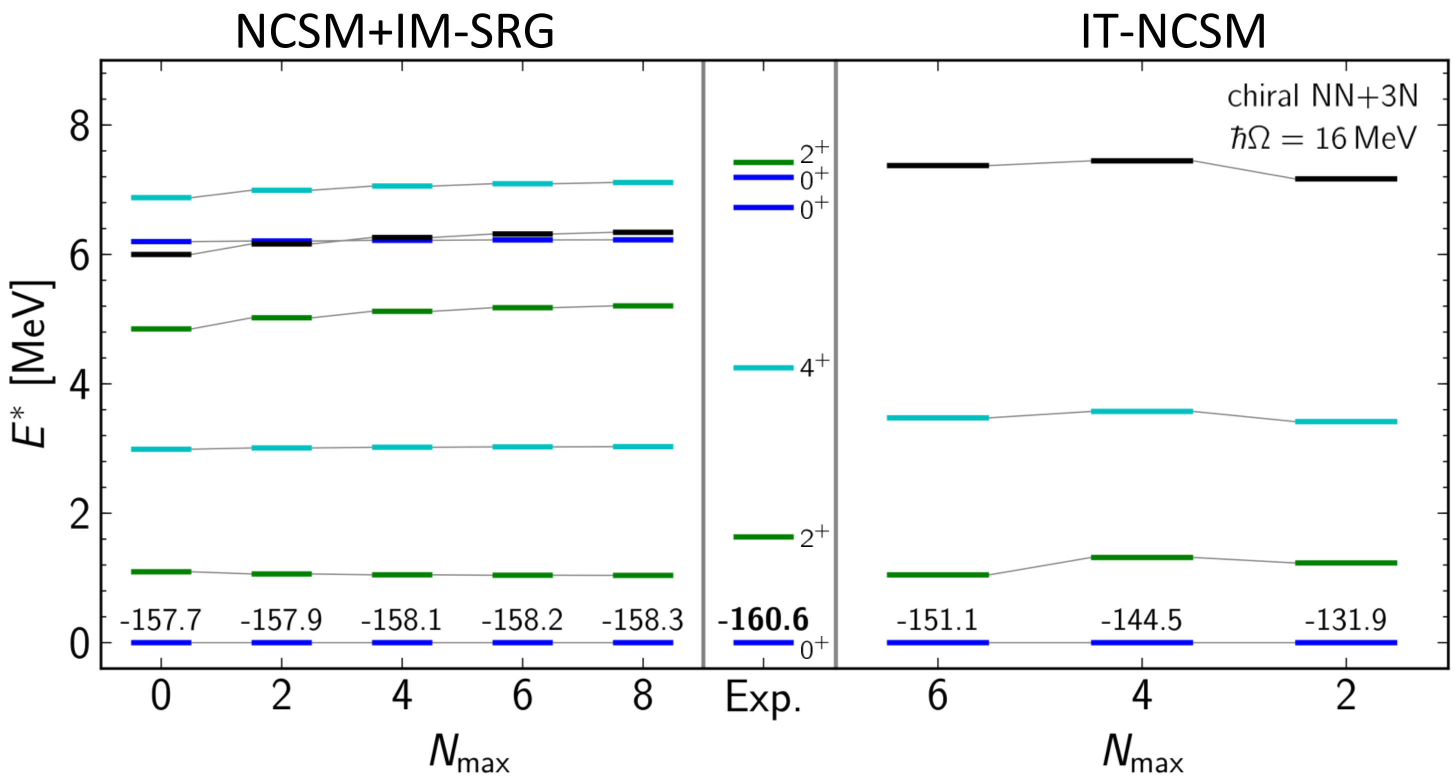
Spectra





- ground-state energy perfectly converged for NCSM+IM-SRG
- two different classes of states
  - fast N_{max} convergence –> states with dominant N_{max}=0 component
  - slow N_{max} convergence –> states with dominant N_{max}≠0 component

Results
Spectra



chiral NN+$3N_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08\,\text{fm}^4$
$\hbar\Omega = 20$ MeV

Imag. Time
$N_{max}^{ref} = 0$

^{20}**Ne**
$e_{max} = 12$
$\lambda_{Hcm} = 1$
$s_{opt} = 1.01$

Summary

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- ✓ introduced novel many-body technique NCSM+IM-SRG
- ✓ exploits the advantages of both approaches
- ✓ IM-SRG decouples **reference state** from higher N_{max}
- ✓ extremely enhanced N_{max} convergence
- ✓ small $N_{max} \leq 4$ sufficient to extract converged ground-state for evolved Hamiltonians
- ✓ NCSM+IM-SRG: **variational principle** valid for **excitation energies** since ground-state converged

Outlook

- variation of several parameters: generator, $N_{\max}^{\text{ref}}$, $\hbar\Omega$, …
- consistent evolution radius, electromagnetic, … operators
- detailed analysis of the Hoyle state in ^{12}C
- extend applicability of NCSM+IM-SRG to odd nuclei
  - particle-attached or particle-removed formalism (first study very promising)
  - include non-scalar densities for the IM-SRG evolution
- include three-body operators in IM-SRG: explicit or perturbative treatment

Thank You For Your Attention

TECHNISCHE UNIVERSITÄT DARMSTADT

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DFG

HIC for FAIR
Helmholtz International Center

HELMHOLTZ GEMEINSCHAFT

JURECA	LOEWE-CSC	LICHTENBERG
JÜLICH FORSCHUNGSZENTRUM	CSC Center for Scientific Computing Frankfurt	HRZ Hochschulrechenzentrum

COMPUTING TIME