Ab Initio Method: In-Medium No-Core Shell Model

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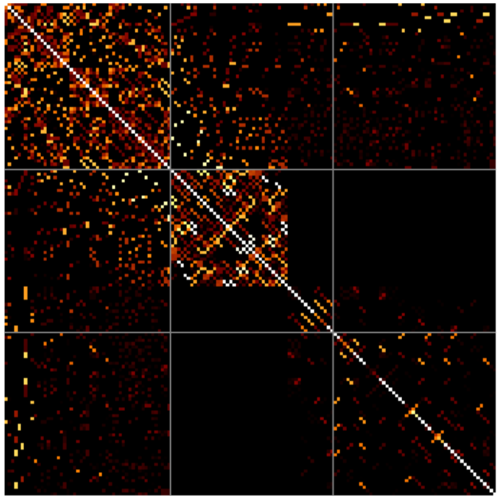
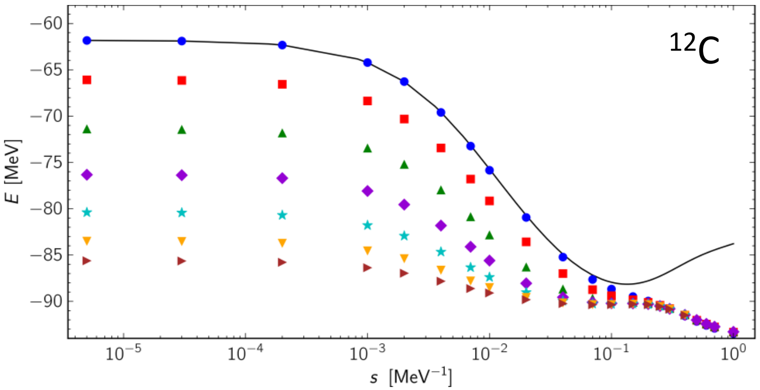
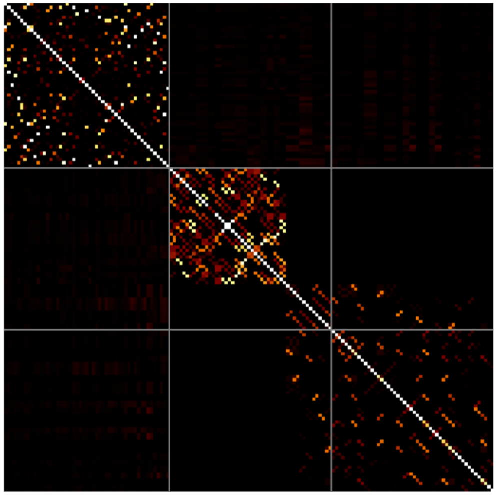


accepted on PRL, arXiv:1610.05254





Overview

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

Barrett, Vary, Navratil, ...

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

- construct matrix representation of Hamiltonian using **basis of HO/HF Slater determinants** truncated w.r.t. 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

Basics

Tsukiyama, Bogner, Schwenk, Hergert,..

… uses flow equation for normal-ordered Hamiltonian to decouple the **reference state** from its excitations

flow parameter

generator designed to decouple the reference state $|\Psi_{\mathrm{ref}}\rangle$

flow equation for Hamiltonian:

$$\frac{\mathrm{d}}{\mathrm{d}s} H(s) = [\eta(s), H(s)]$$

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H in multi-reference normal-ordered form w.r.t. $|\Psi_{\text{ref}}\rangle$ [Kutzelnigg,Mukherjee]

$$H(0) = E(0) + \sum f^{\circ}_{\circ}(0)\tilde{a}^{\circ}_{\circ} + \tfrac{1}{4}\sum \Gamma^{\circ\circ}_{\circ\circ}(0)\tilde{a}^{\circ\circ}_{\circ\circ} + \tfrac{1}{36}\sum W^{\circ\circ\circ}_{\circ\circ\circ}(0)\tilde{a}^{\circ\circ\circ}_{\circ\circ\circ}$$

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$$\langle\Psi_{\text{ref}}|H(s)|\Psi_{\text{ref}}\rangle = E(s)$$

Why should we merge…

IM-SRG

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

- not exact method
- only for ground state
- spectroscopy not straight forward

NCSM

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

+ exact method
+ easy access to excited states
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How should we merge...

NCSM
define reference state

- diagonalize Hamiltonian in small model space
- ground state defines reference state

IM-SRG
evolve operators

- evolve Hamiltonian and other operators
- pre-diagonalization in *A*-body space

NCSM
extract observables

- diagonalize IM-SRG evolved Hamiltonian
- obtain eigenstates and extract observables

IM-NCSM is different from …

NCSM
define
reference state

↓

IM-SRG
evolve
operators

↓

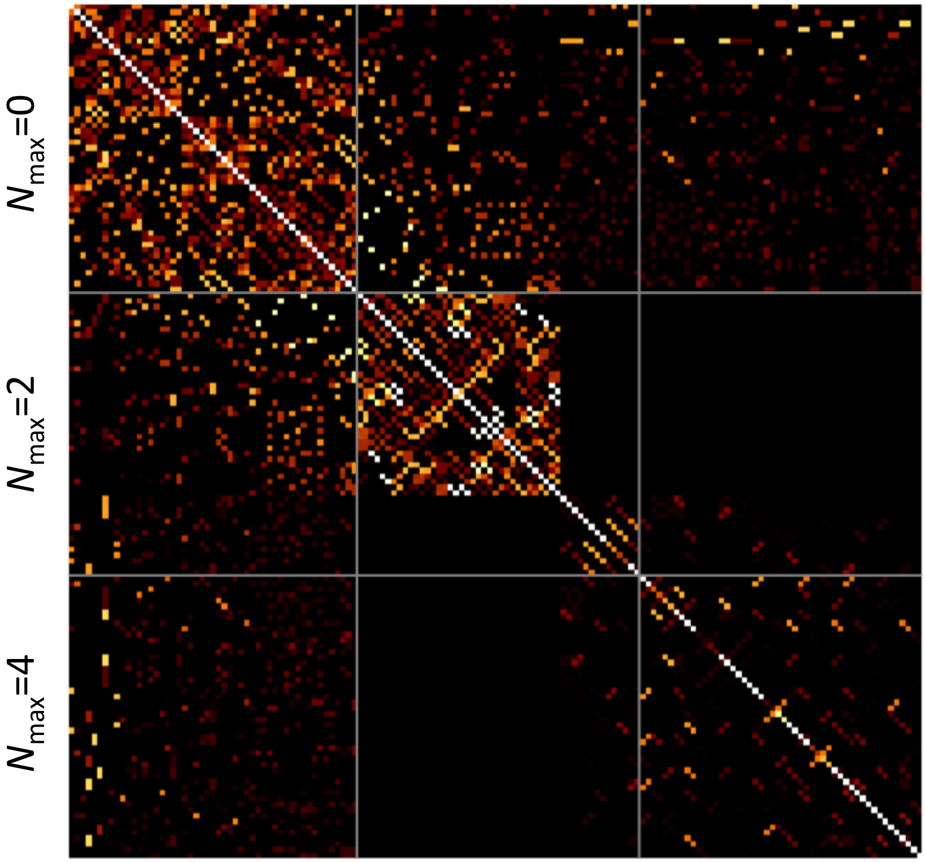
NCSM
extract
observables

IM-NCSM is different from
IM-SRG for valence-space interactions:

- build on explicit multi-reference formulation
- full no-core approach
- all model-space truncations are converged

In-Medium No-Core Shell Model
Hamiltonian Matrix in *A*-Body Basis: ^{12}C

$s = 0.00\ \text{MeV}^{-1}$



N_{max}=0 Slater determinants
N_{max}=2 Slater determinants
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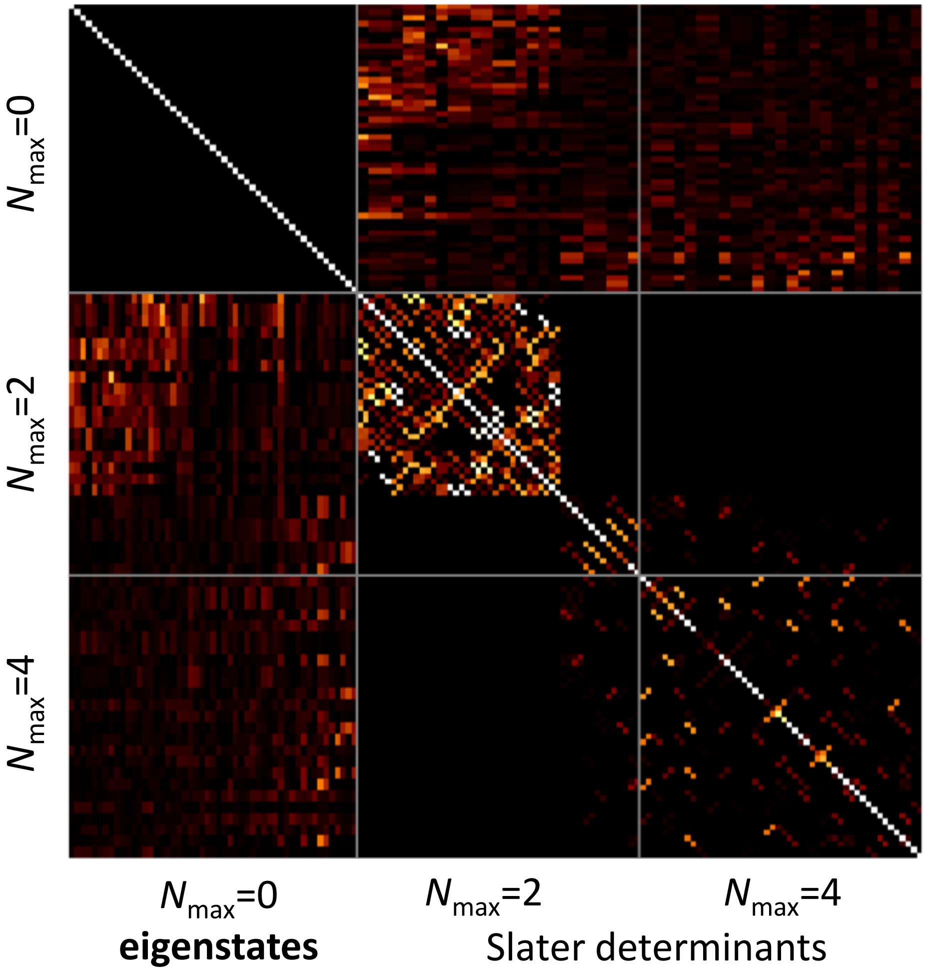

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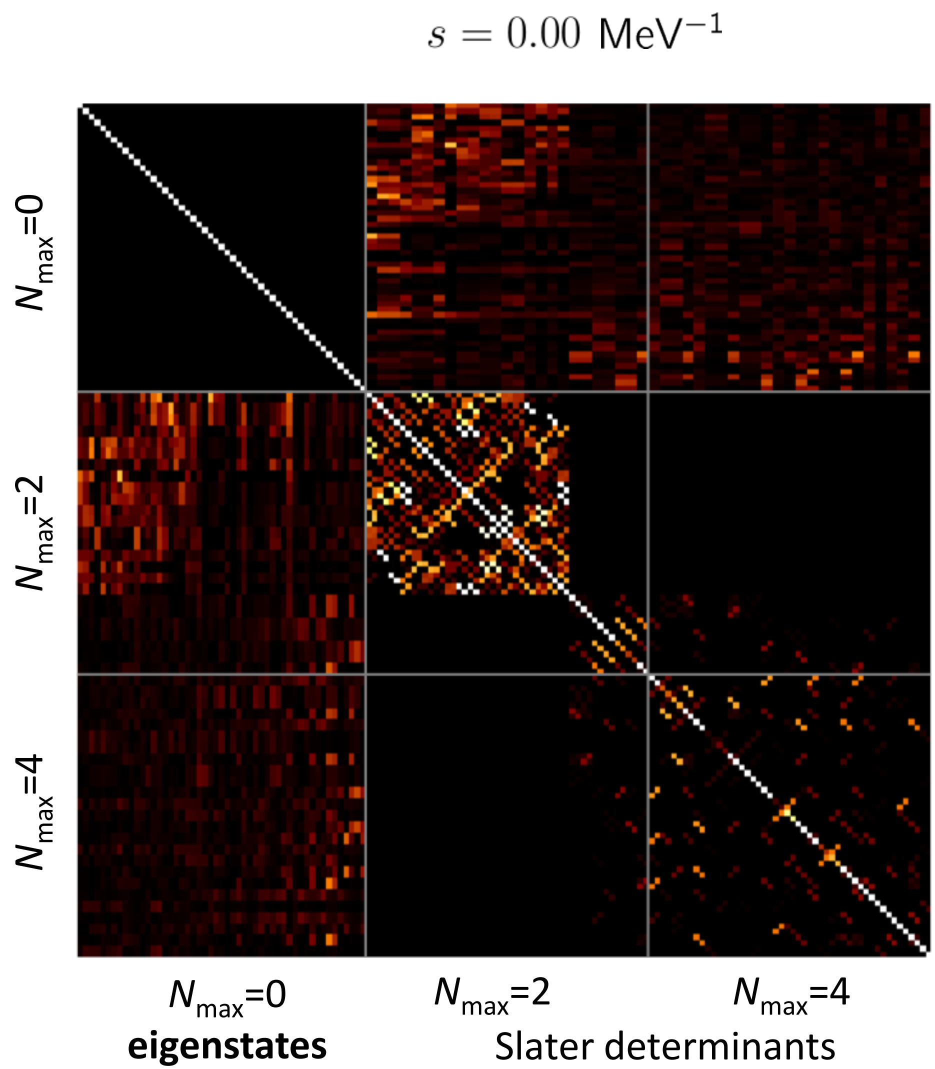

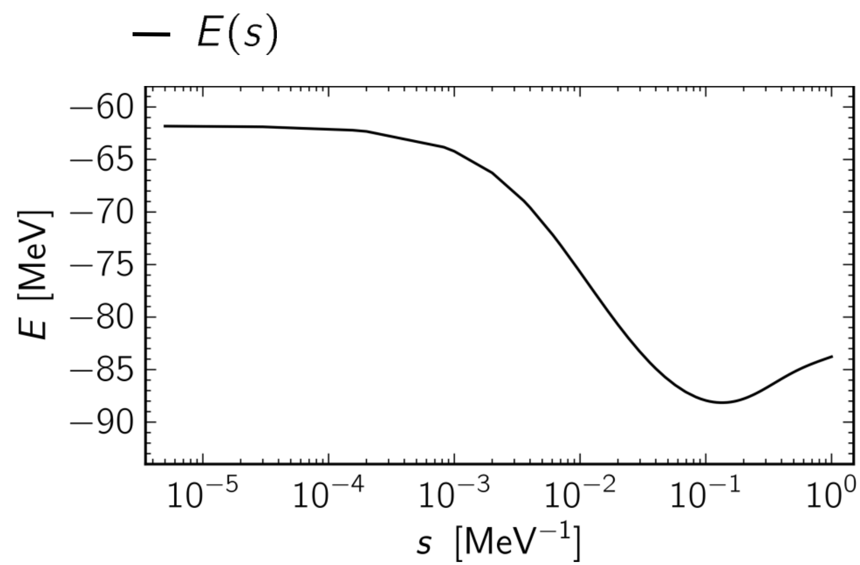

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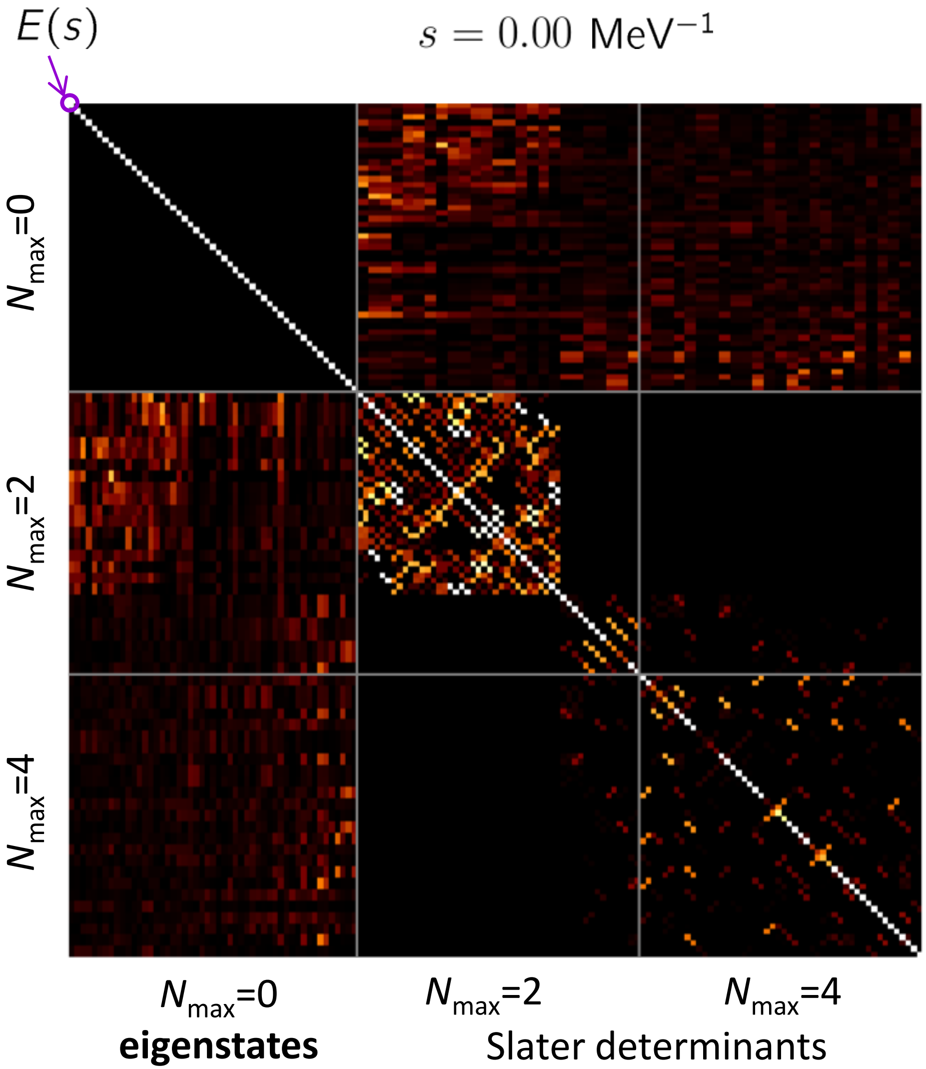
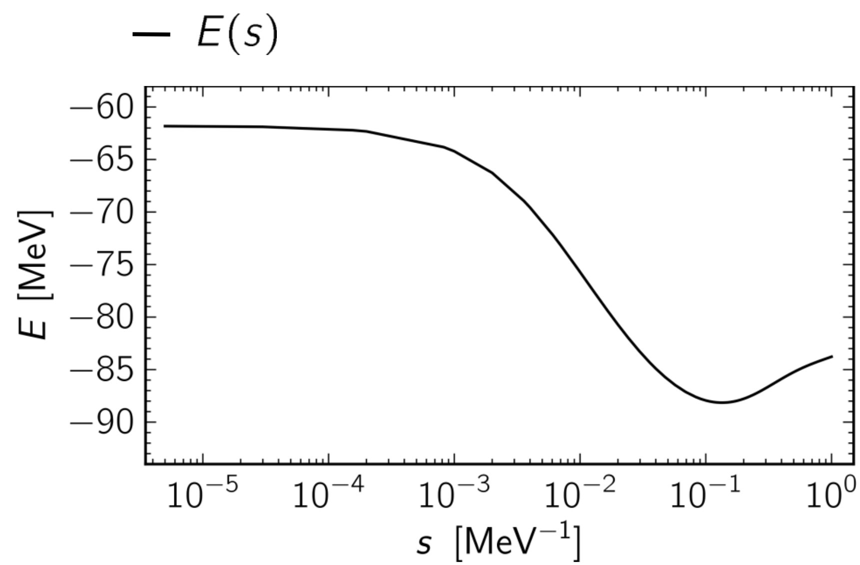
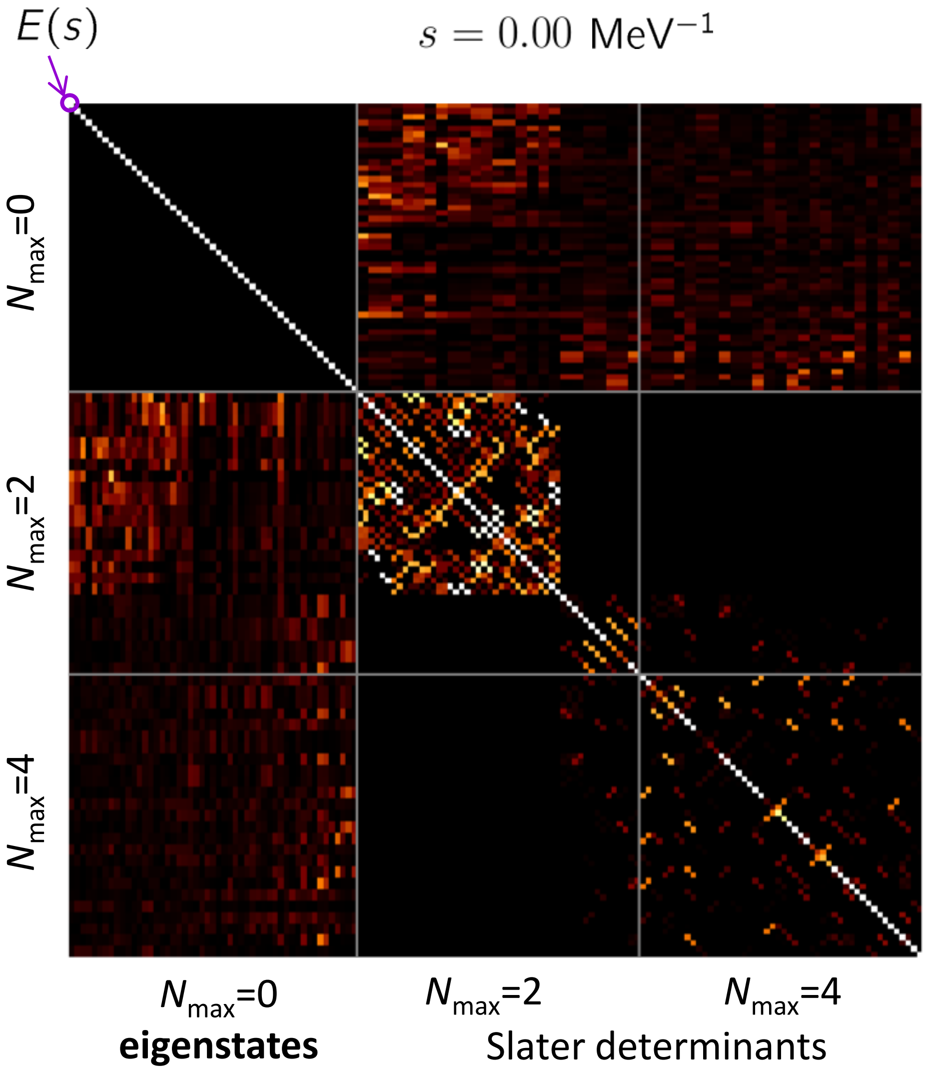
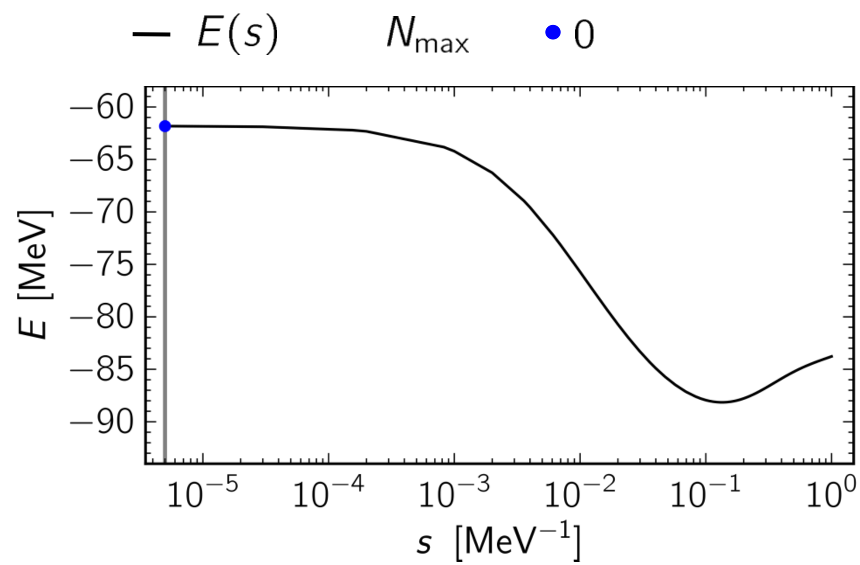




In-Medium No-Core Shell Model
Hamiltonian Matrix in A-Body Basis: ^{12}C





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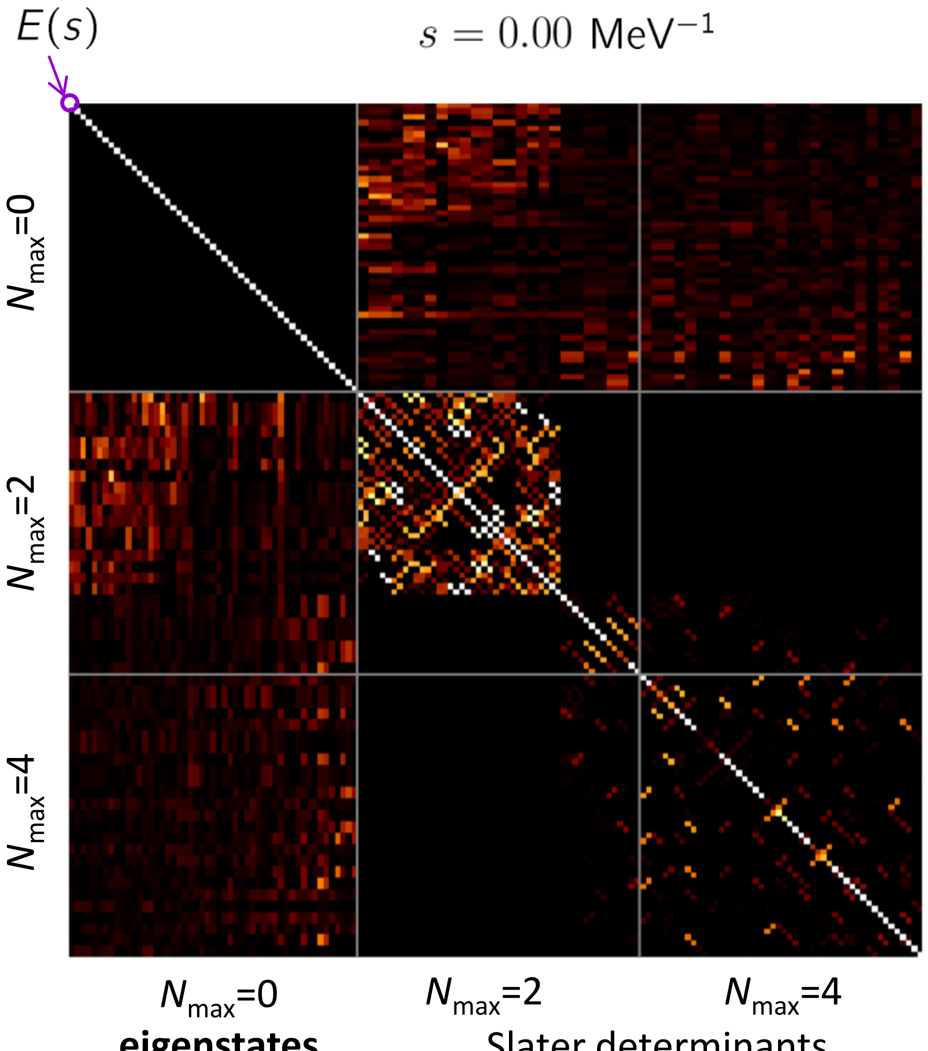

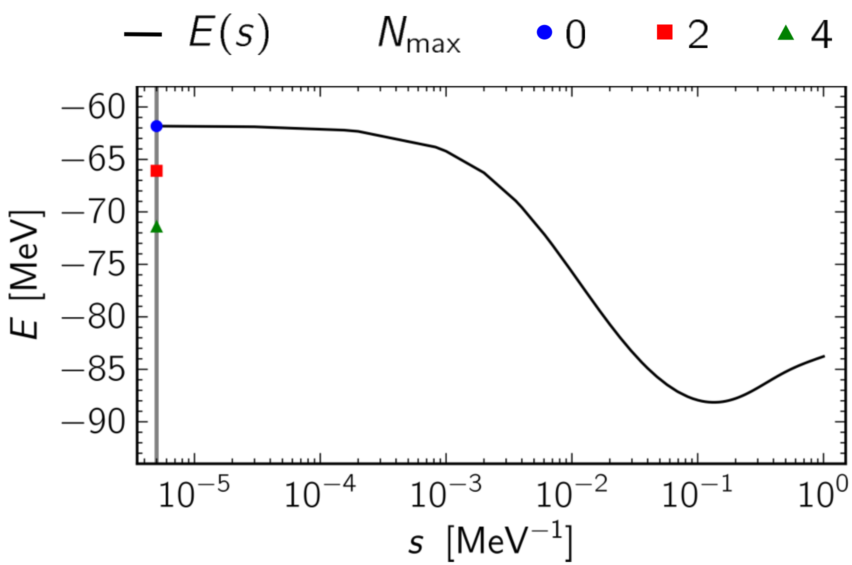

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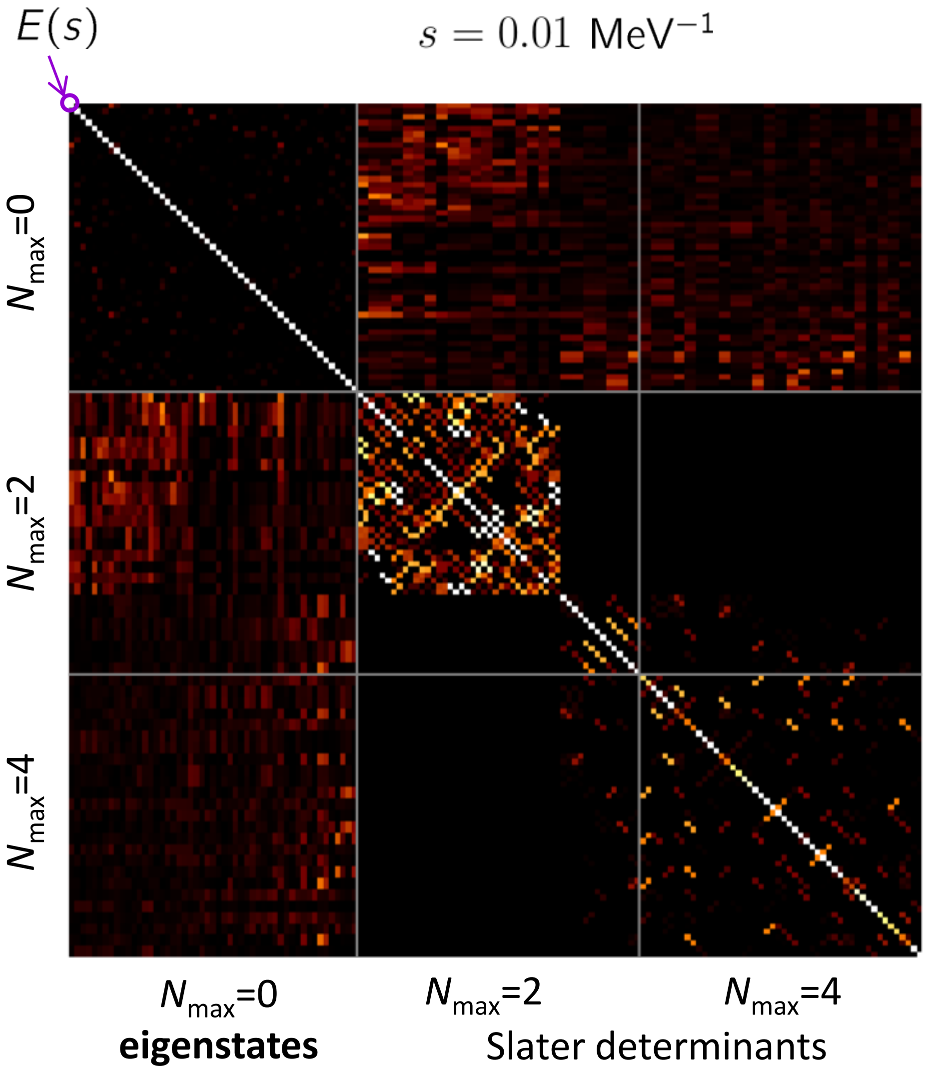

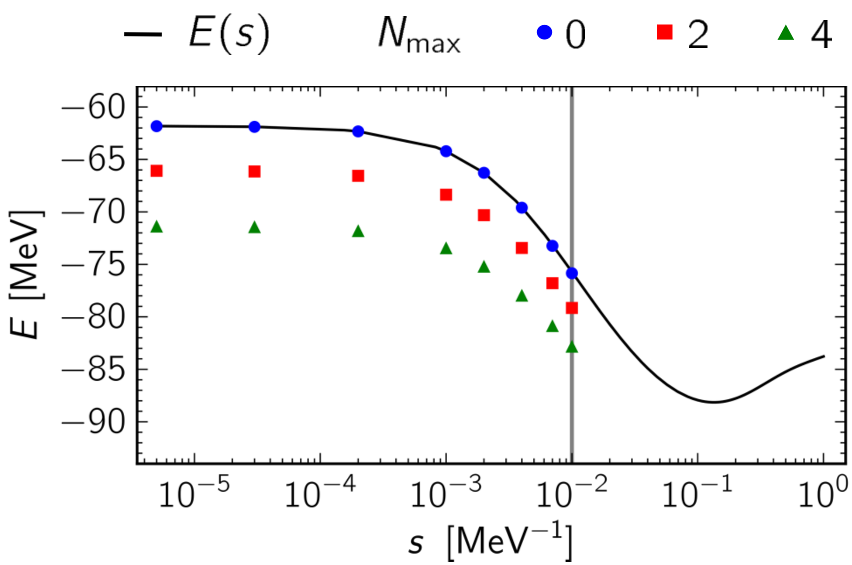

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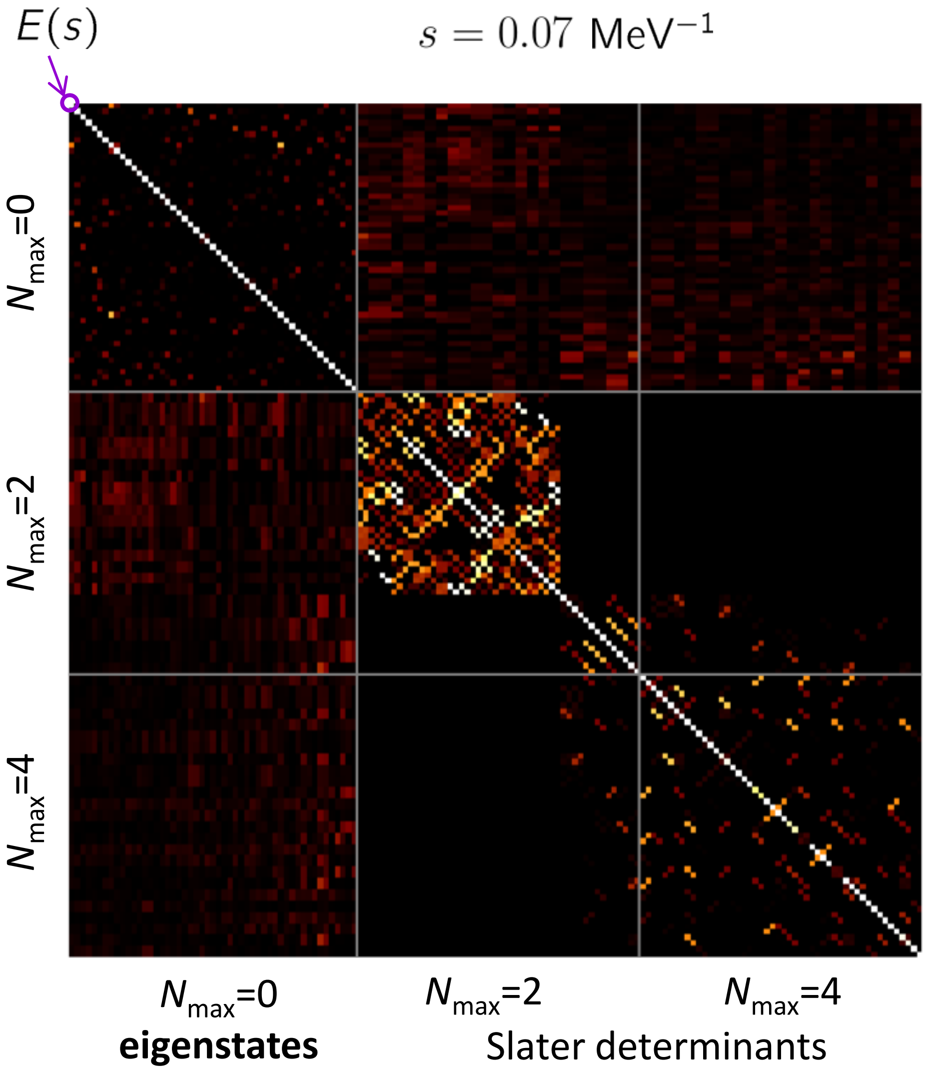

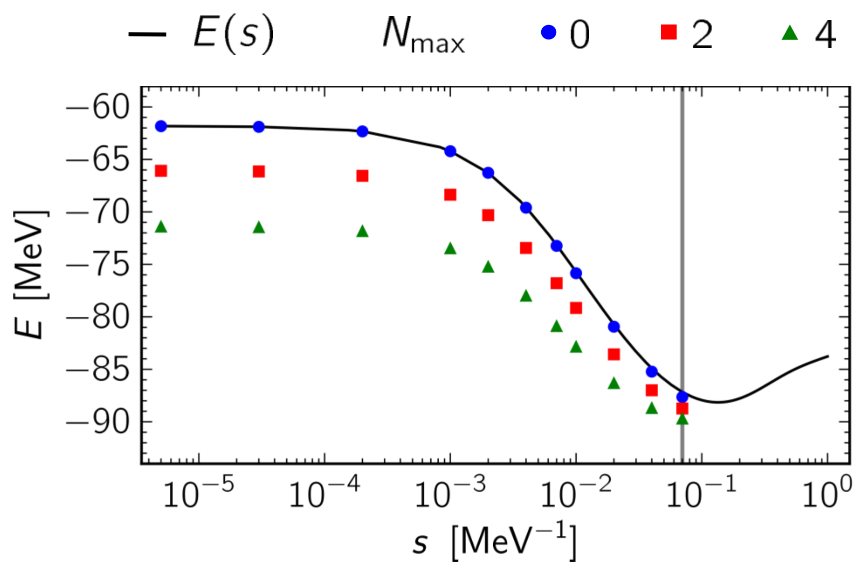

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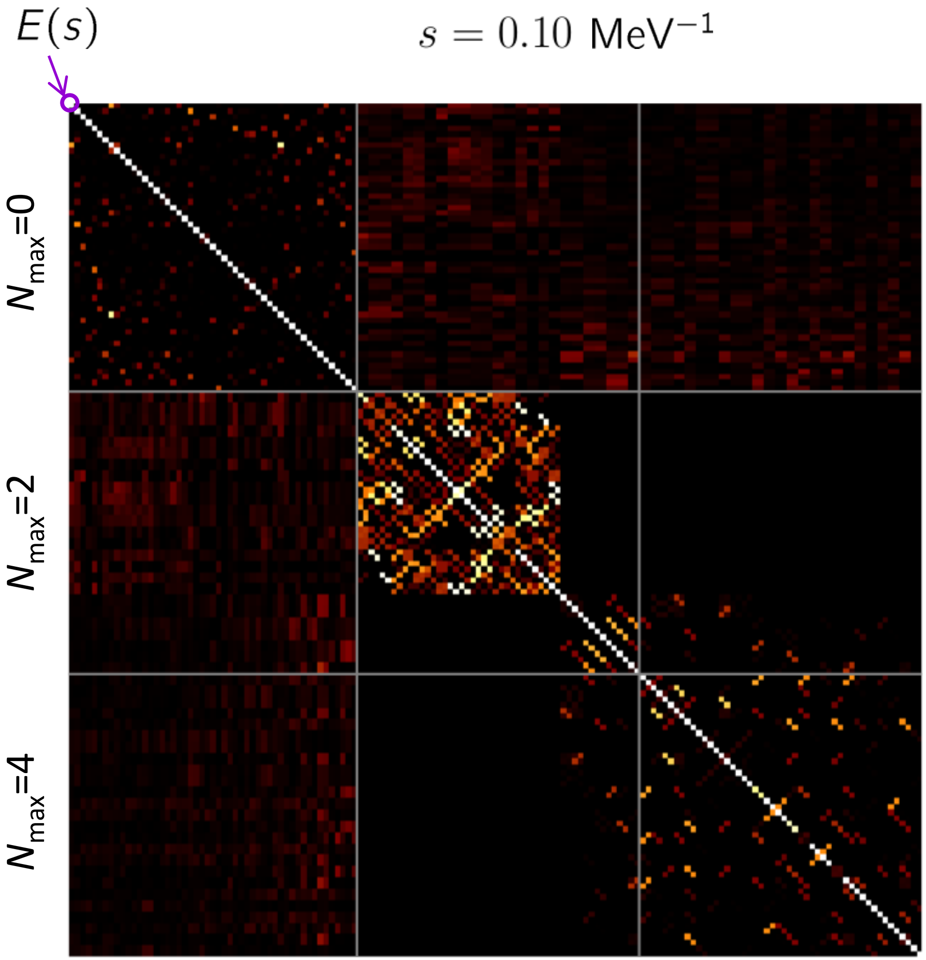
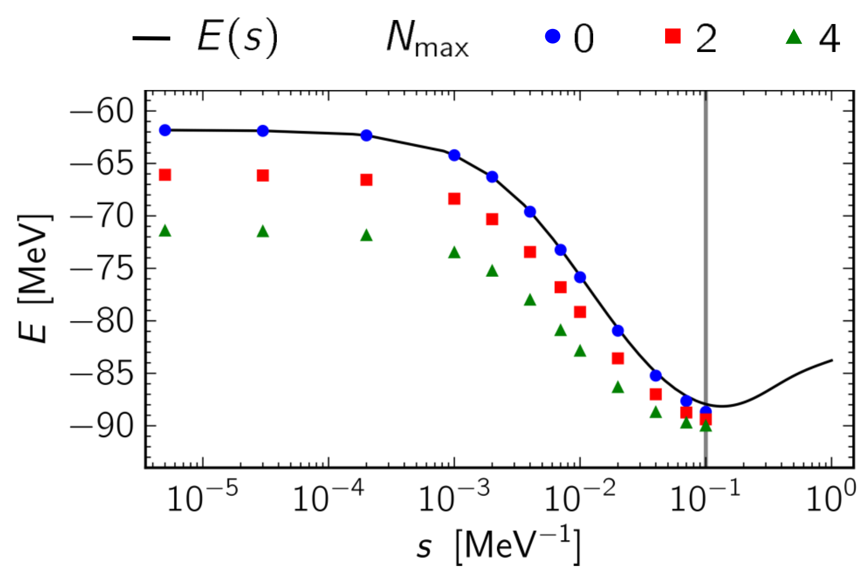


N_{max}=0 **eigenstates** | N_{max}=2 N_{max}=4 Slater determinants



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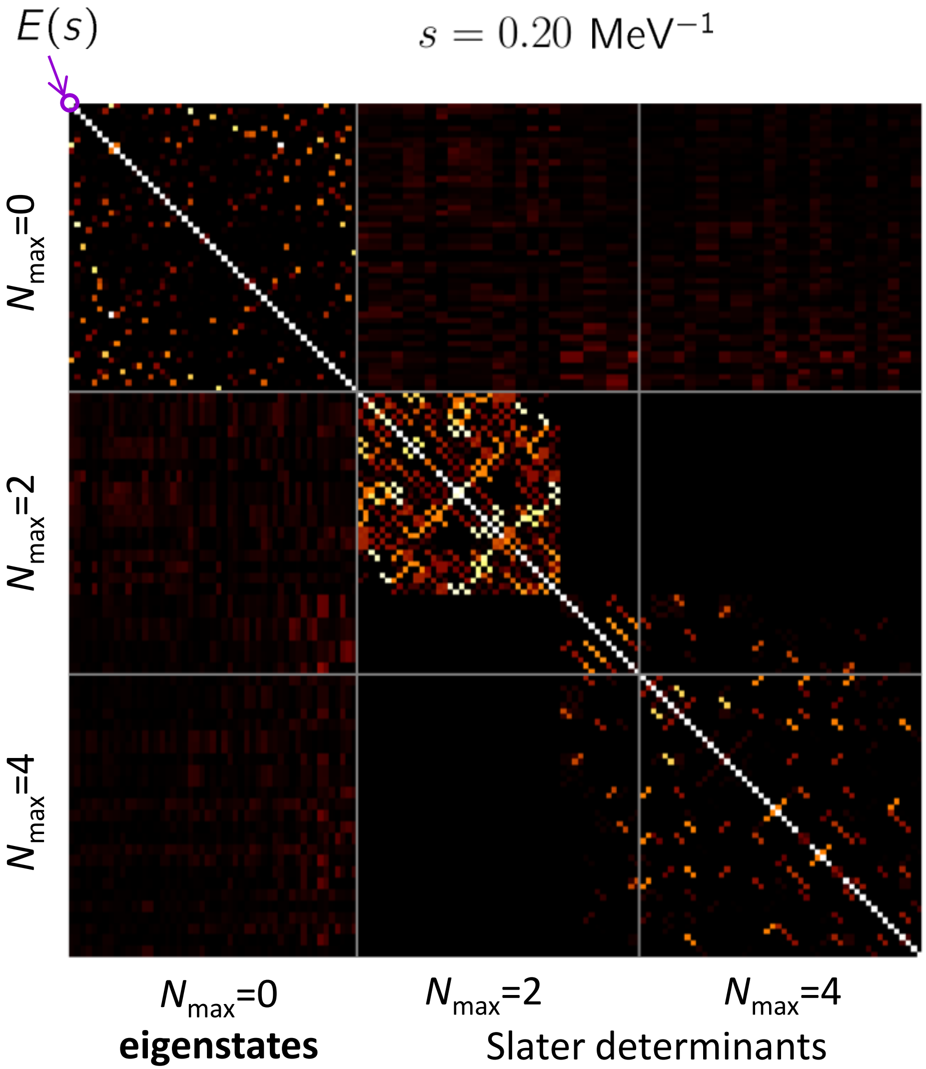

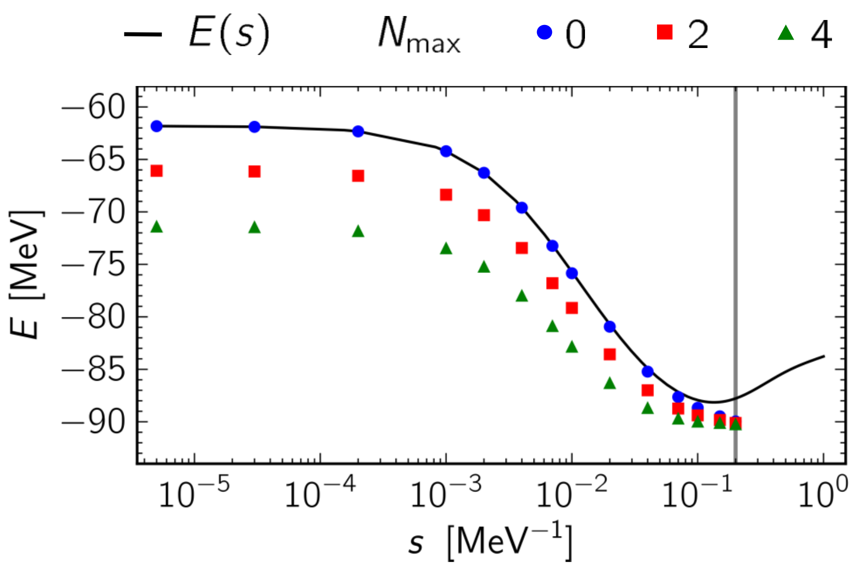

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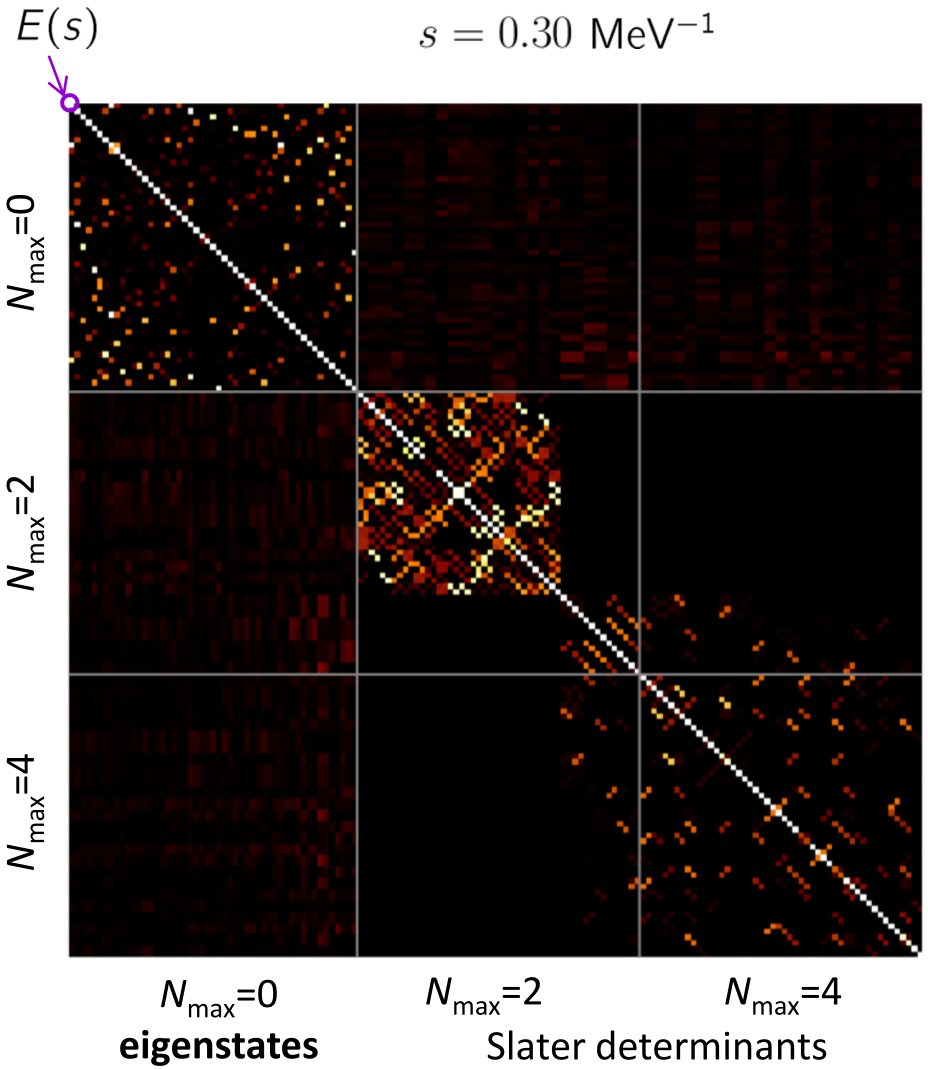

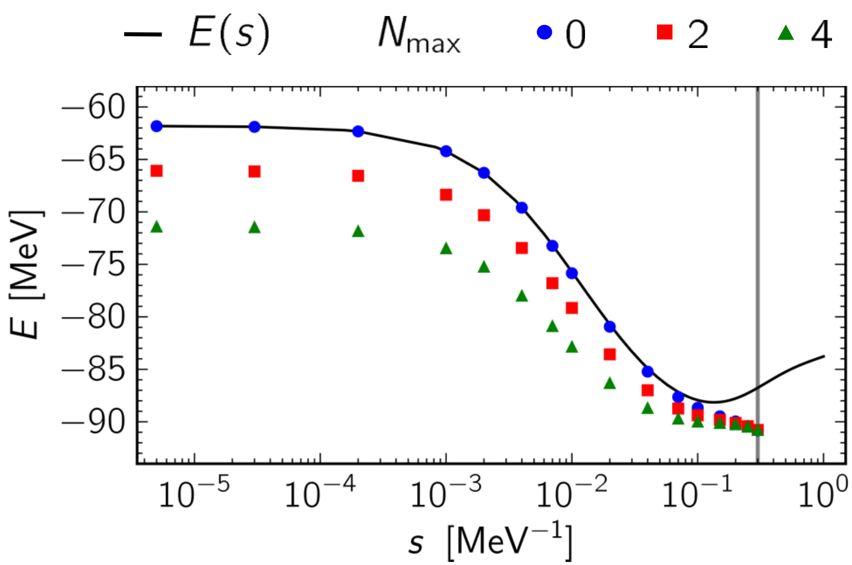

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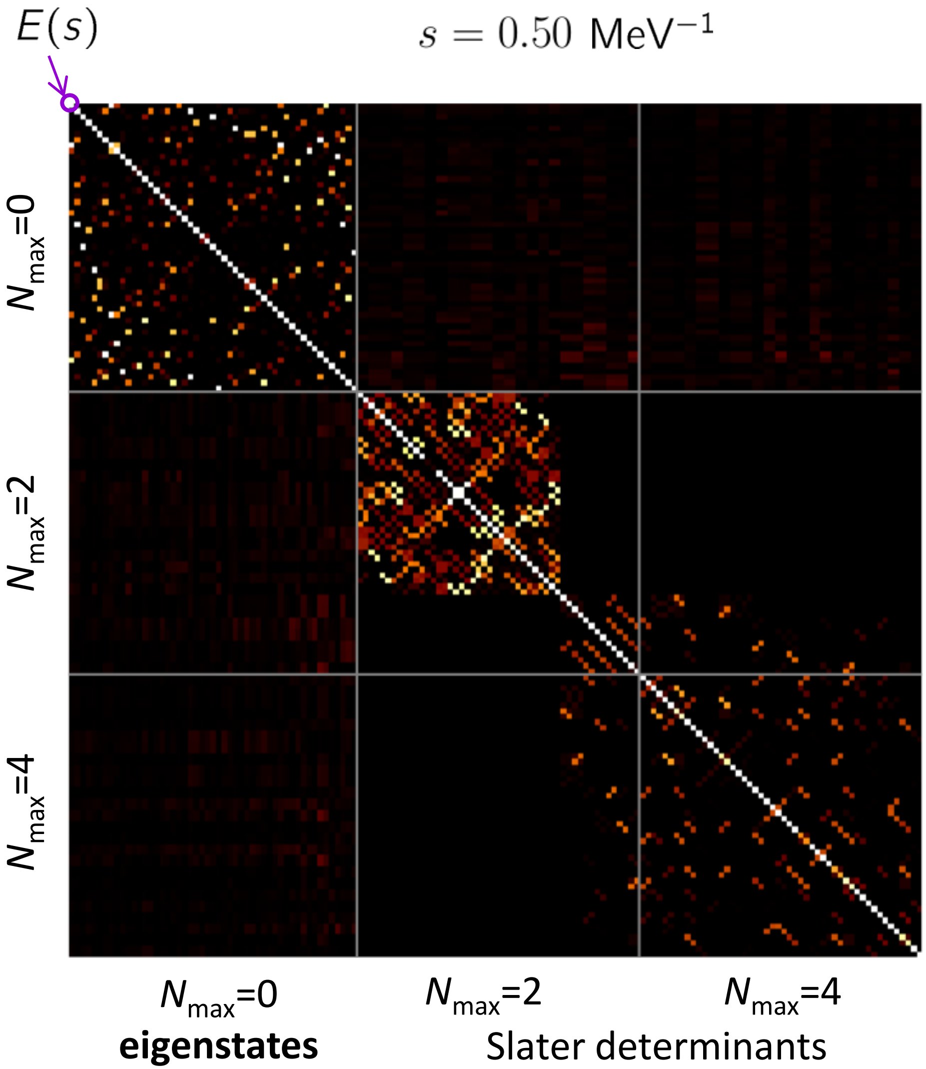

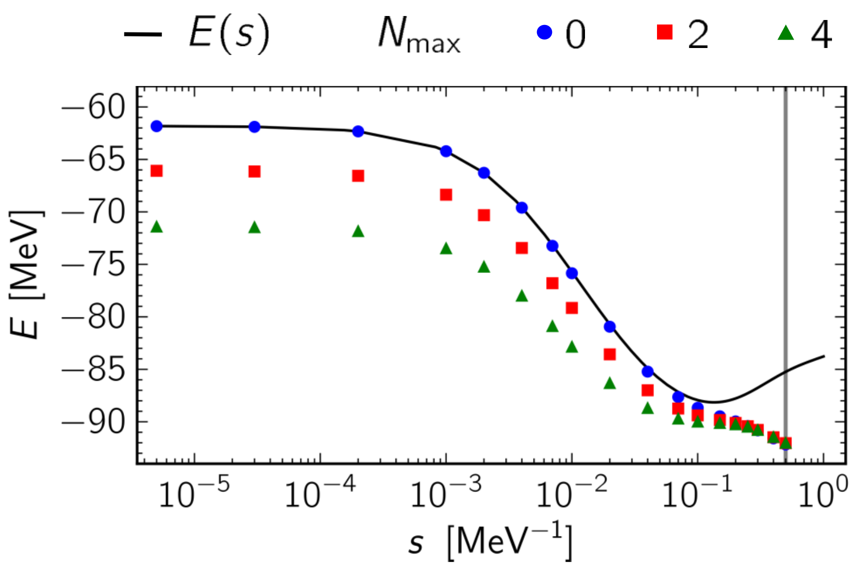

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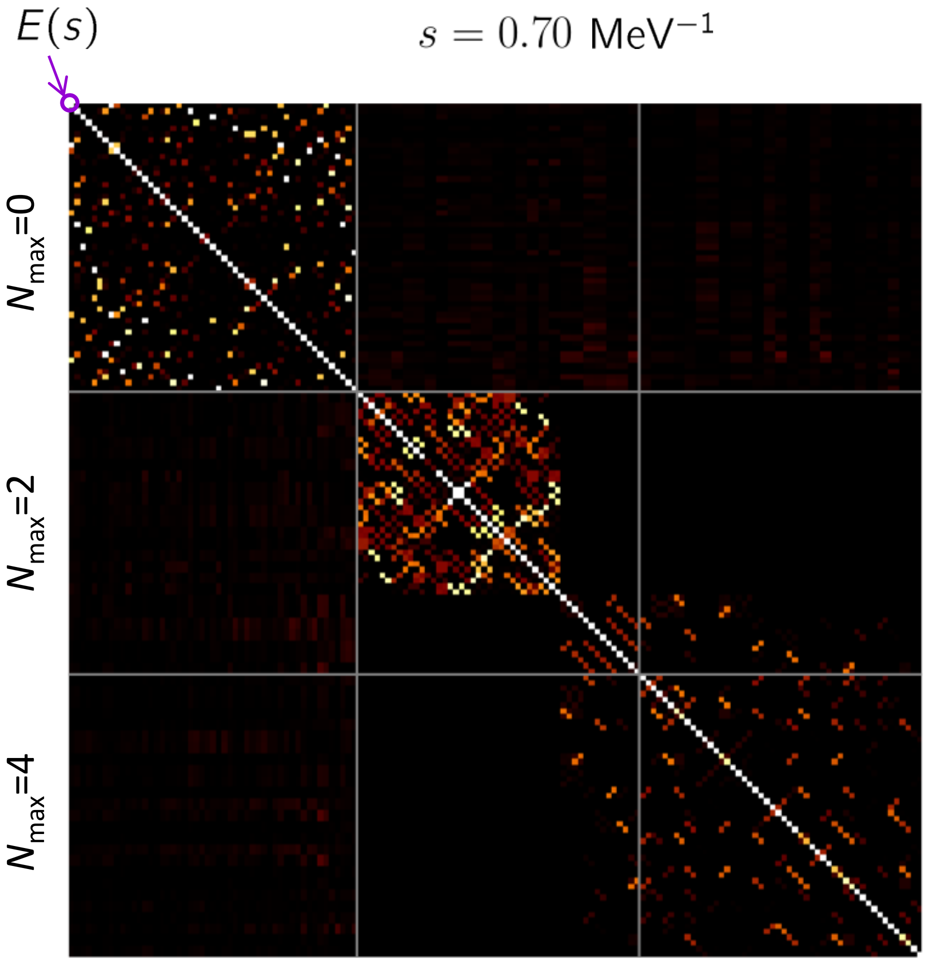

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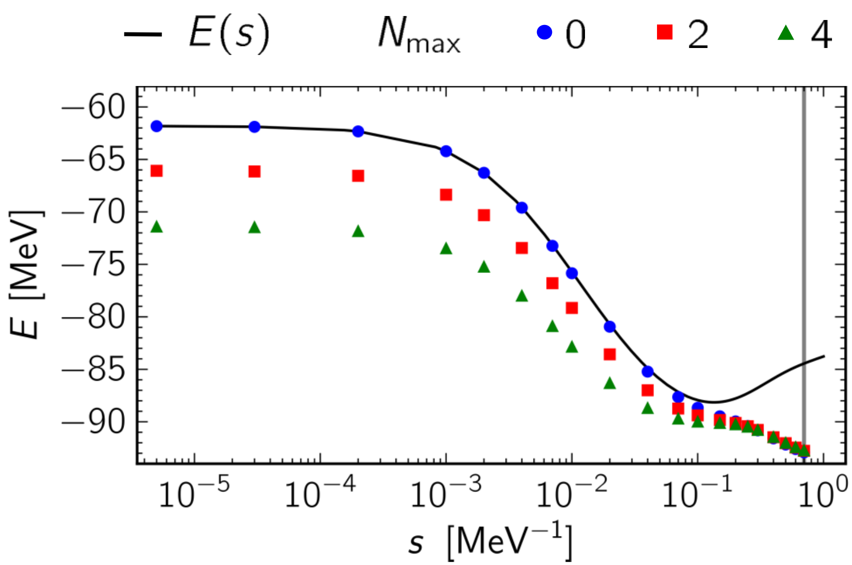

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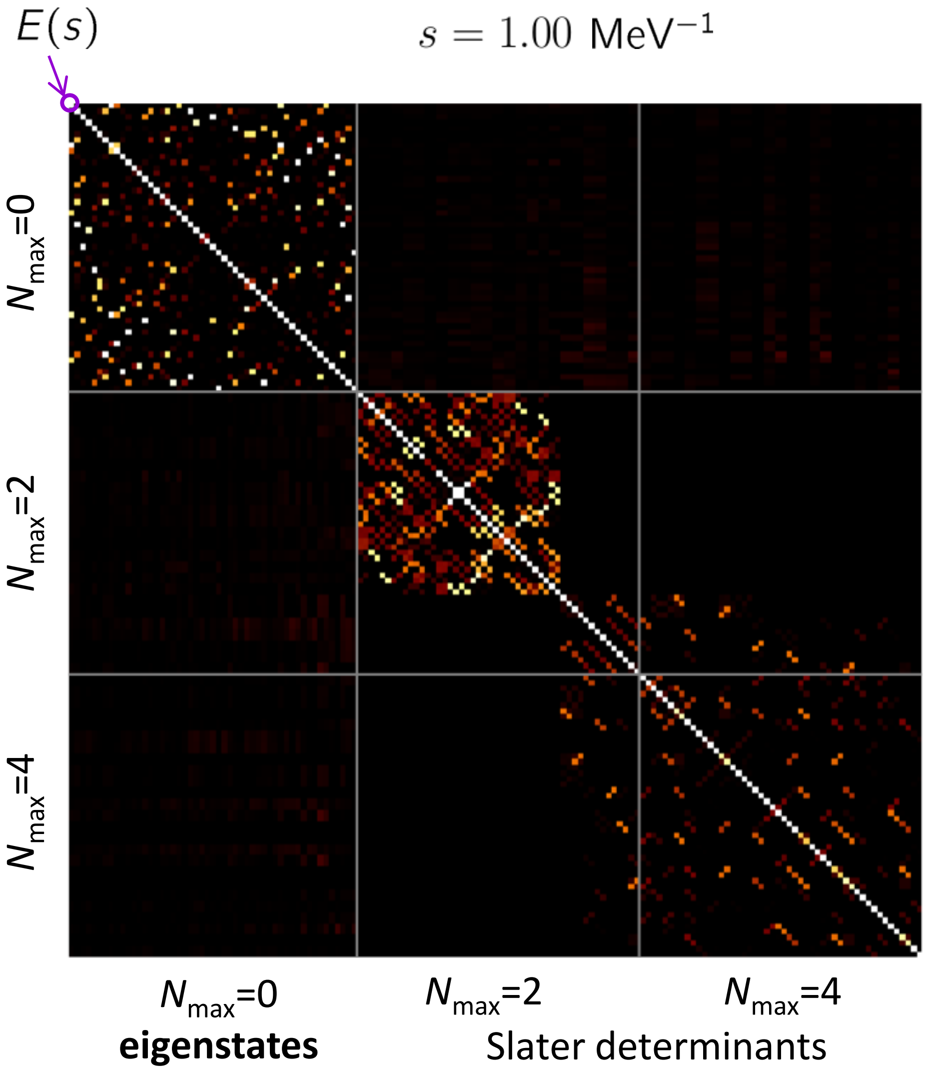

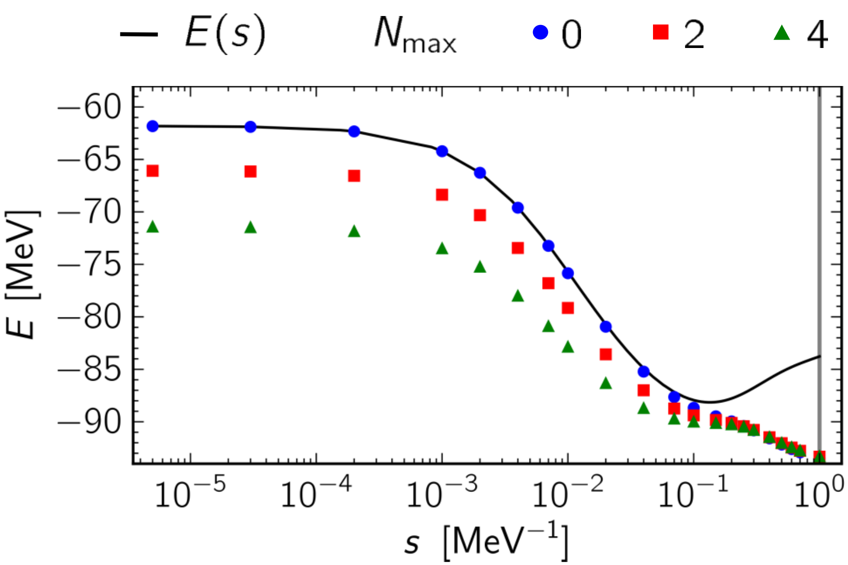

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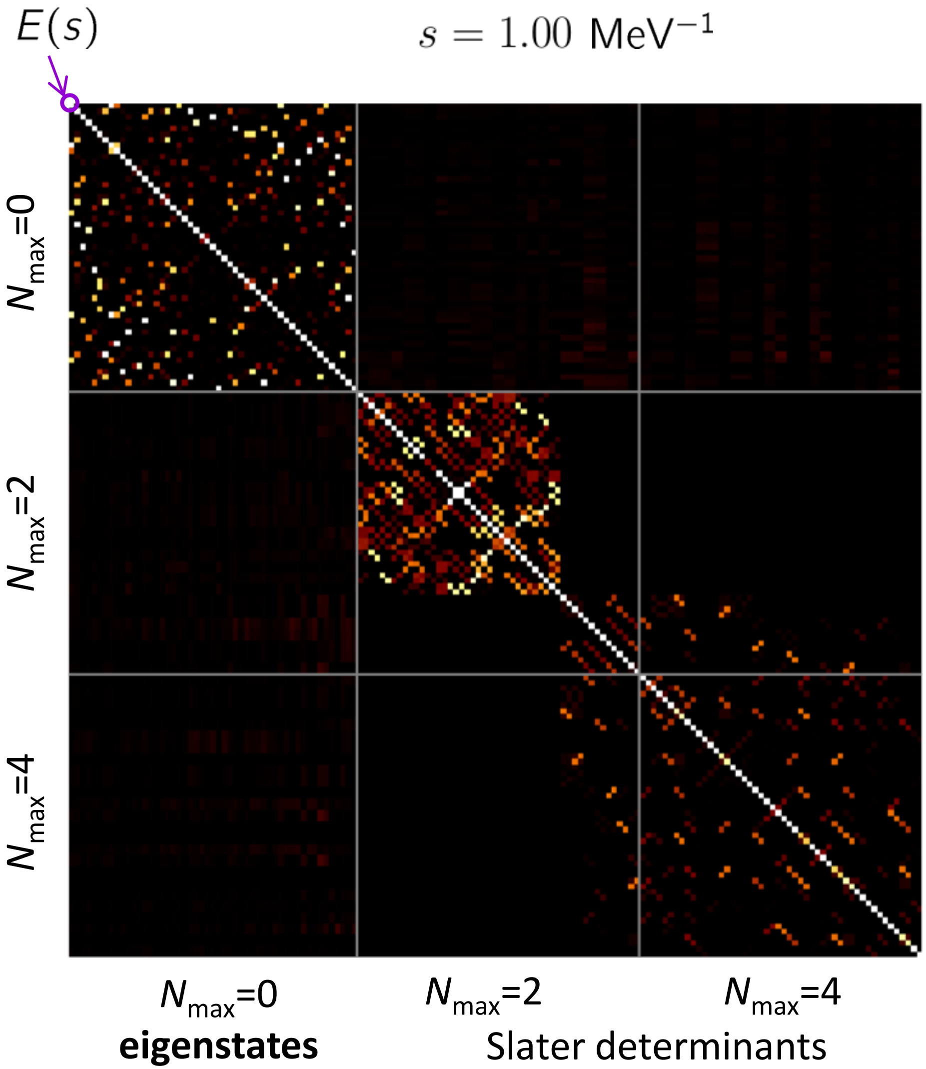

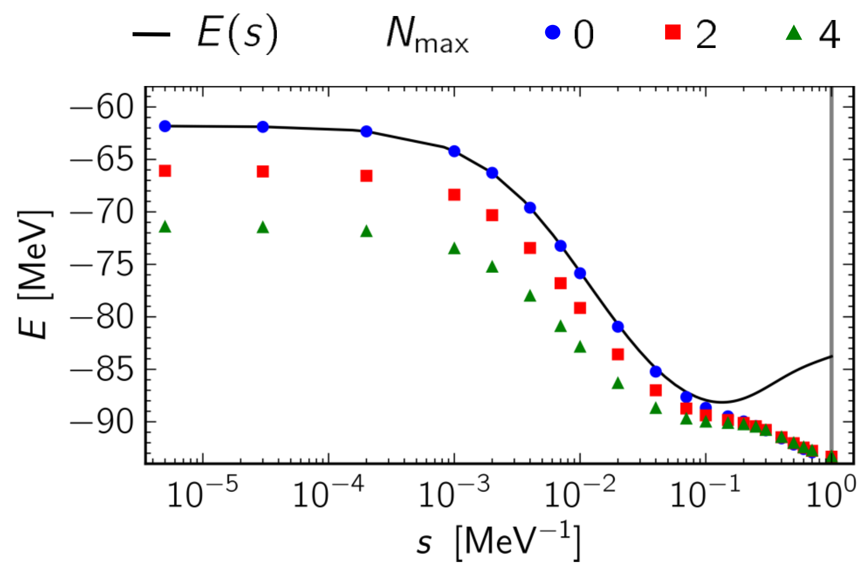

for sufficiently large flow parameter eigenvalues in N_{max}=0, 2 and 4 equal

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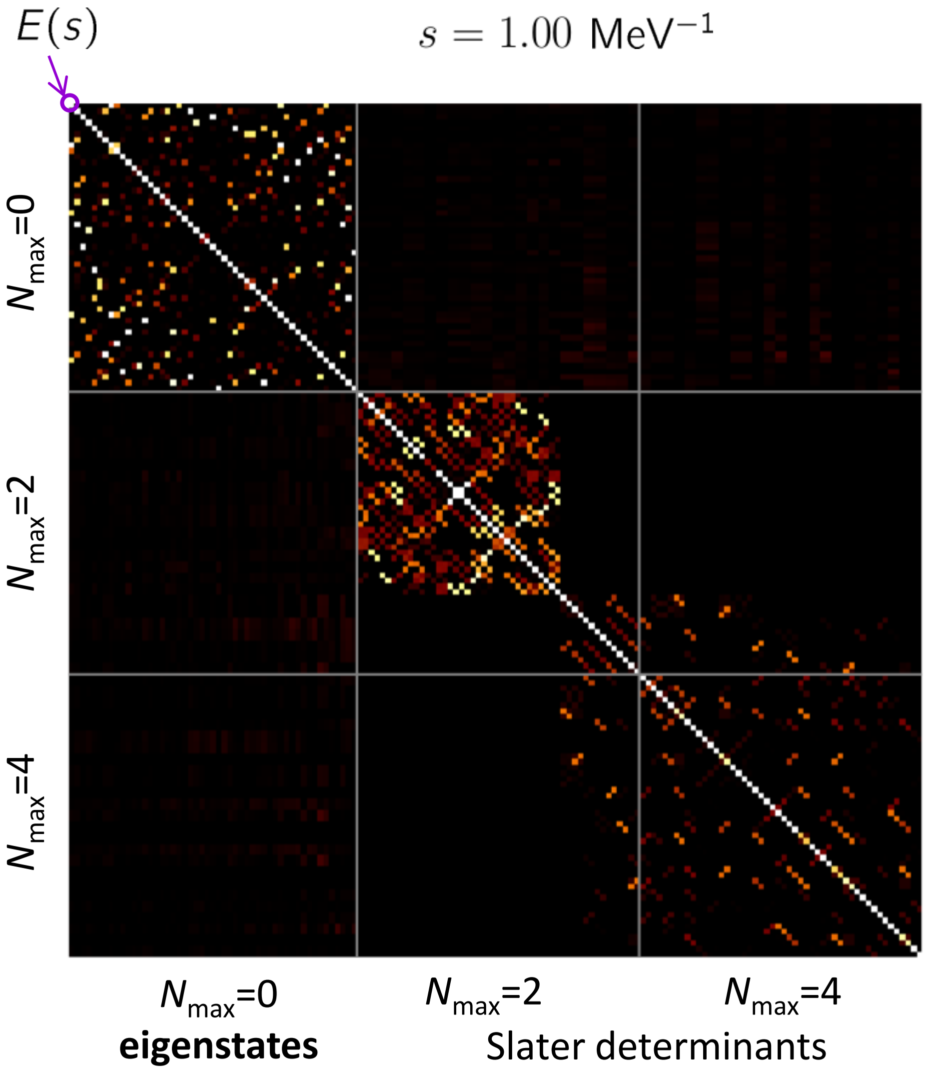

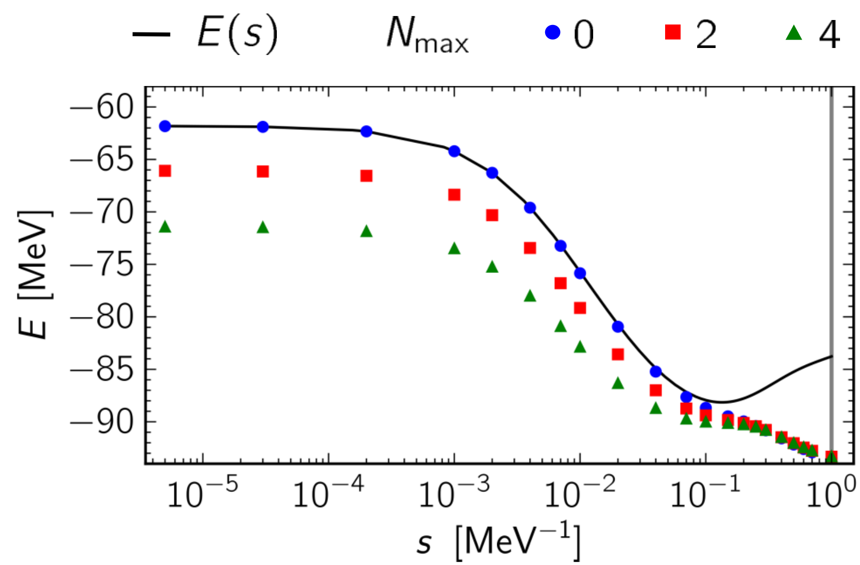

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IM-SRG decouples reference state from N_{max}=2 and 4 spaces

In-Medium No-Core Shell Model

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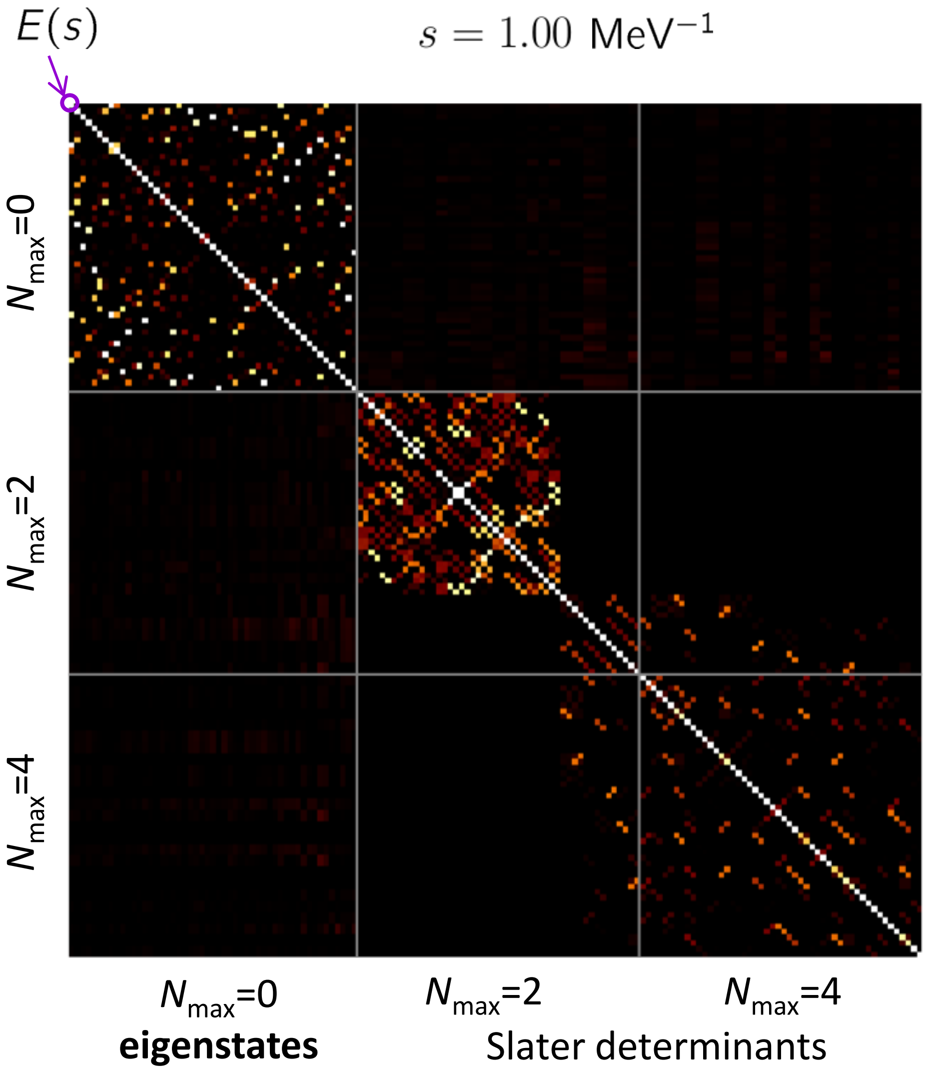

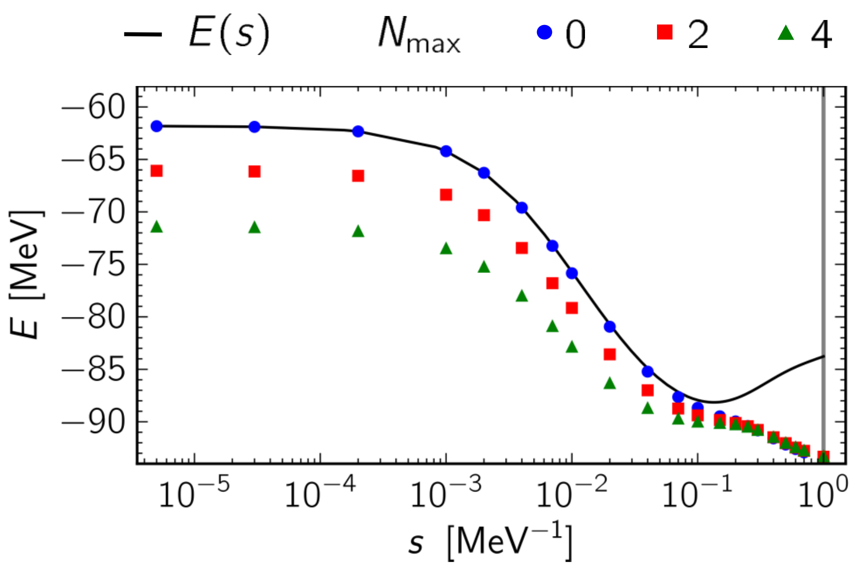

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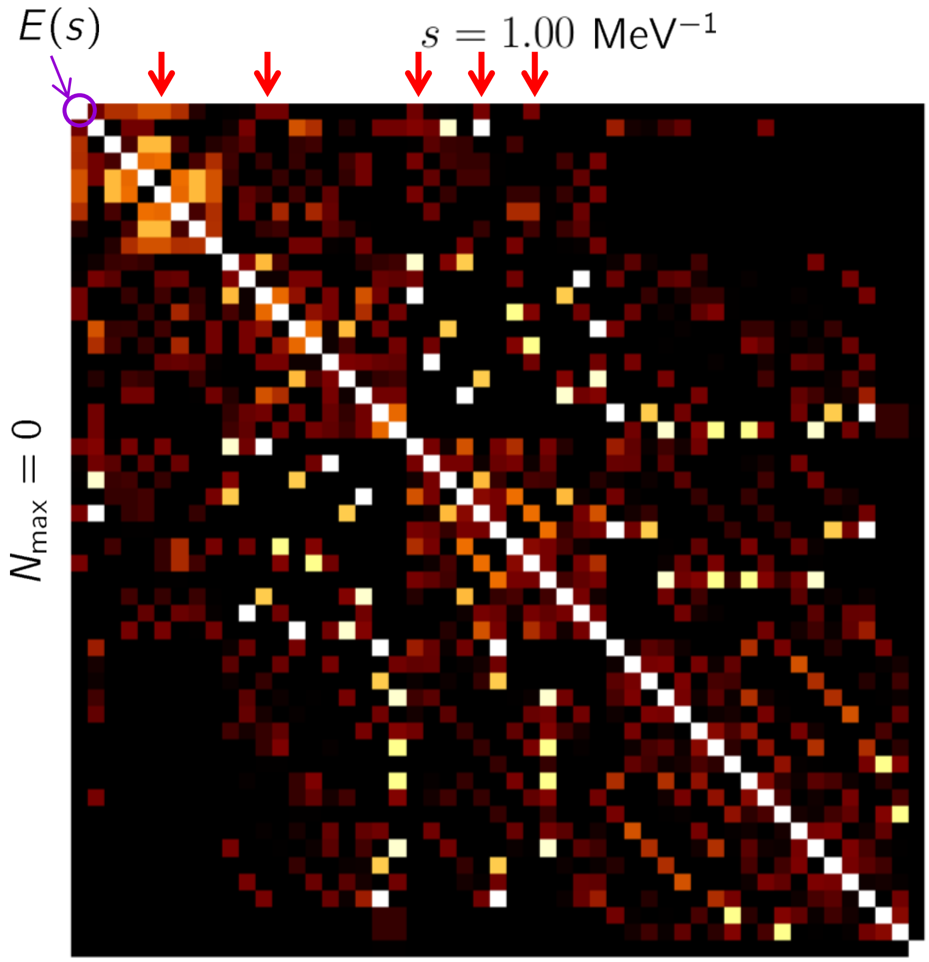
IM-SRG decouples reference state from N_{max} =2 and 4 spaces

→ Why do $E(s)$ and N_{max}=0 eigenvalue differ?

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



N_{max}=0 eigenstates

first basis state = reference state

- N_{max}=0 states couple to reference state $|\Psi_{ref}\rangle$
- $E(s)$ and N_{max}=0 eigenvalue not identical

diagonalization of evolved Hamiltonian necessary

Evolution of Ground-State Energy

chiral NN+$3N_{NO2B}$

$\Lambda_{3N} = 400\,\text{MeV}$

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

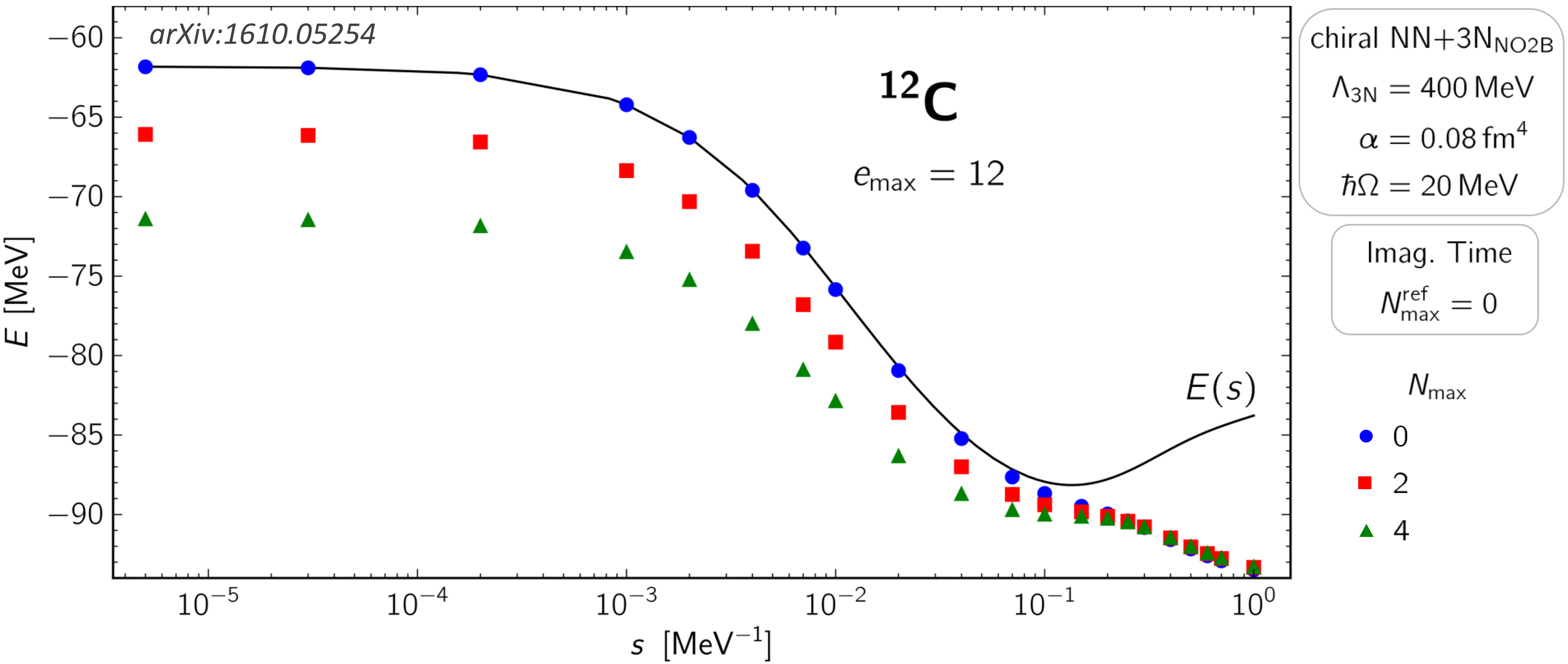
$\hbar\Omega = 20\,\text{MeV}$

Imag. Time

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

Results

Evolution of Ground-State Energy



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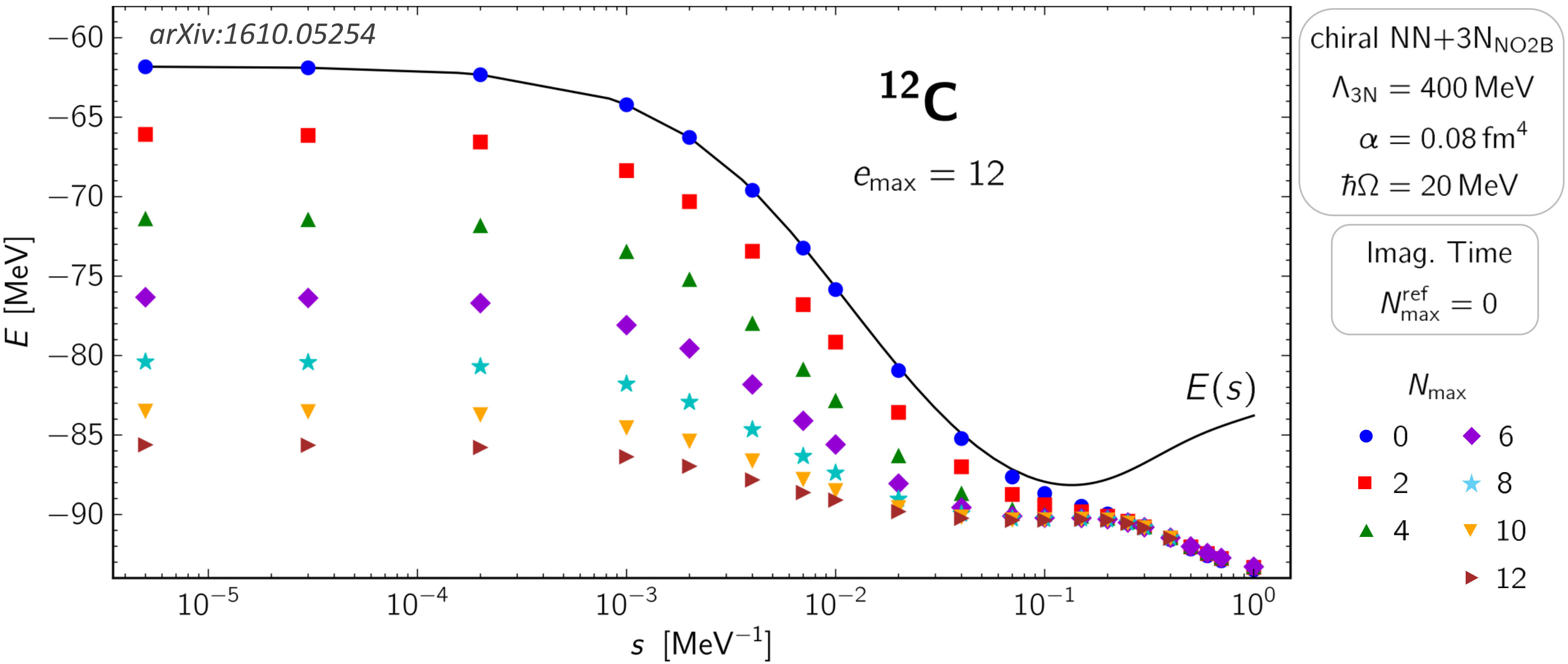

- drastically enhanced model-space convergence for IM-NCSM

Results
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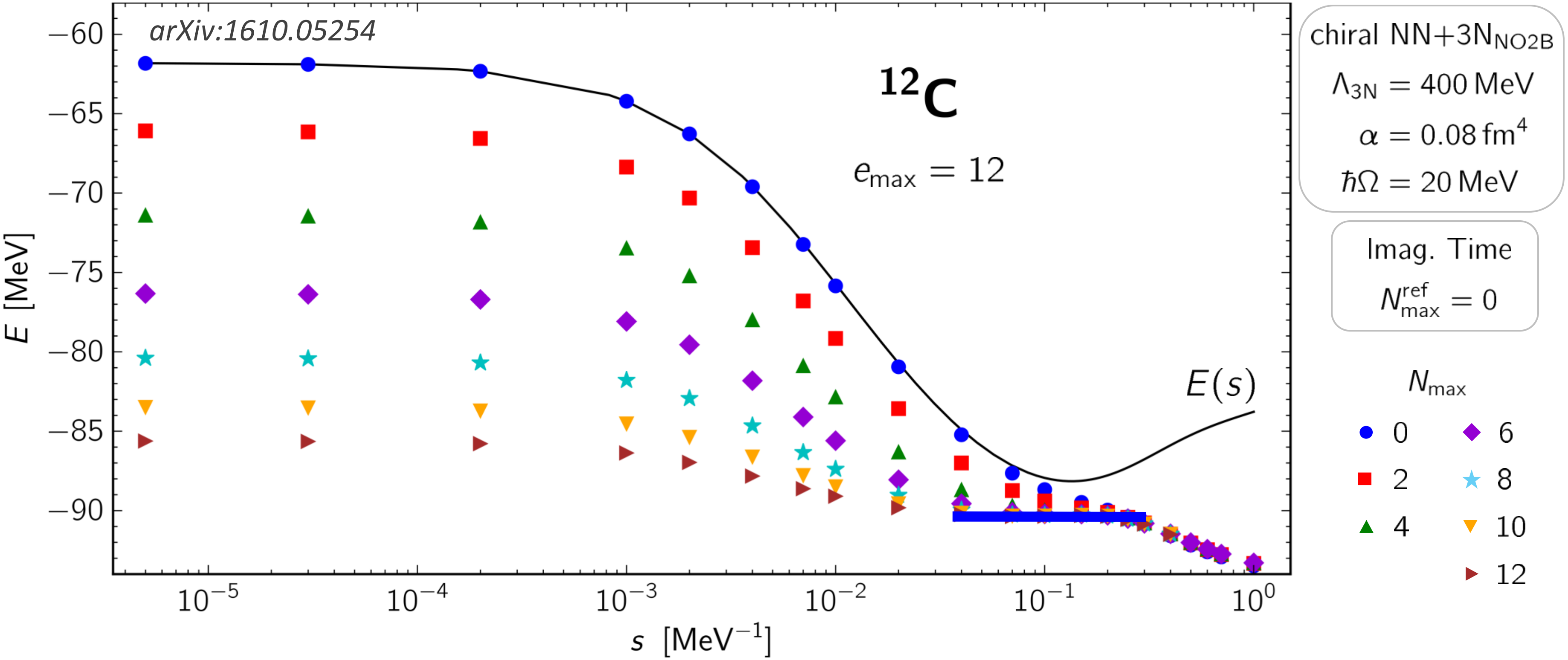

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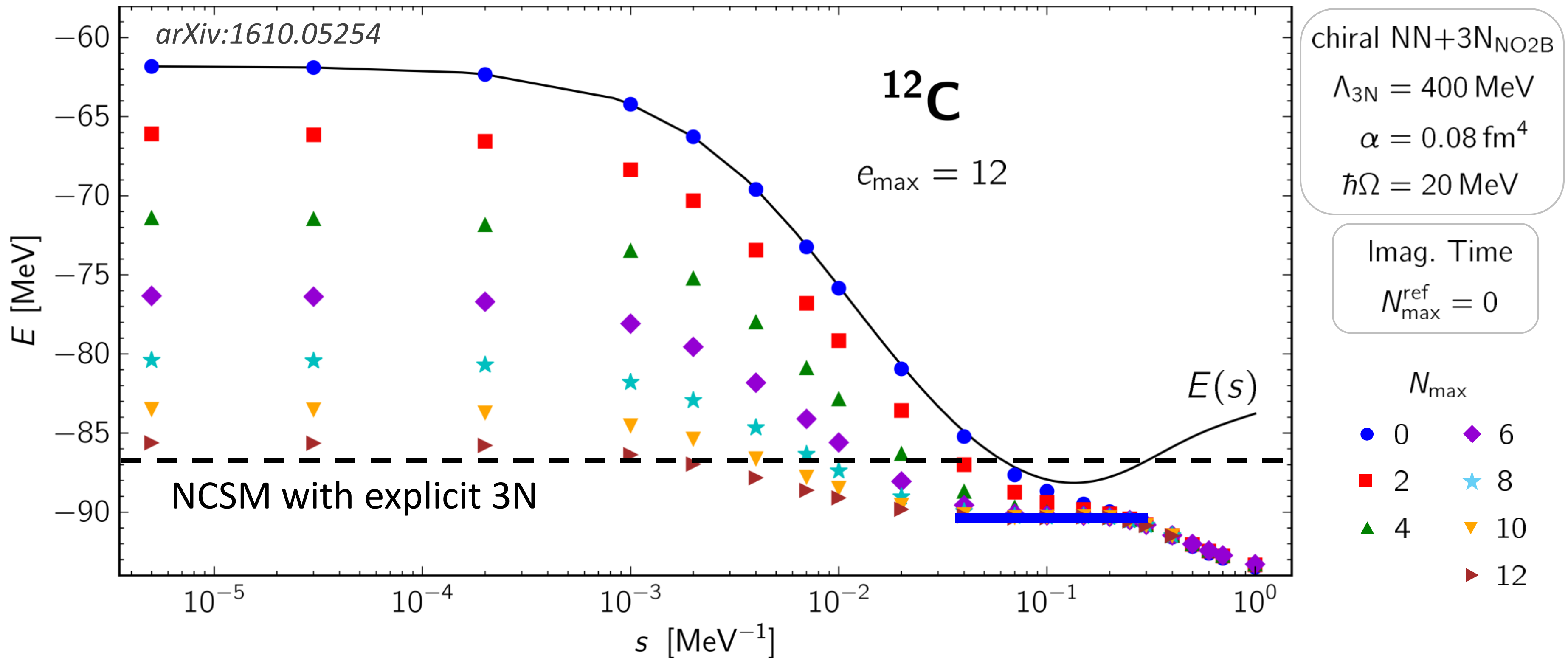

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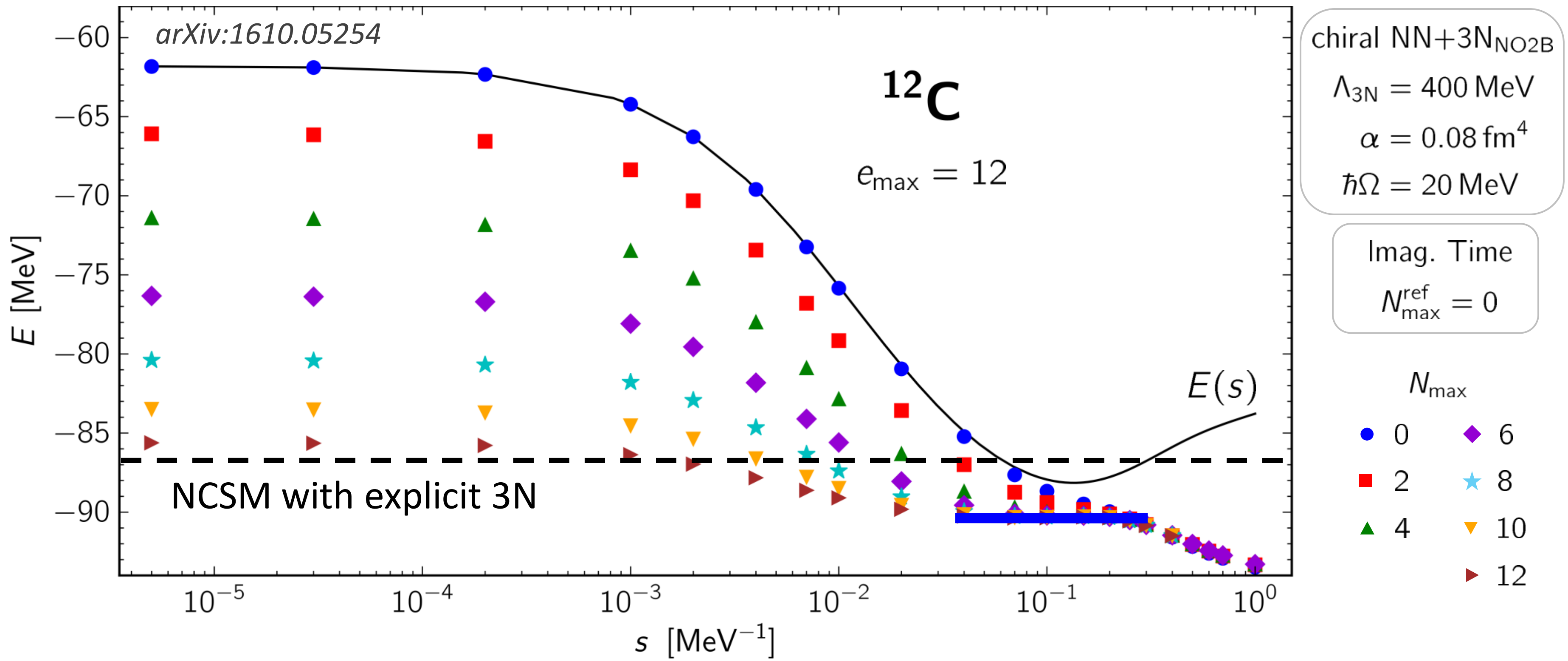

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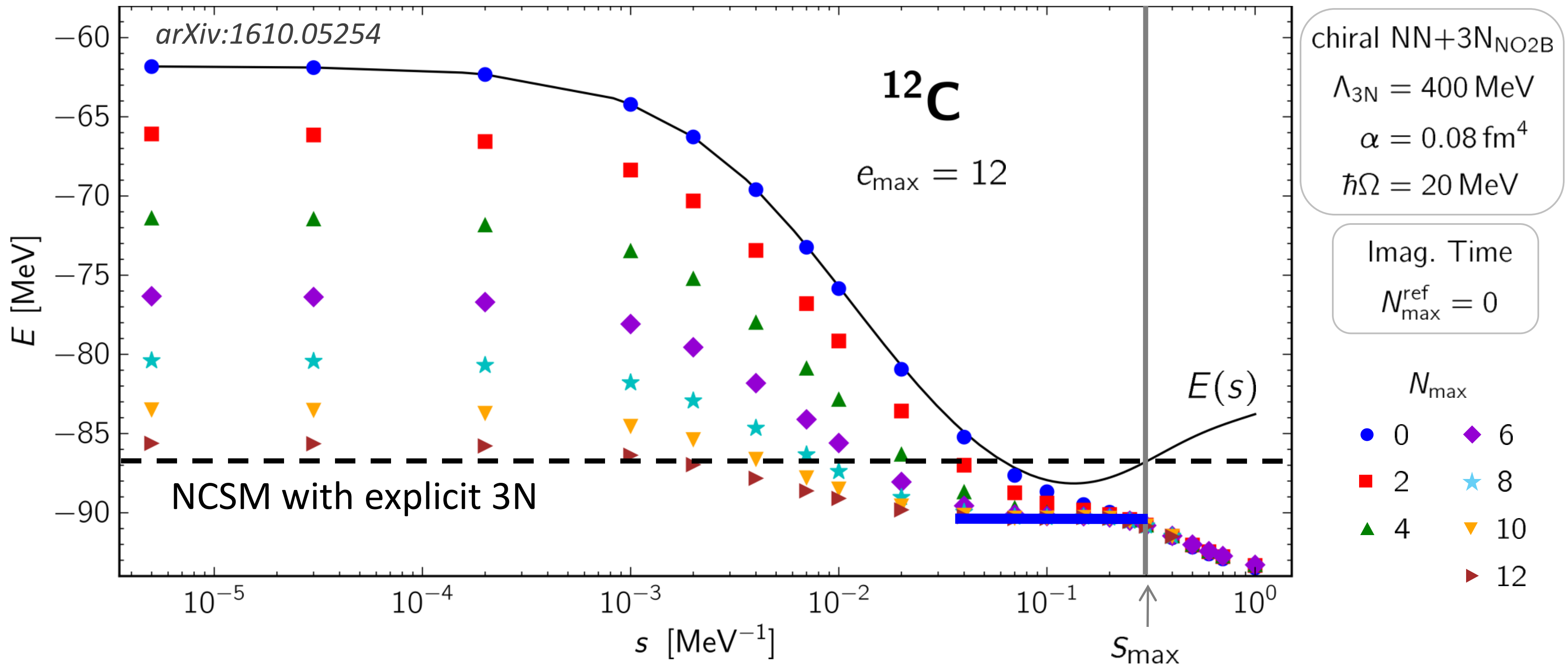

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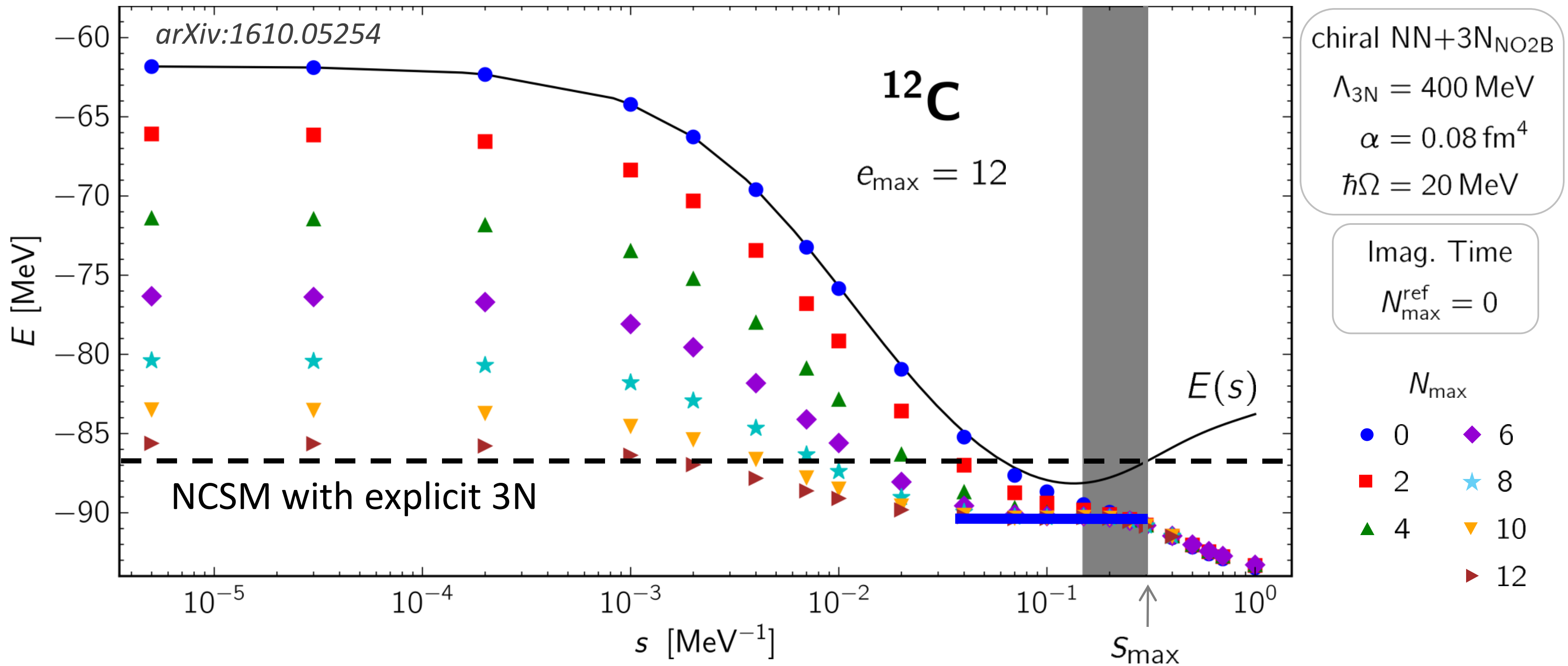

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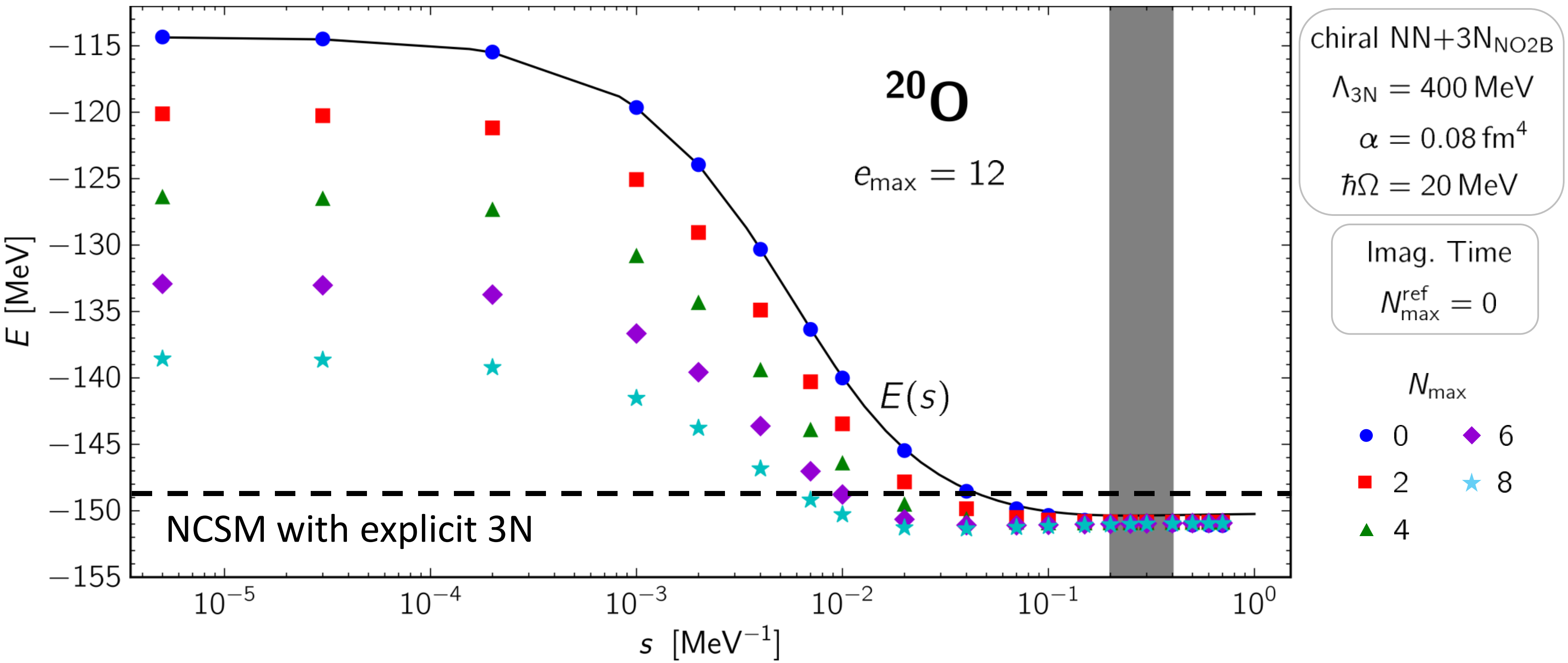
- for $s > 0.3\ \mathrm{MeV}^{-1}$ induced many-body contribution becomes significant

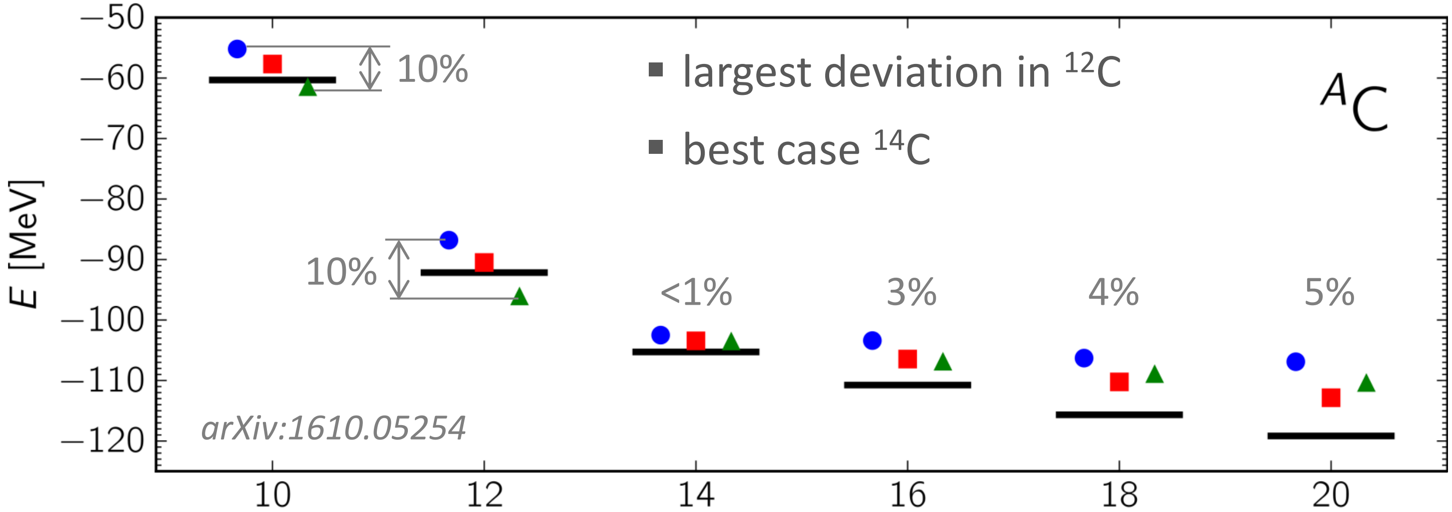
Evolution of Ground-State Energy

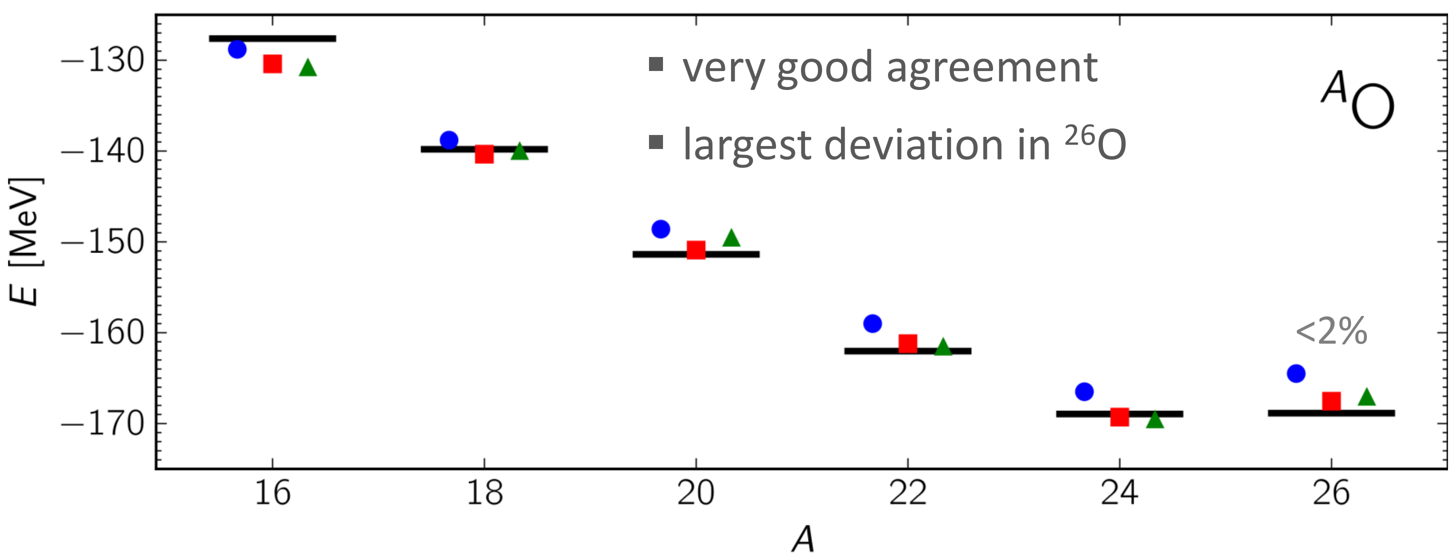


- $E(s)$ more robust than in ^{12}C case
- NO2B approximation + induced many-body contribution = 2.3 MeV (< 2 %)

Results

NCSM vs. IM-NCSM vs. MR-IM-SRG





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

$\Lambda_{3N} = 400$ MeV

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

$\hbar\Omega = 20$ MeV

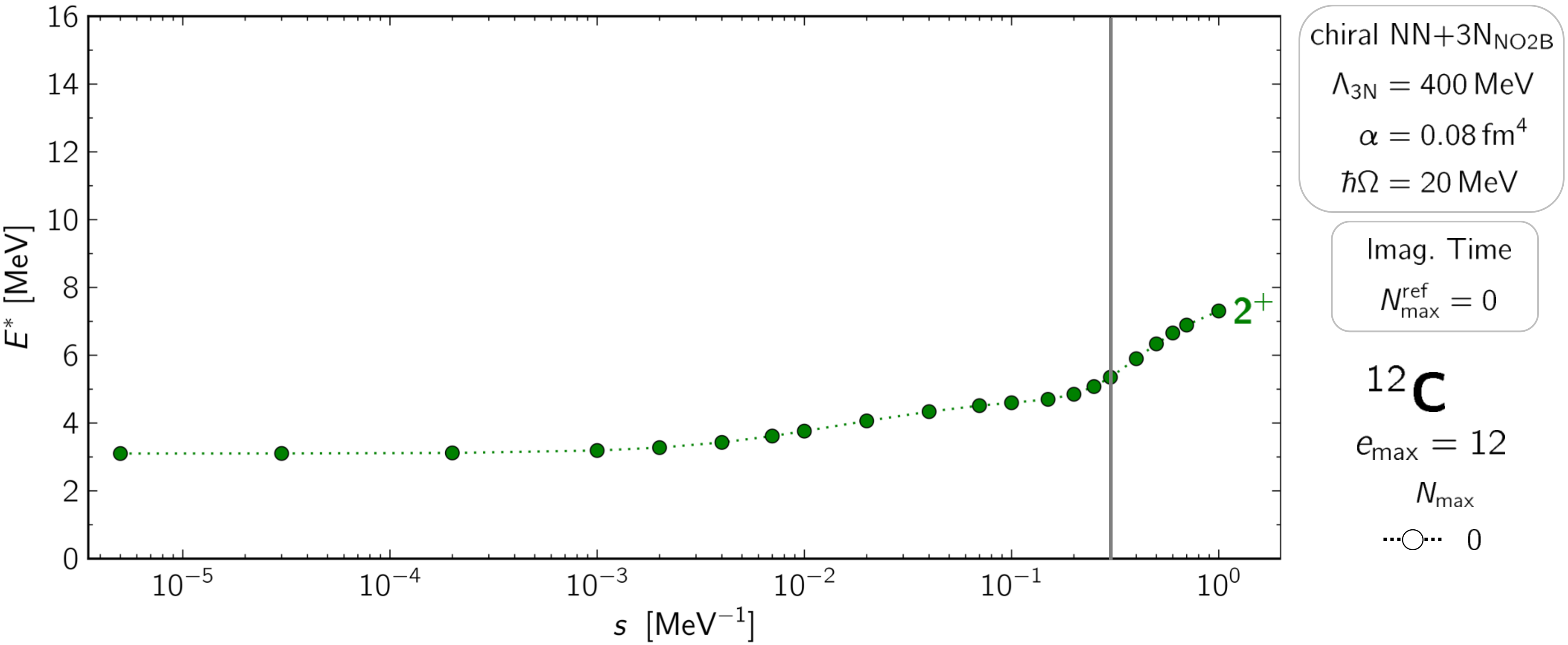
Imag. Time

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

$e_{\max} = 12$

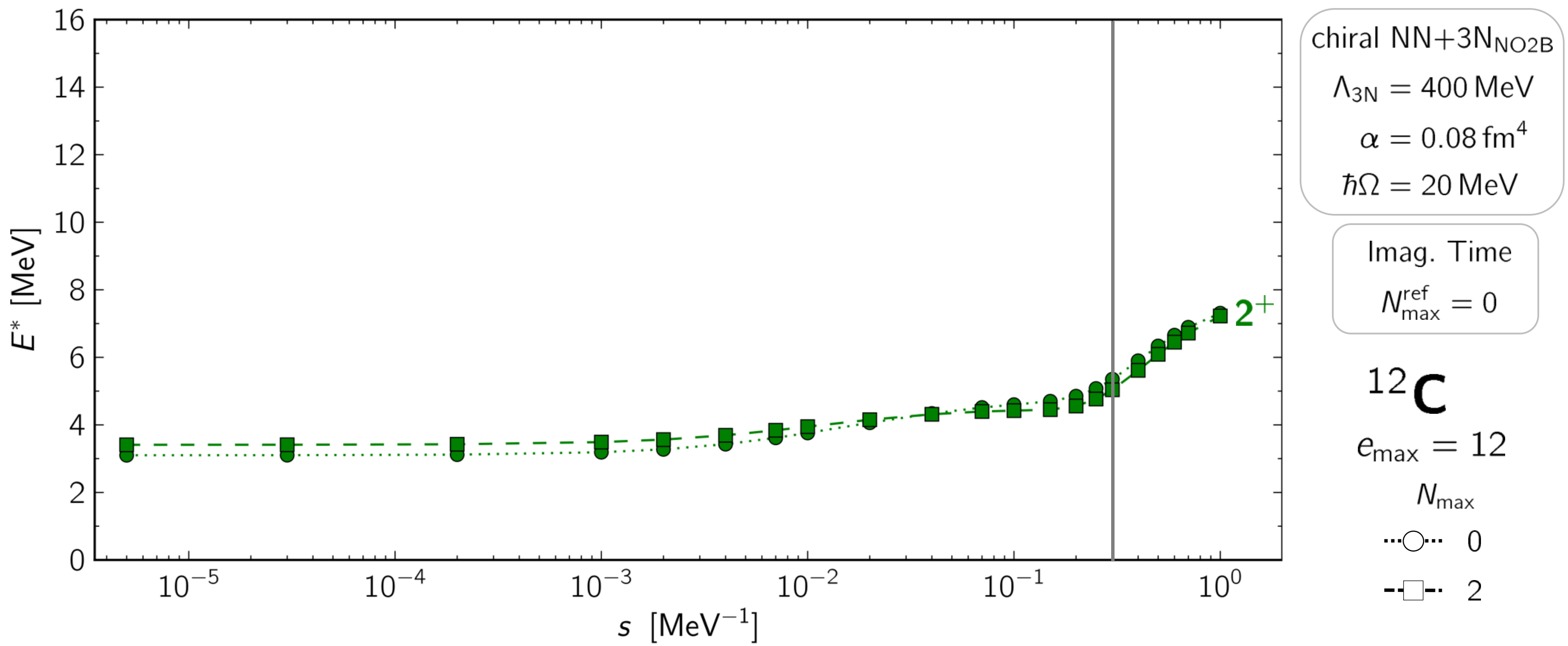
- ● NCSM @ $N_{\max}$ extrap.
- ■ IM-NCSM @ $N_{\max}$=4
- ▲ MR-IM-SRG (HFB, White)
- — Experiment

Evolution of Excitation Energies



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

Evolution of Excitation Energies



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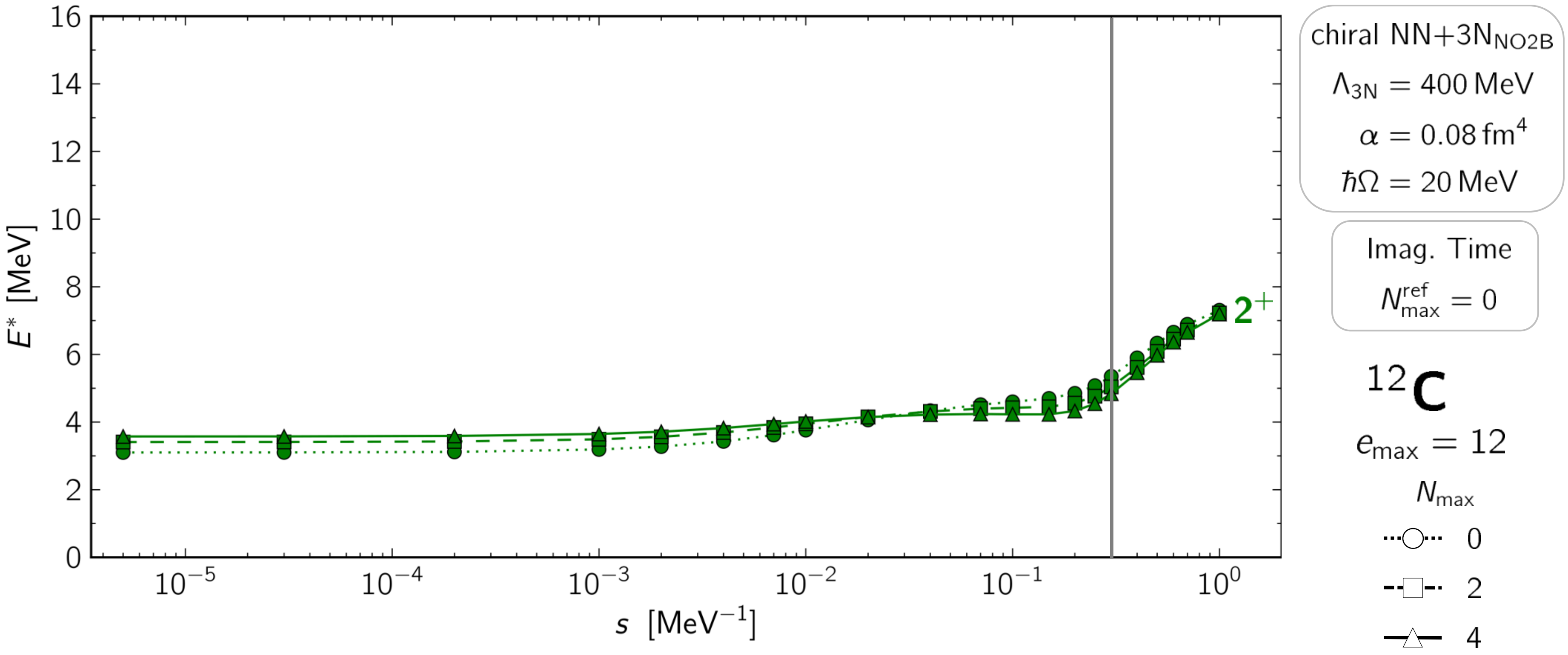
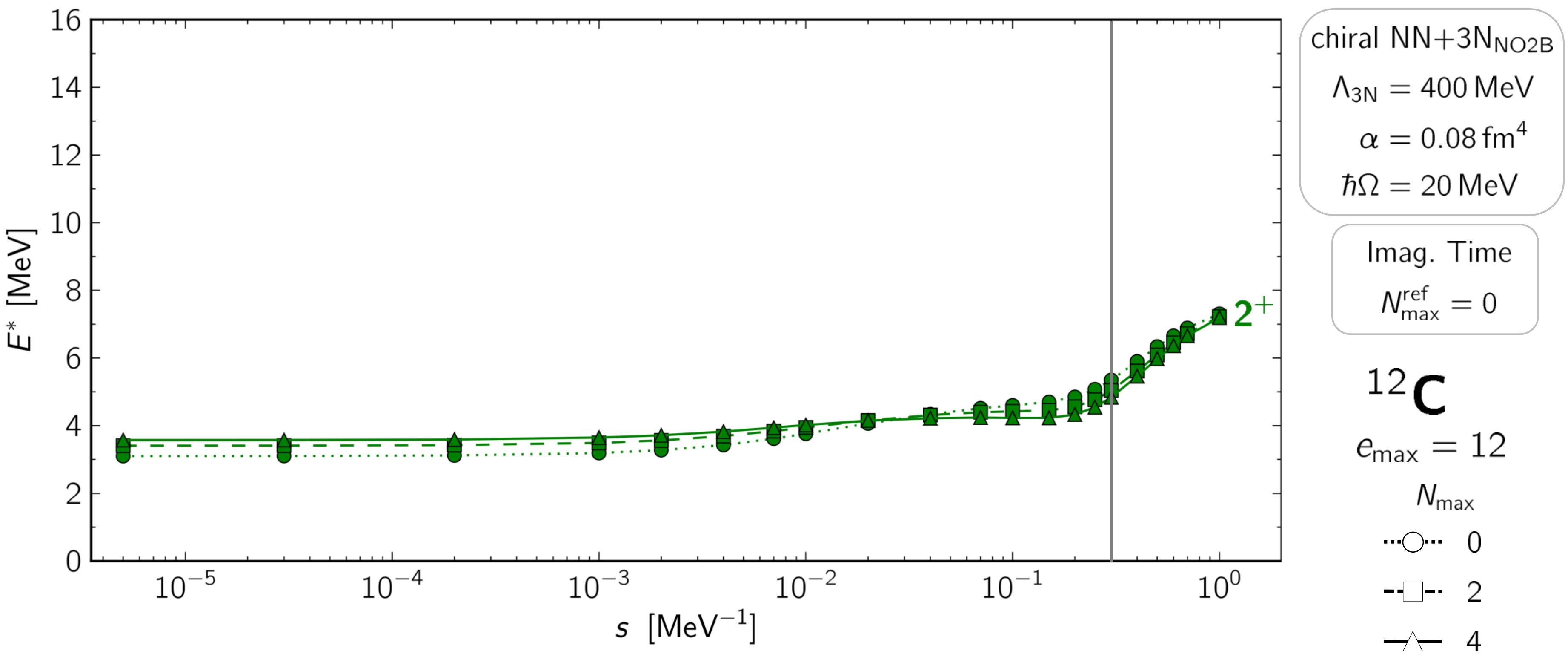
Evolution of Excitation Energies



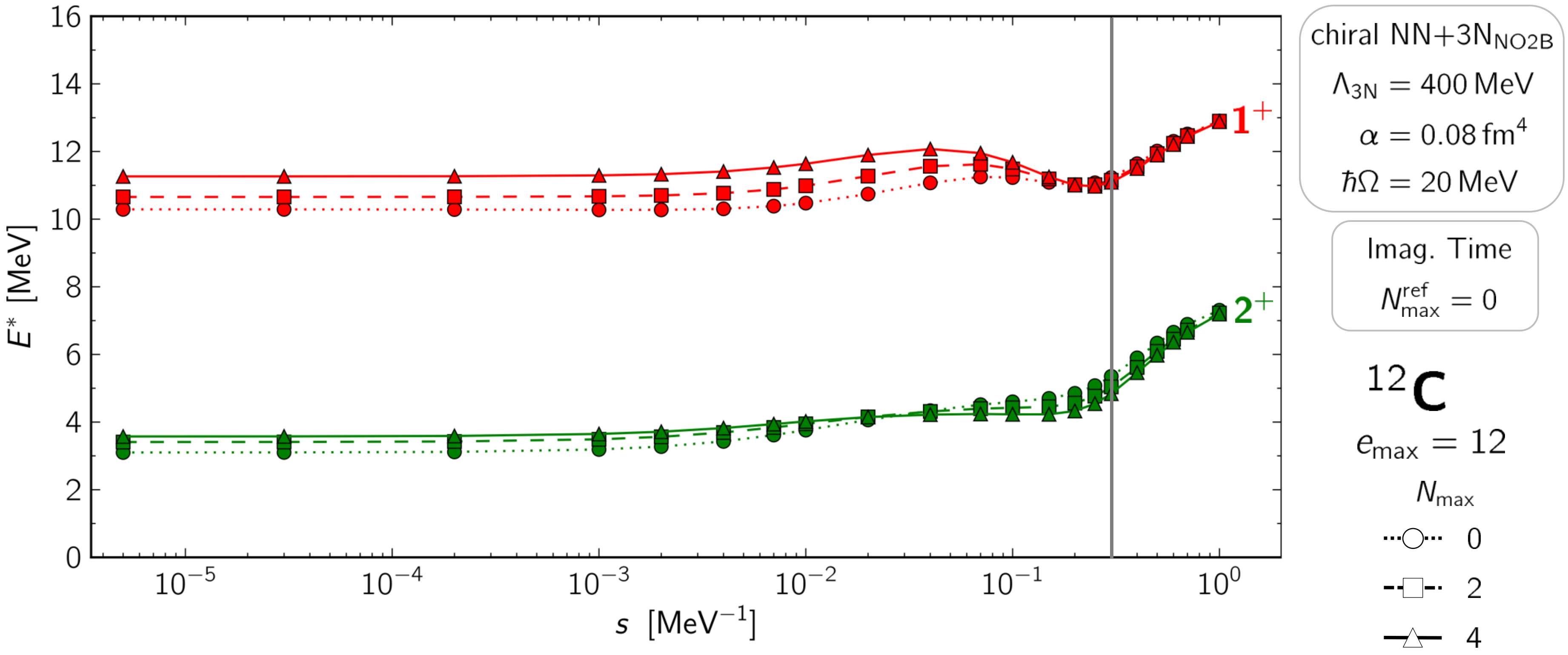
- E^* of 2^+ increases abruptly at the end due to kink in ground-state energy

Results
Evolution of Excitation Energies



- E^* of 2^+ increases abruptly at the end due to kink in ground-state energy
- N_{max} convergence **from above in decoupled regime** → variational principle

Results
Evolution of Excitation Energies



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Results
Evolution of Excitation Energies

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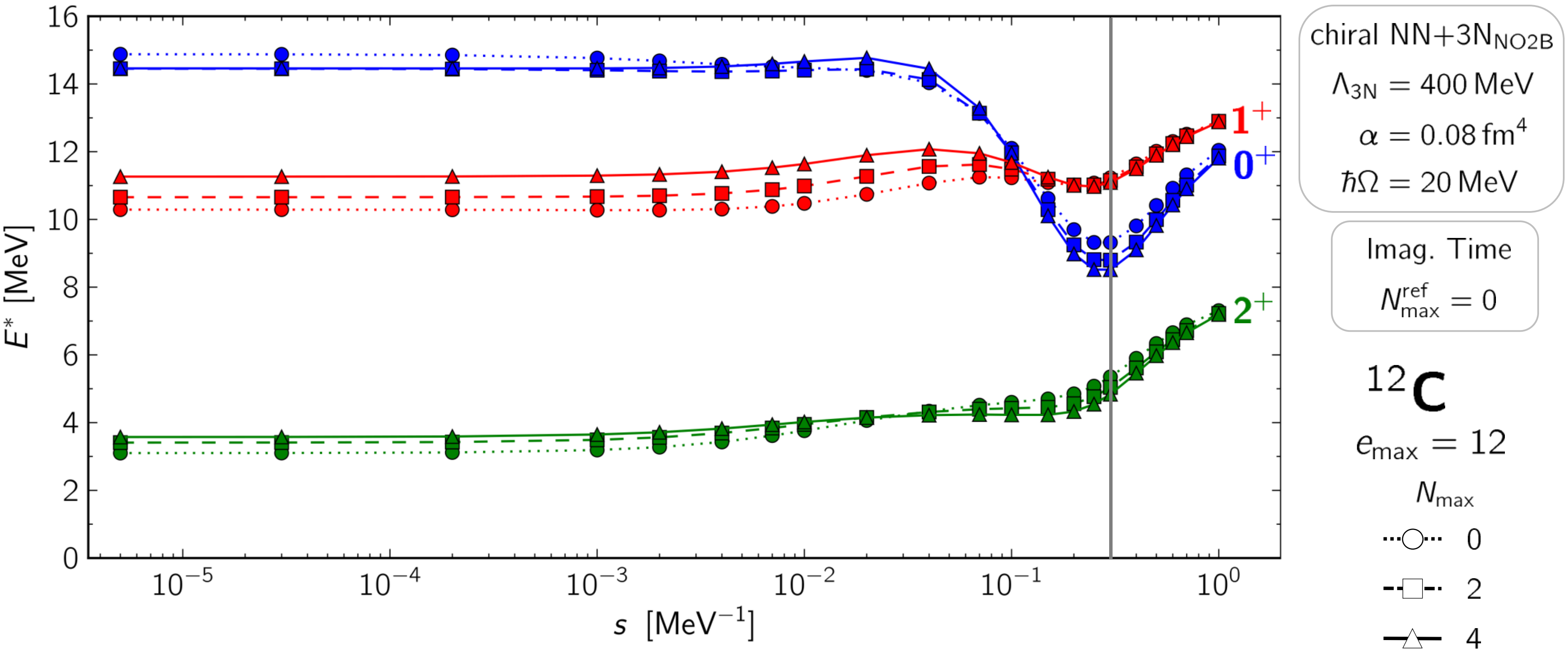

- E^* of 2^+ increases abruptly at the end due to kink in ground-state energy
- N_{max} convergence **from above in decoupled regime** → variational principle
- first excited 0^+ behaves differently and drops by ≈5 MeV → **Hoyle state?**

Signatures of Hoyle State in ^{12}C

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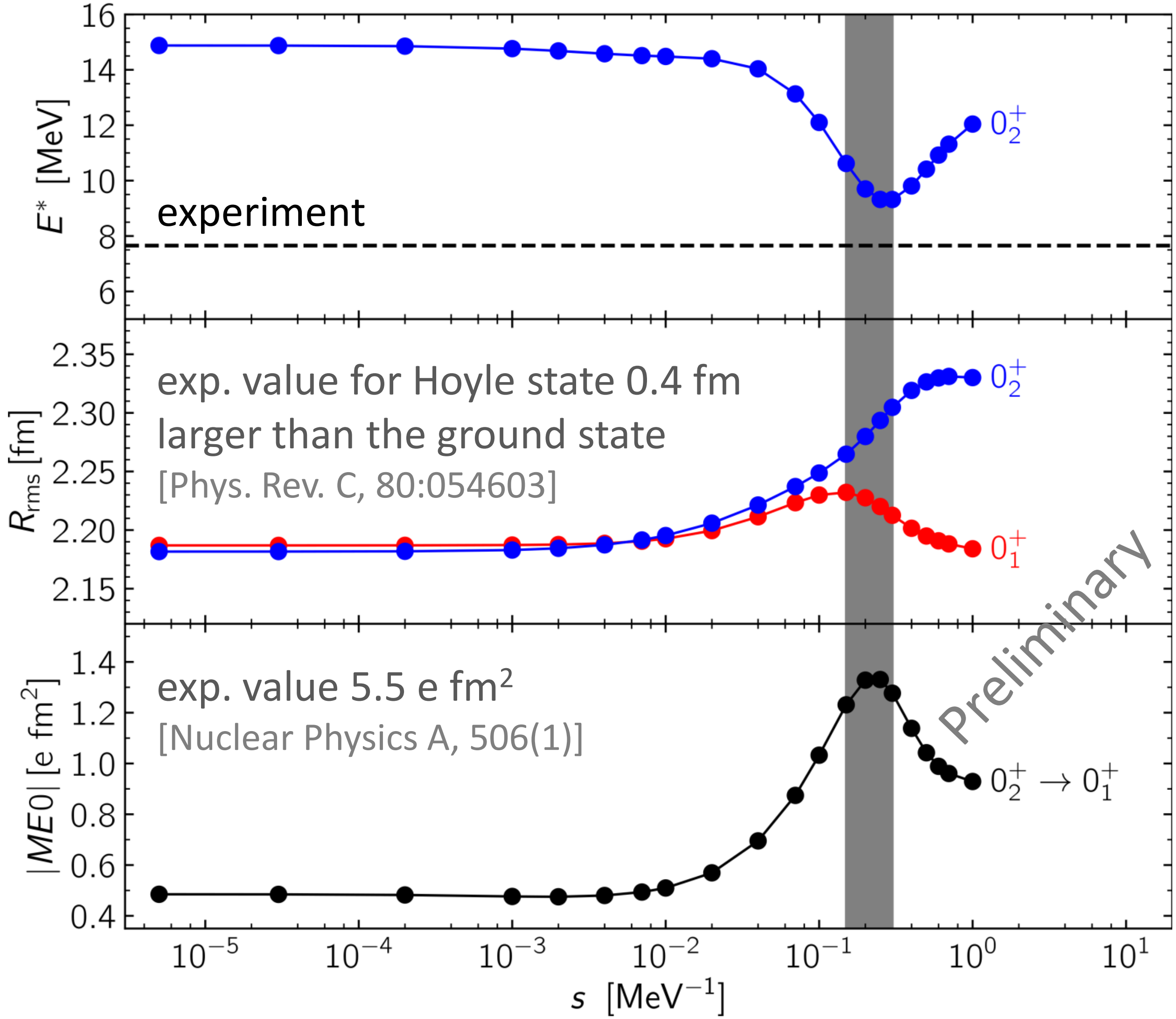


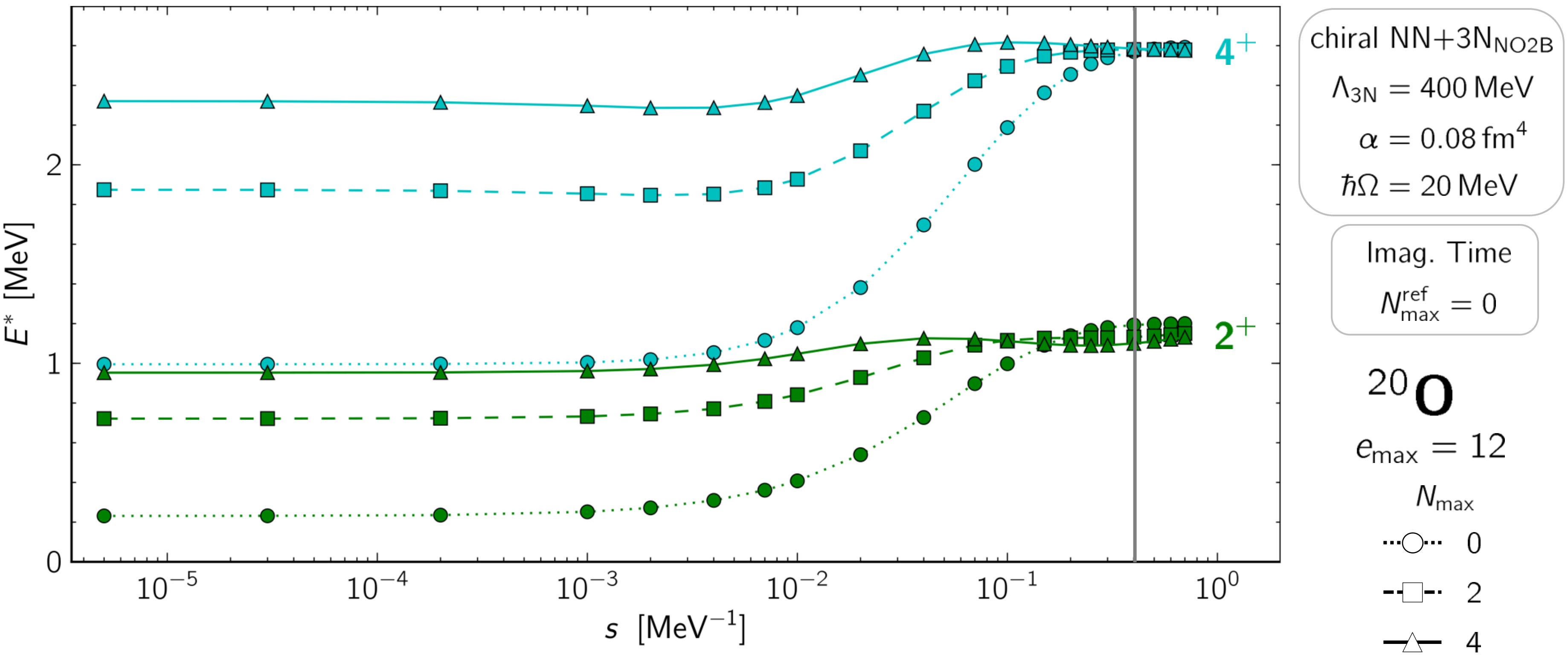
chiral NN+3N$_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08$ fm^4
$\hbar\Omega = 20$ MeV

$N_{max} = 0$
$e_{max} = 12$

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

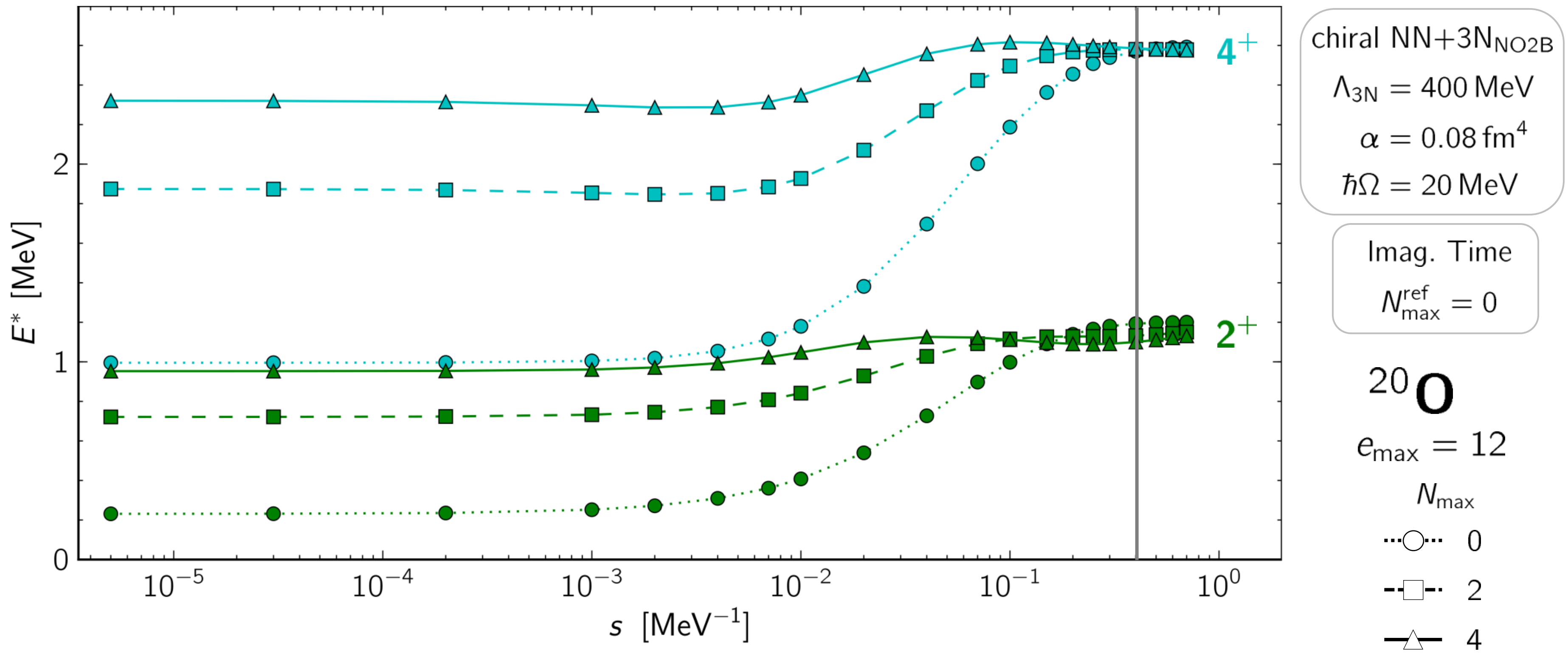
- trends are compatible with Hoyle-state interpretation
- need better control of induced many-body terms for quantitative statements

Results
Evolution of Excitation Energies



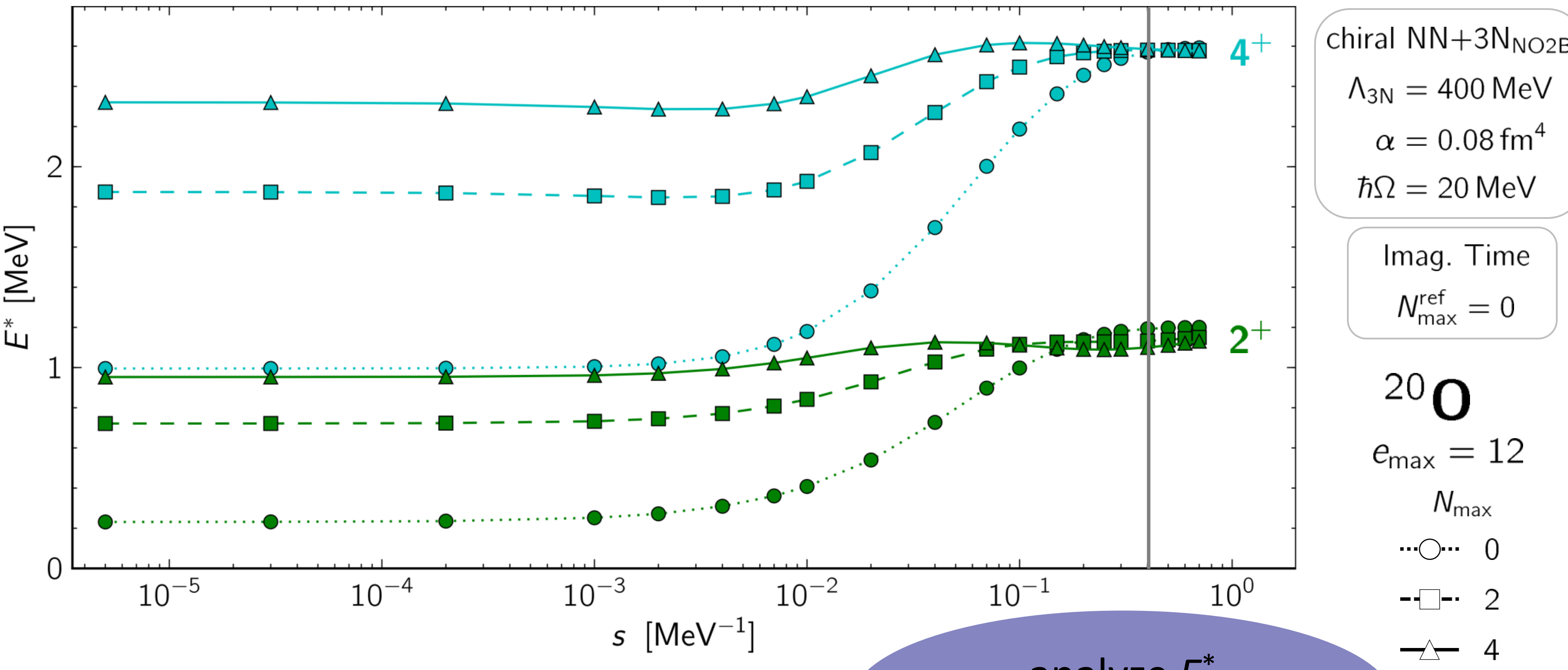
- large dependence on s in N_{max}=0
- dependence on s reduces with increasing N_{max}

Results
Evolution of Excitation Energies



- large dependence on s in N_{max}=0
- dependence on s reduces with increasing N_{max}
- E^* converges **monotonically from above** for evolved Hamiltonian

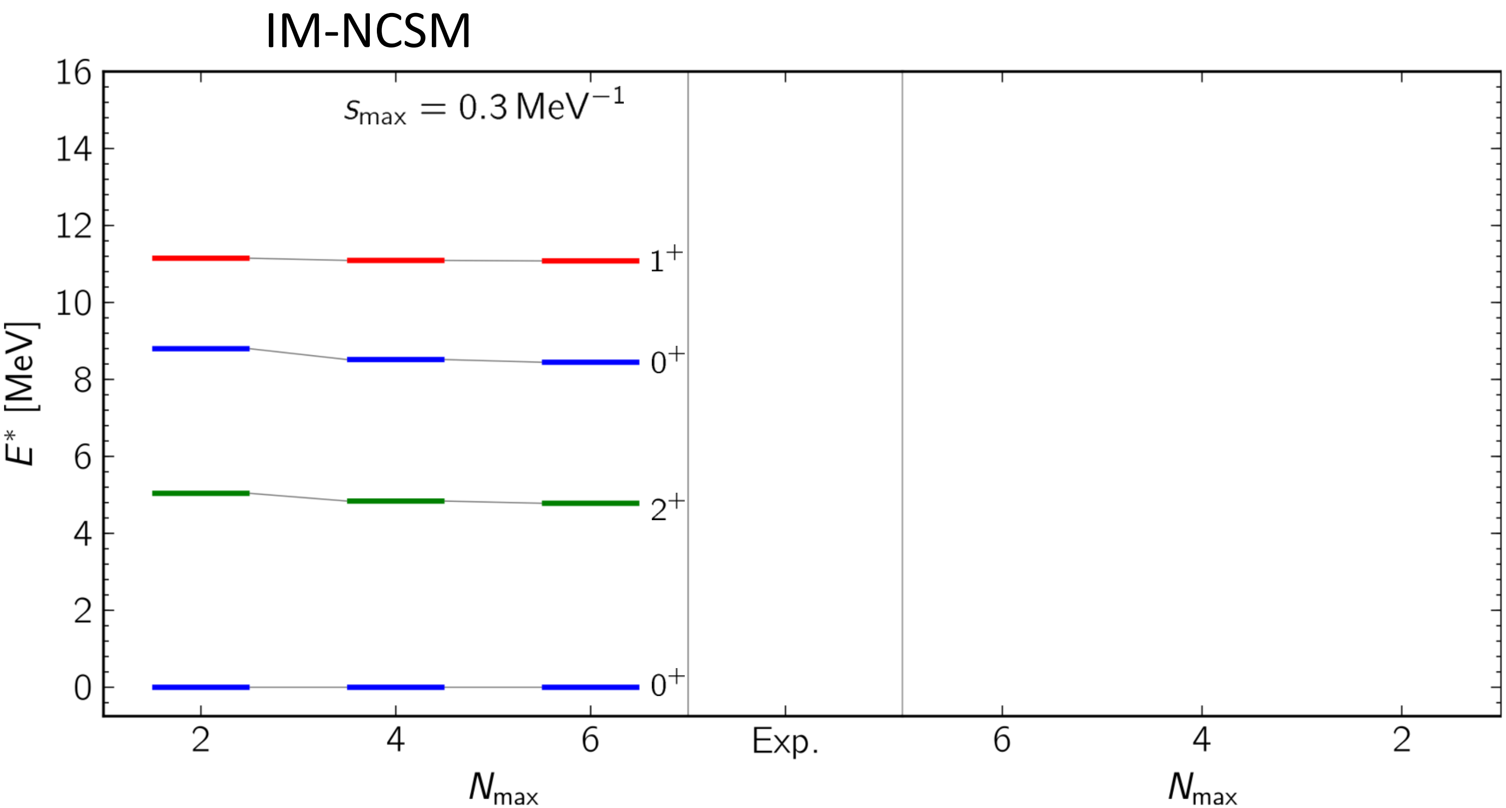
Evolution of Excitation Energies



analyze E^* as function of N_{max}

- large dependence on s in N_{max}=0
- dependence on s reduces with increasing N_{max}
- E^* converges **monotonically from above** for evolved Hamiltonian

Results
Spectra



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

$\hbar\Omega = 20\,\mathrm{MeV}$

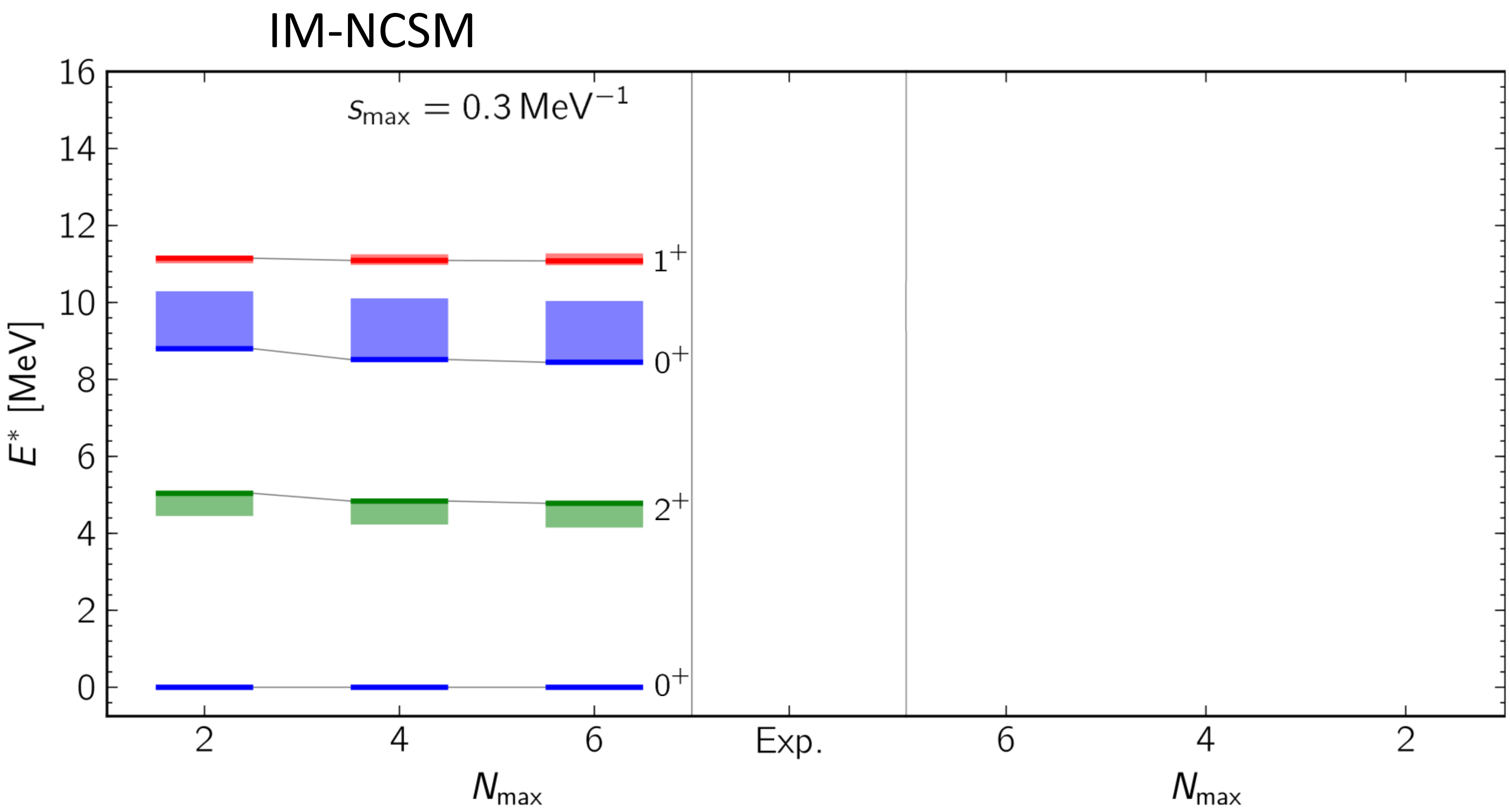
Imag. Time

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

^{12}**C**

$e_{\max} = 12$

Spectra



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$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20\,\mathrm{MeV}$

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

^{12}C
$e_{\max} = 12$

- uncertainty band due to flow-parameter variation between $s_{\max}/2$ and $s_{\max}$

Results
Spectra

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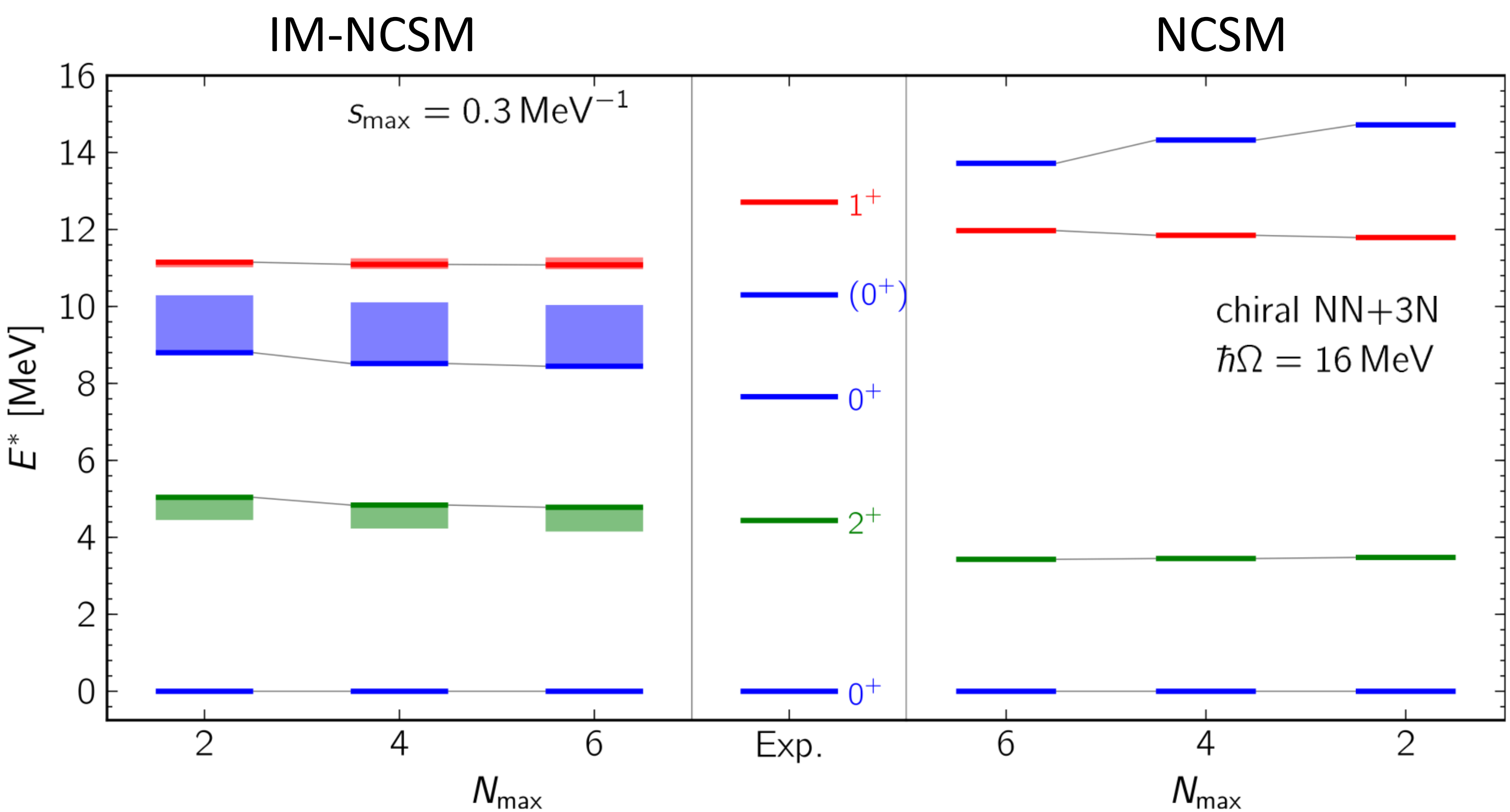

chiral $NN+3N_{NO2B}$

$\Lambda_{3N} = 400\,\mathrm{MeV}$

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

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Imag. Time

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

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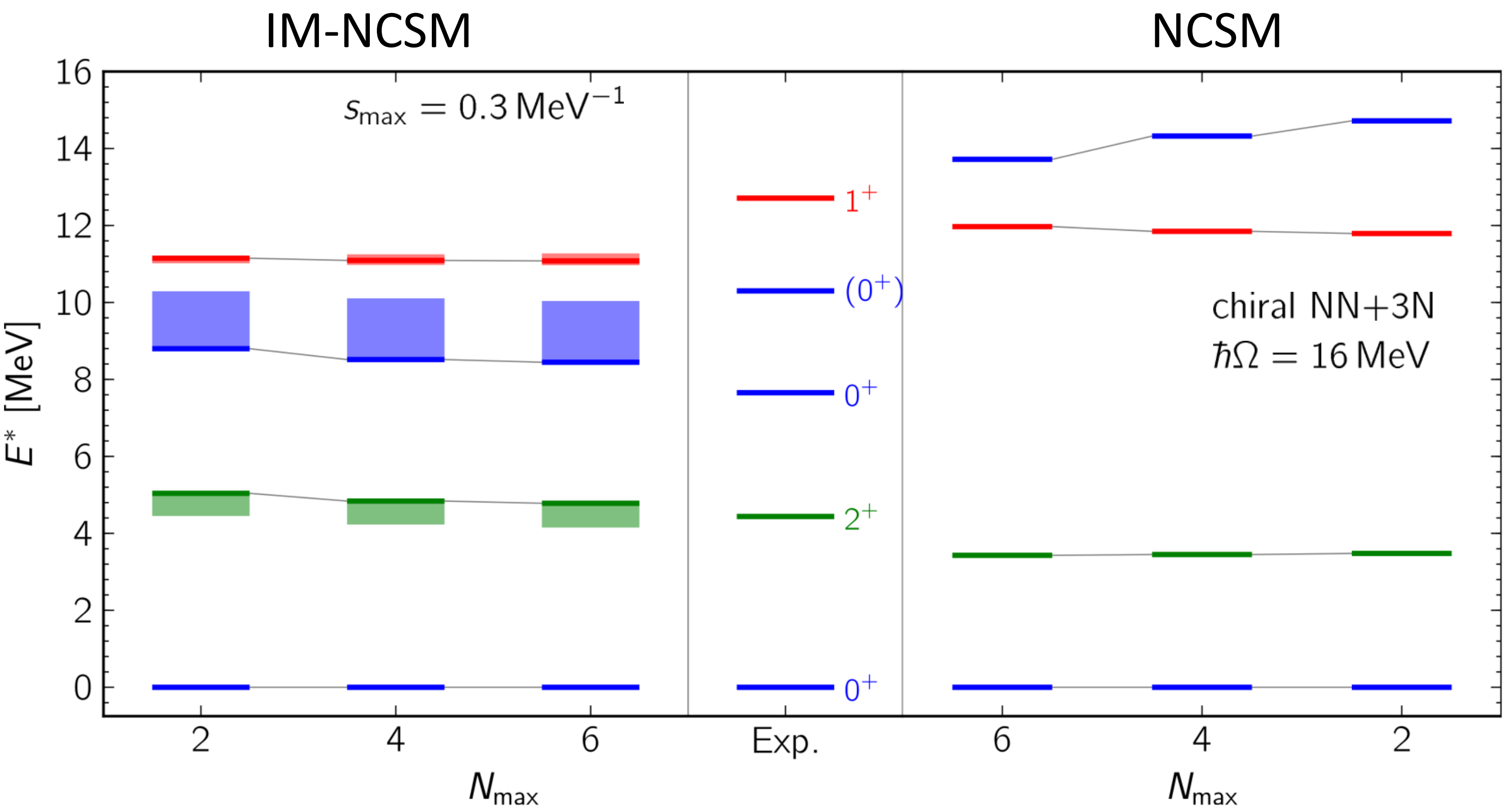
Spectra



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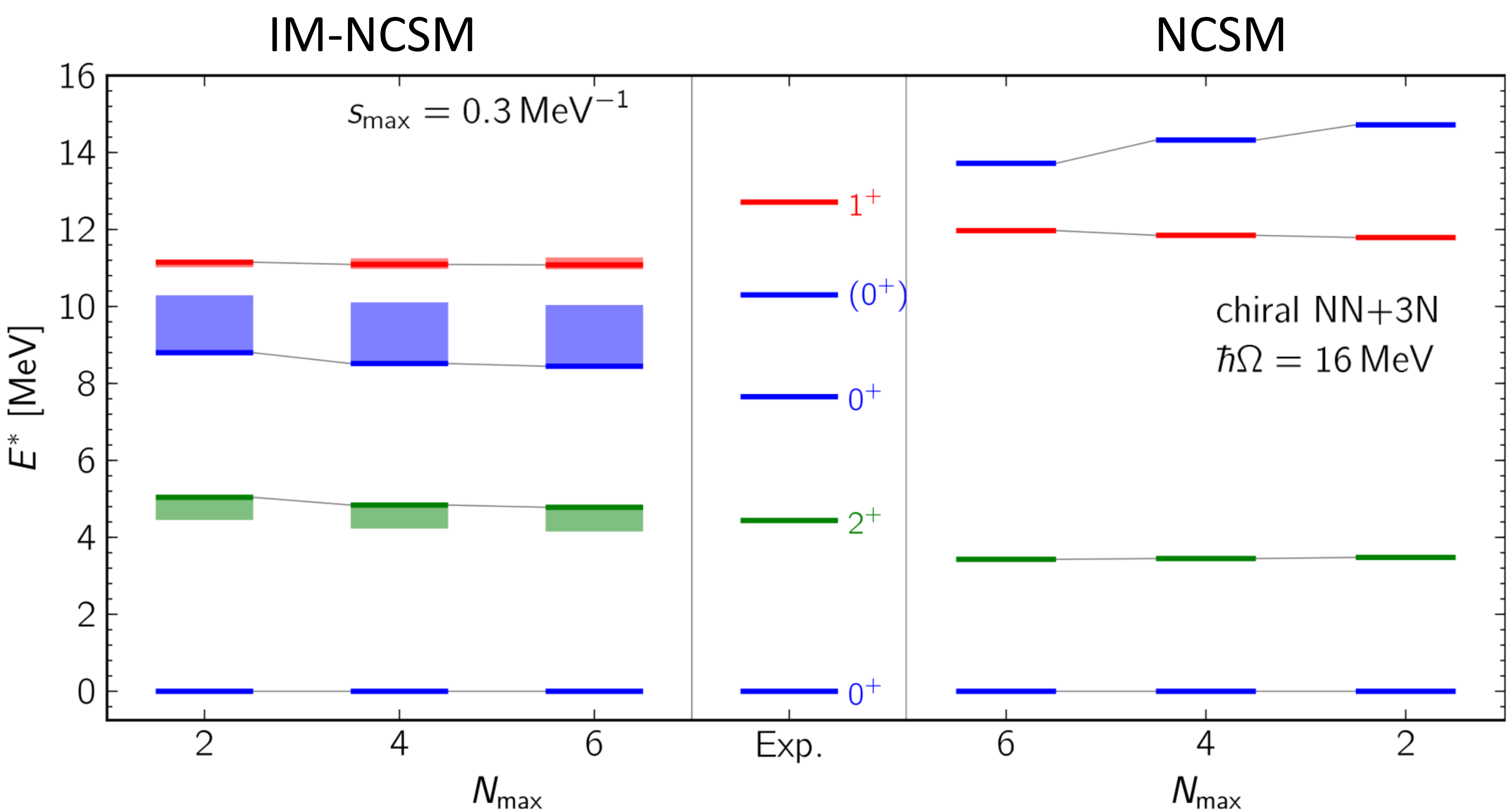
$\Lambda_{3N} = 400\,\mathrm{MeV}$
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20\,\mathrm{MeV}$

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

^{12}C
$e_{max} = 12$

- uncertainty band due to flow-parameter variation between $s_{max}/2$ and s_{max}
- 2^+ and 1^+ in IM-NCSM and NCSM in good agreement

Spectra



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$\Lambda_{3N} = 400\,\mathrm{MeV}$
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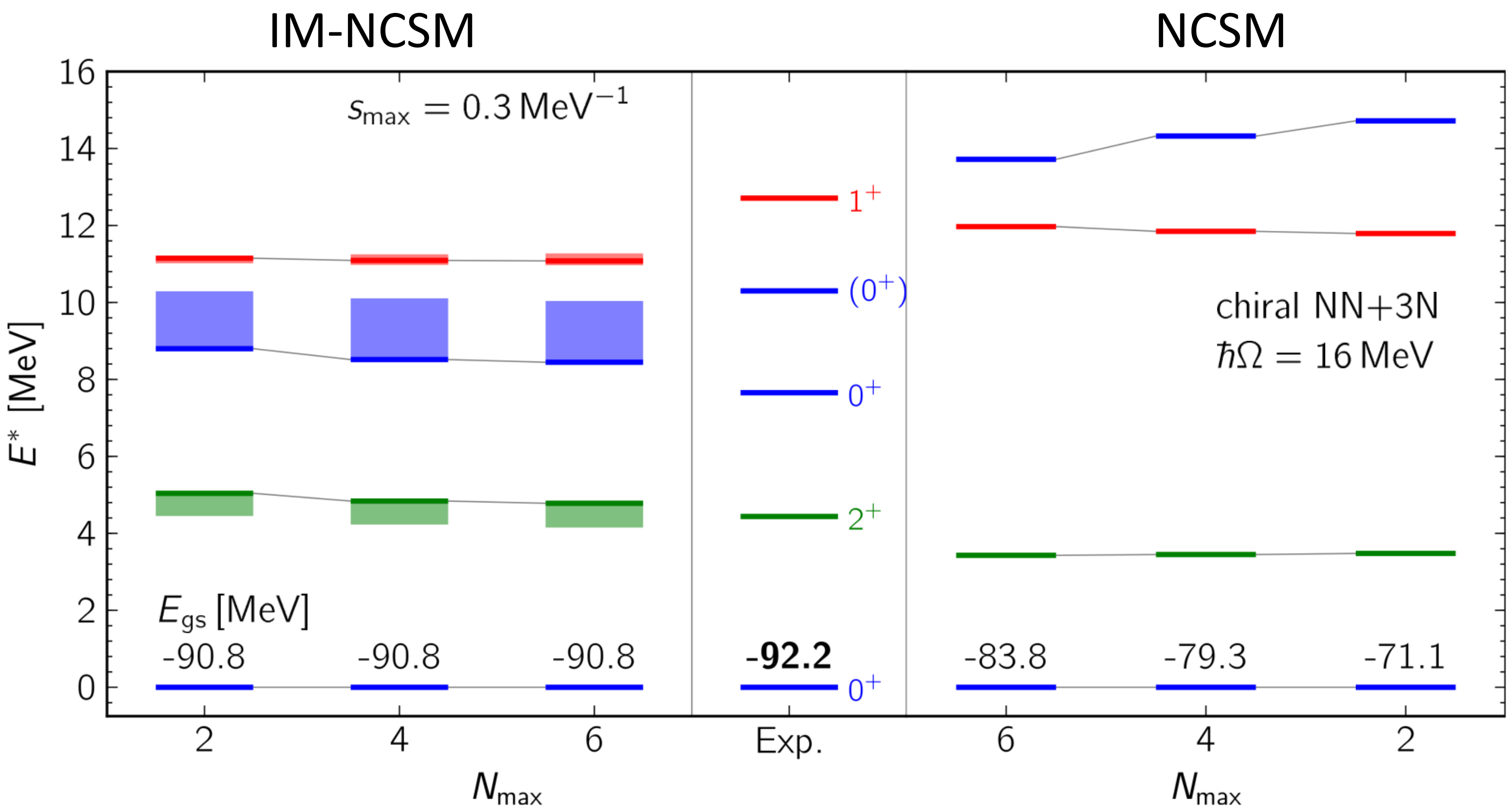
$\hbar\Omega = 20\,\mathrm{MeV}$

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

^{12}C
$e_{max} = 12$

- uncertainty band due to flow-parameter variation between $s_{max}/2$ and s_{max}
- 2^+ and 1^+ in IM-NCSM and NCSM in good agreement
- second 0^+ in NCSM (**Hoyle**?) slow convergence, IM-NCSM closer to experiment

Spectra



chiral NN+3N$_{NO2B}$

$\Lambda_{3N} = 400\,\mathrm{MeV}$

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

$\hbar\Omega = 20\,\mathrm{MeV}$

Imag. Time

$N^{ref}_{max} = 0$

^{12}**C**

$e_{max} = 12$

- uncertainty band due to flow-parameter variation between $s_{max}/2$ and s_{max}
- 2^+ and 1^+ in IM-NCSM and NCSM in good agreement
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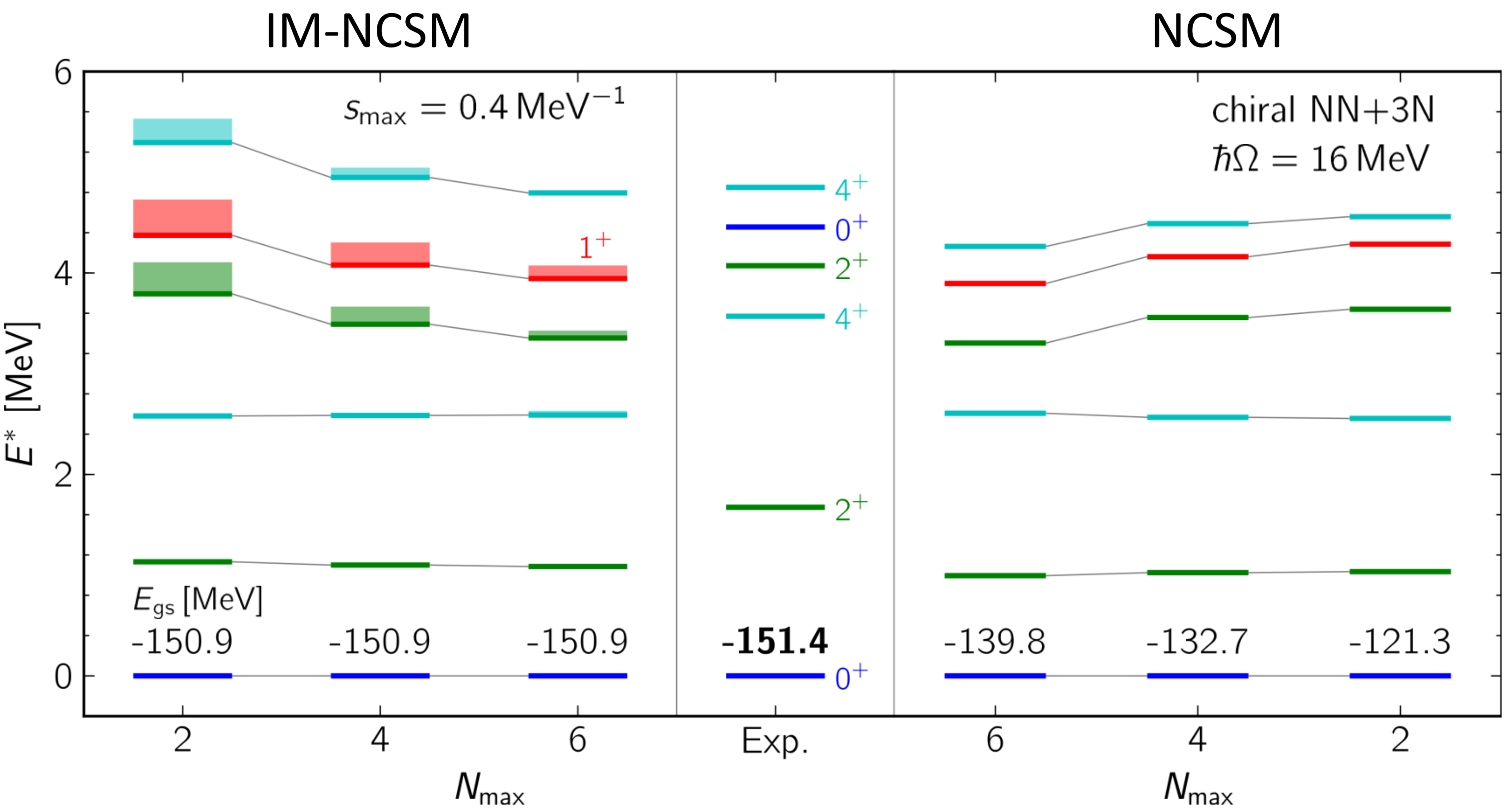

chiral NN+3N$_{NO2B}$

$\Lambda_{3N} = 400$ MeV

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

$\hbar\Omega = 20$ MeV

Imag. Time

$N^{ref}_{max} = 0$

^{20}O

$e_{max} = 12$

- first 2^+ and 4^+ robust and well converged in IM-NCSM
- higher-lying states show small flow-parameter dependence
- 1^+ not yet observed experimentally → theoretical prediction

Summary

TECHNISCHE UNIVERSITÄT DARMSTADT

- ✓ established a many-body technique **IM-NCSM** = IM-SRG + NCSM
- ✓ IM-SRG decouples **reference state** from higher N_{max}
- ✓ extremely **enhanced N_{max} convergence** for subsequent NCSM
- ✓ $N_{max} \leq 4$ sufficient to extract converged ground-state energies
- ✓ **variational principle** becomes valid for **excitation energies** since ground-state energy converged
- ✓ preliminary *ab initio* studies regarding Hoyle state in ^{12}C

Outlook

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- more detailed analysis of the Hoyle state in ^{12}C
- study of exotic nuclei: island-of-inversion physics, …
- evolve vector operator, for instance E1 transition operators
- extend applicability of IM-NCSM to odd nuclei
  using particle-attached particle-removed formalism
- …

Thank You For Your Attention

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Thanks to my group & collaborator

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- **H. Hergert**

  NSCL/FRIB, Michigan State University

SFB 1245

Bundesministerium für Bildung und Forschung

LOEWE

Exzellente Forschung für Hessens Zukunft

Deutsche Forschungsgemeinschaft

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