Ab Initio Description of Open-Shell Nuclei: Merging In-Medium SRG and No-Core Shell Model

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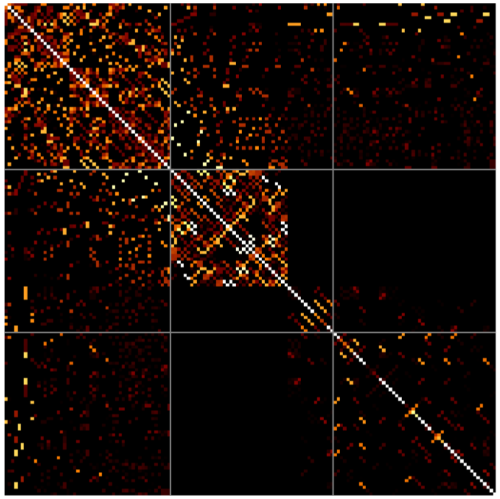

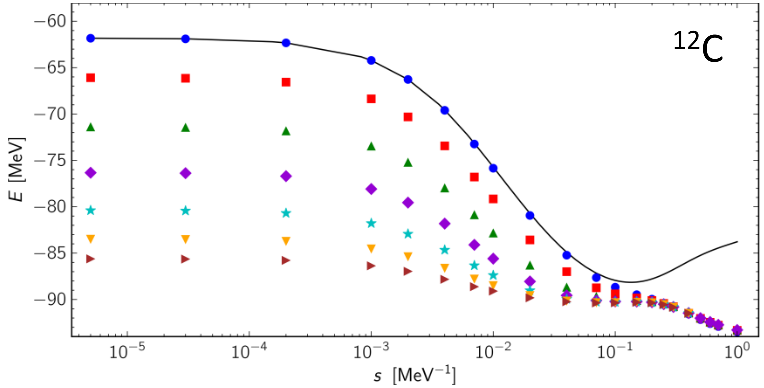

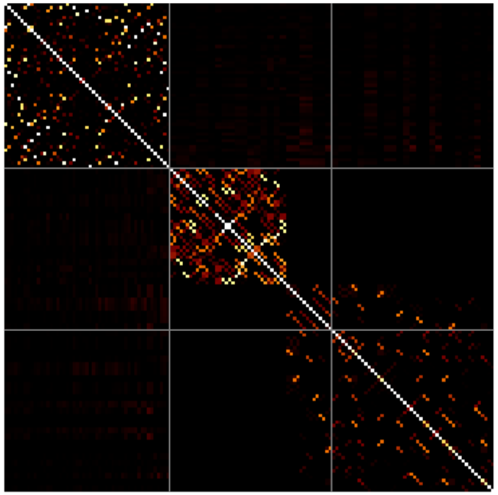

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NCSM

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

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IM-SRG

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

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Motivation

Why should we merge IM-SRG and NCSM?

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- not exact method
- only for ground state
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Overview

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

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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

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- 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

Basics

Tsukiyama, Bogner, Schwenk, Hergert,..

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

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. $|\Phi_{\text{ref}}\rangle$ [Kutzelnigg,Mukherjee]

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

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

Novel Approach: IM-NCSM
How should we merge…

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NCSM
define reference state

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

↓

IM-SRG
evolve operators

↓

NCSM
extract observables

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- evolve Hamiltonian and other operators
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NCSM
extract observables

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

Novel Approach: IM-NCSM

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

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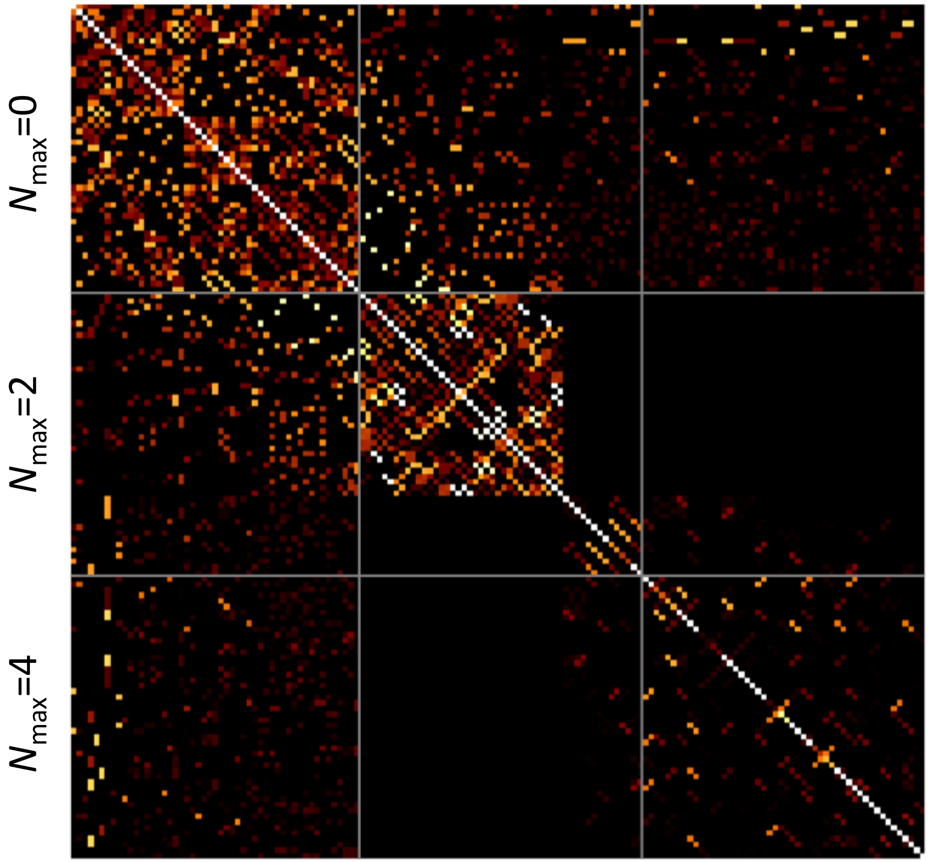
$s = 0.00$



N_{max}=0 N_{max}=2 N_{max}=4

Slater determinants Slater determinants

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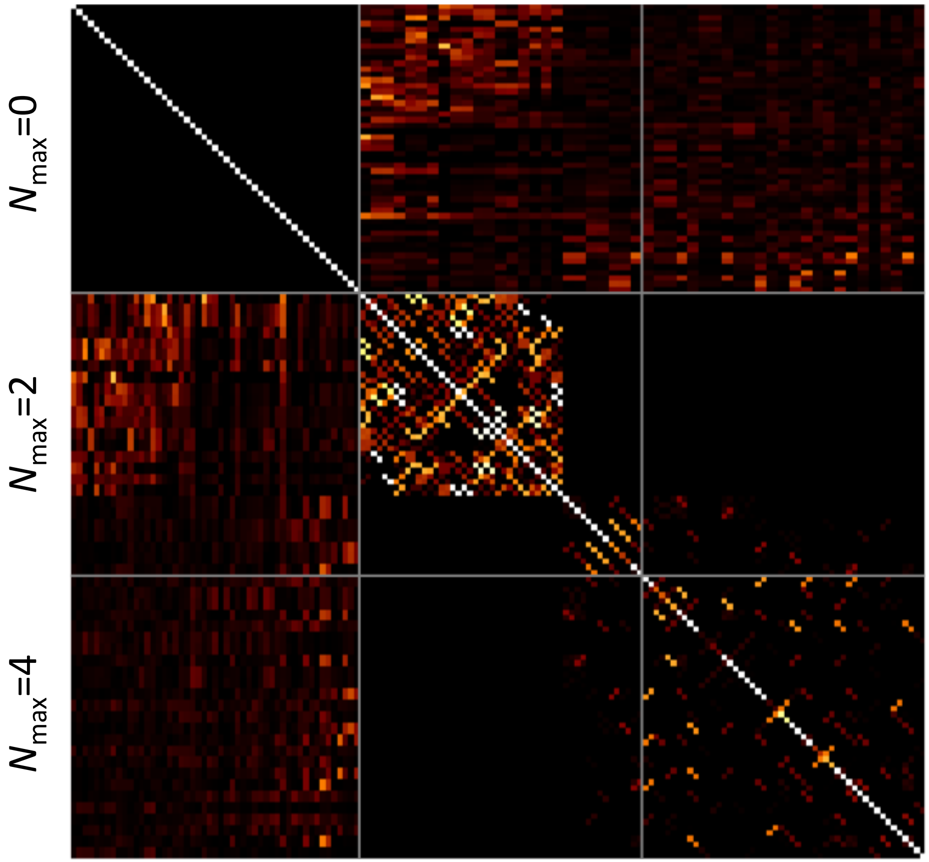

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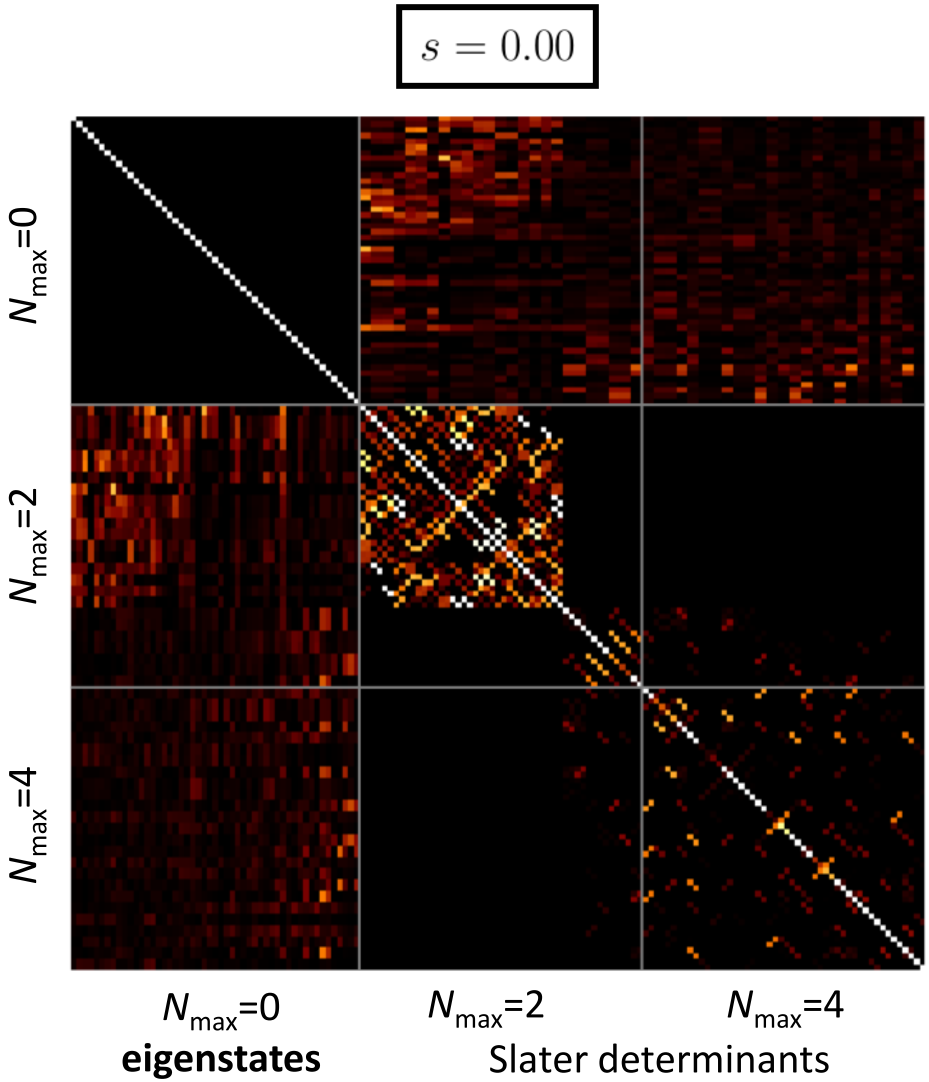

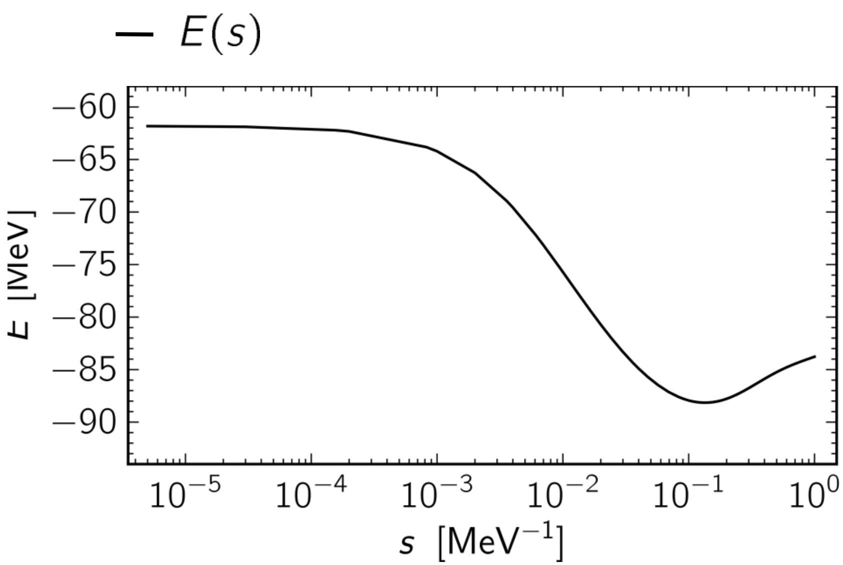

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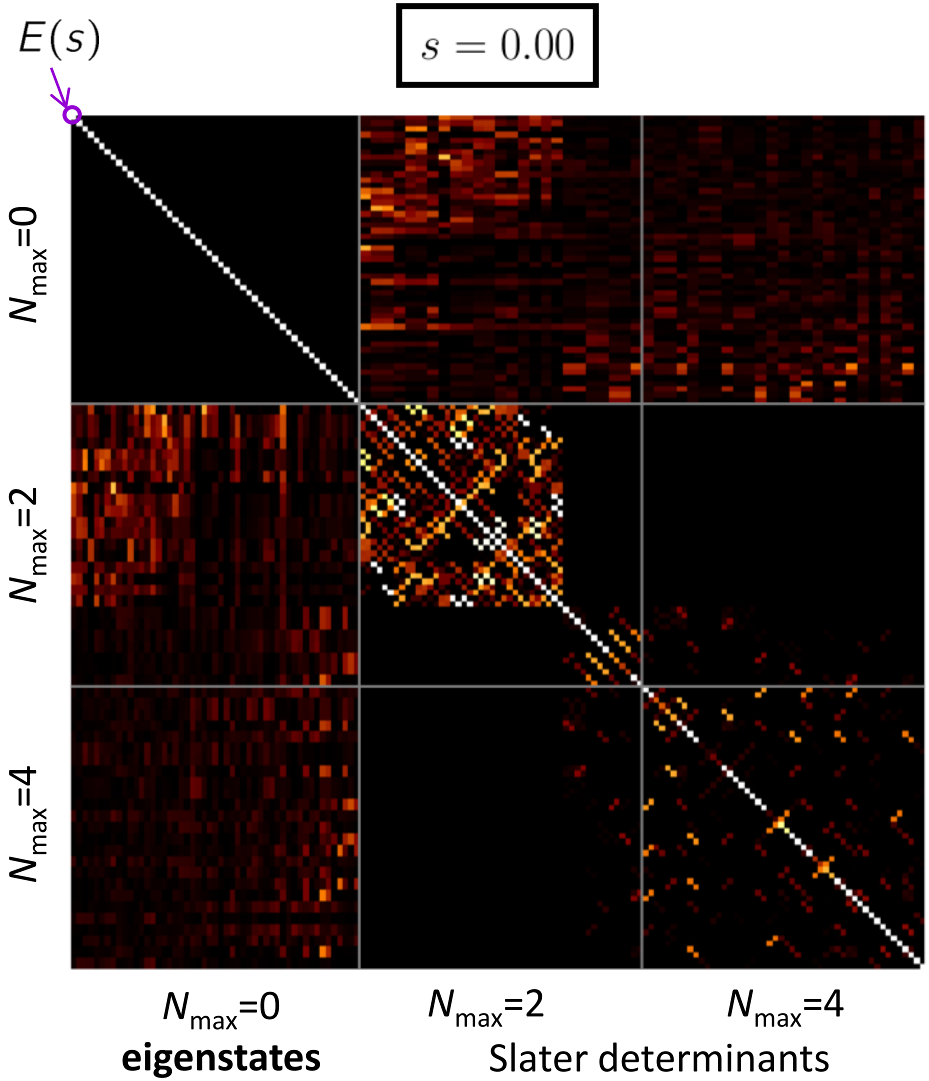

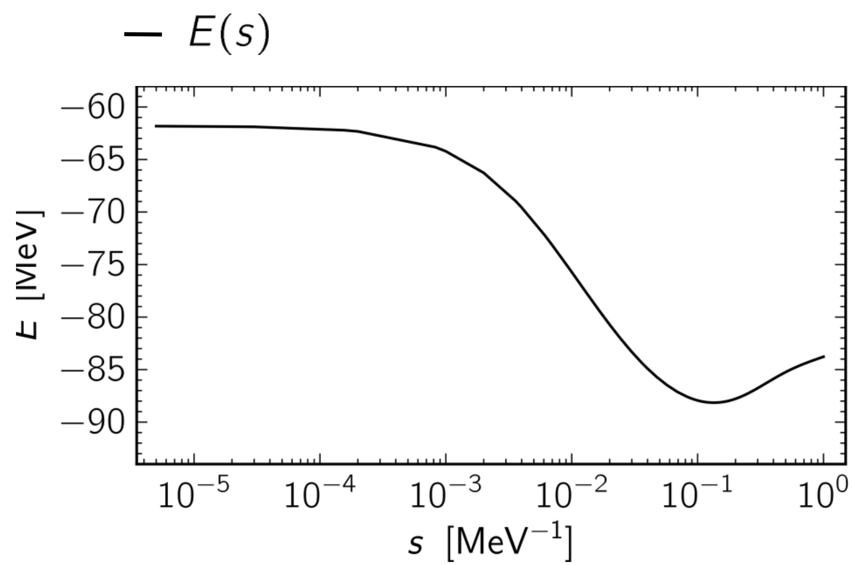

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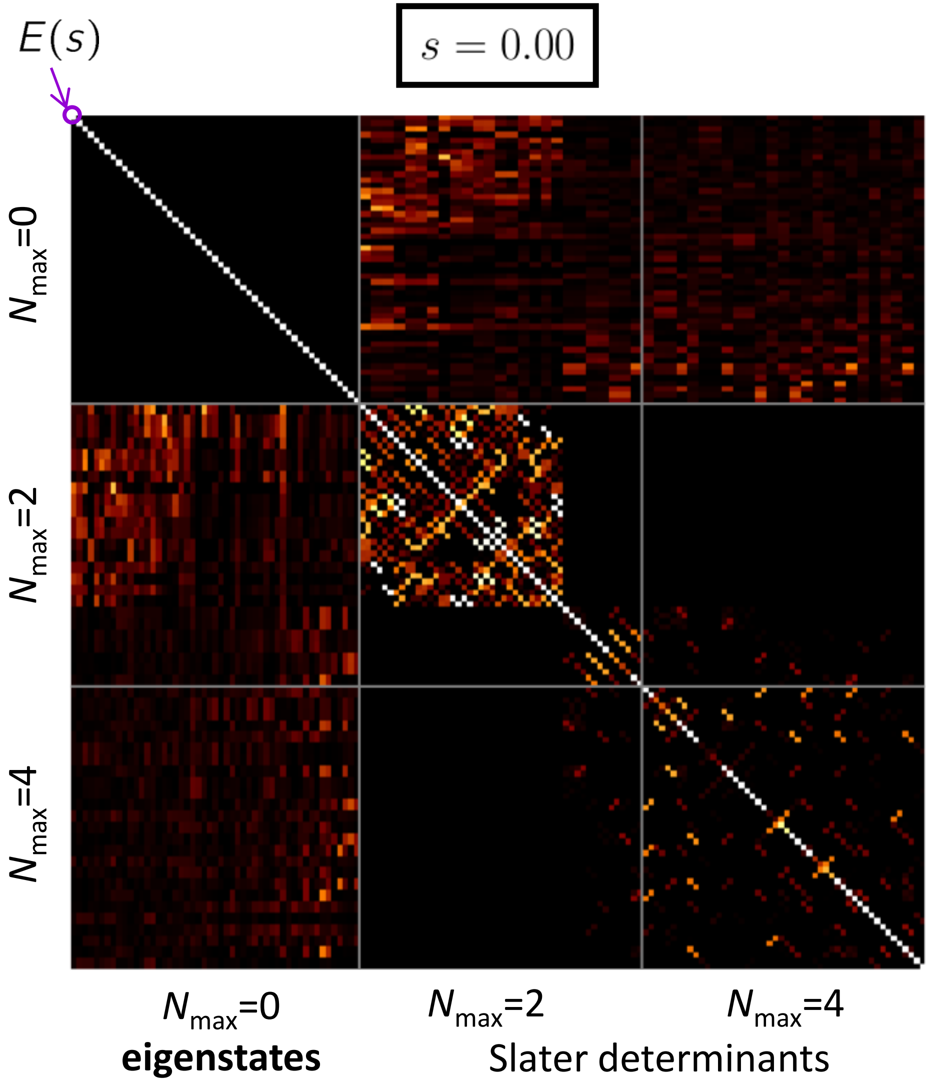

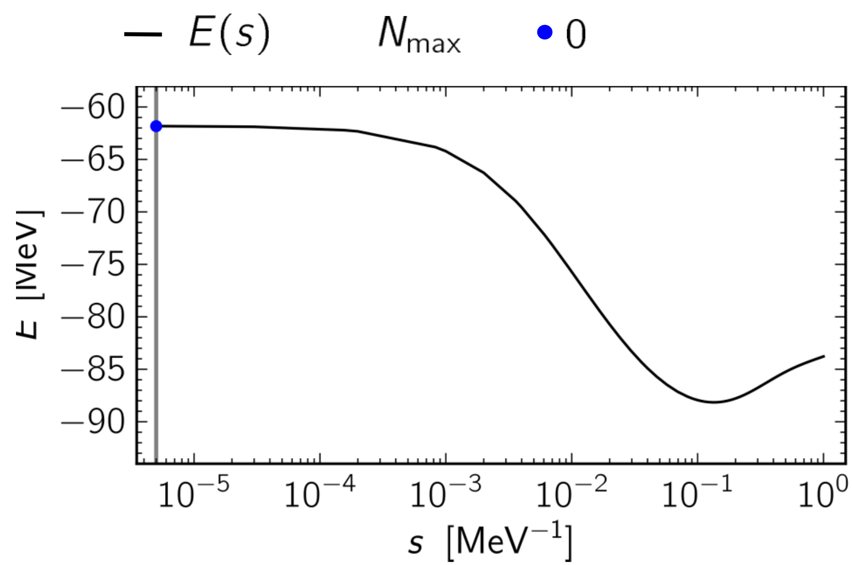

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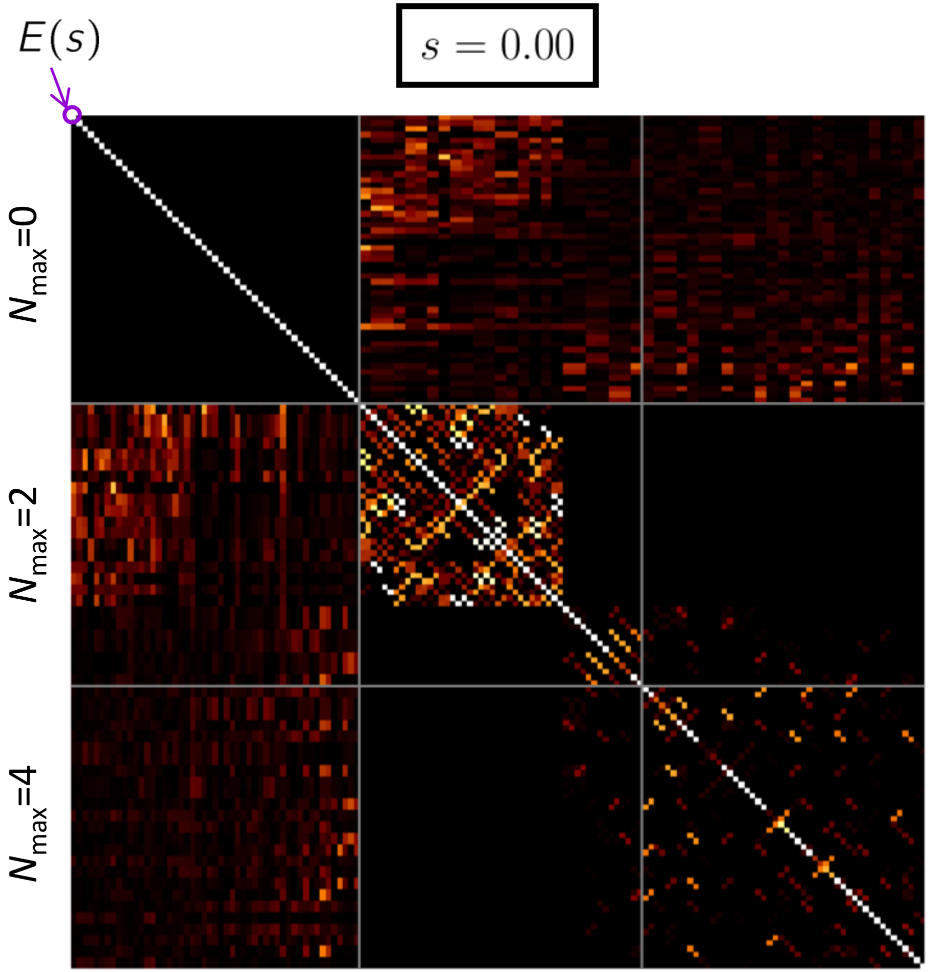

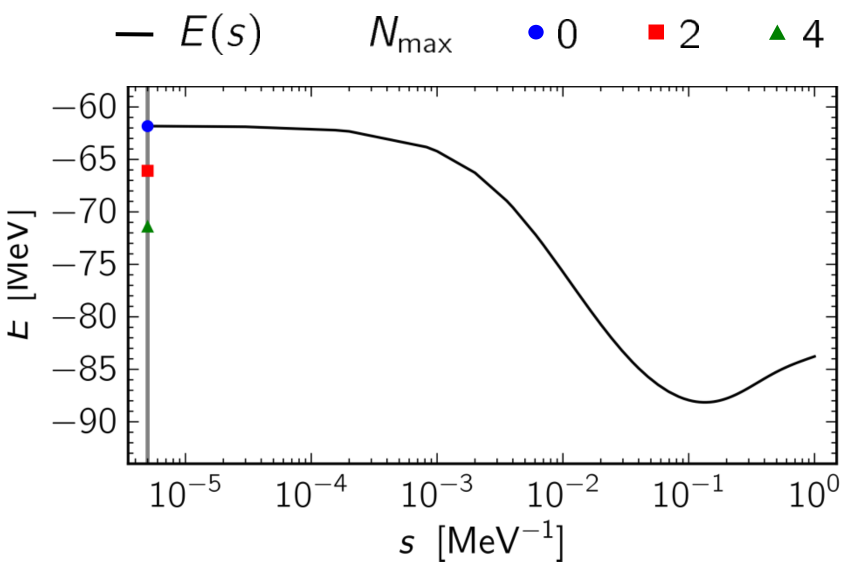

N_{max}=0 **eigenstates** — N_{max}=2, N_{max}=4 Slater determinants

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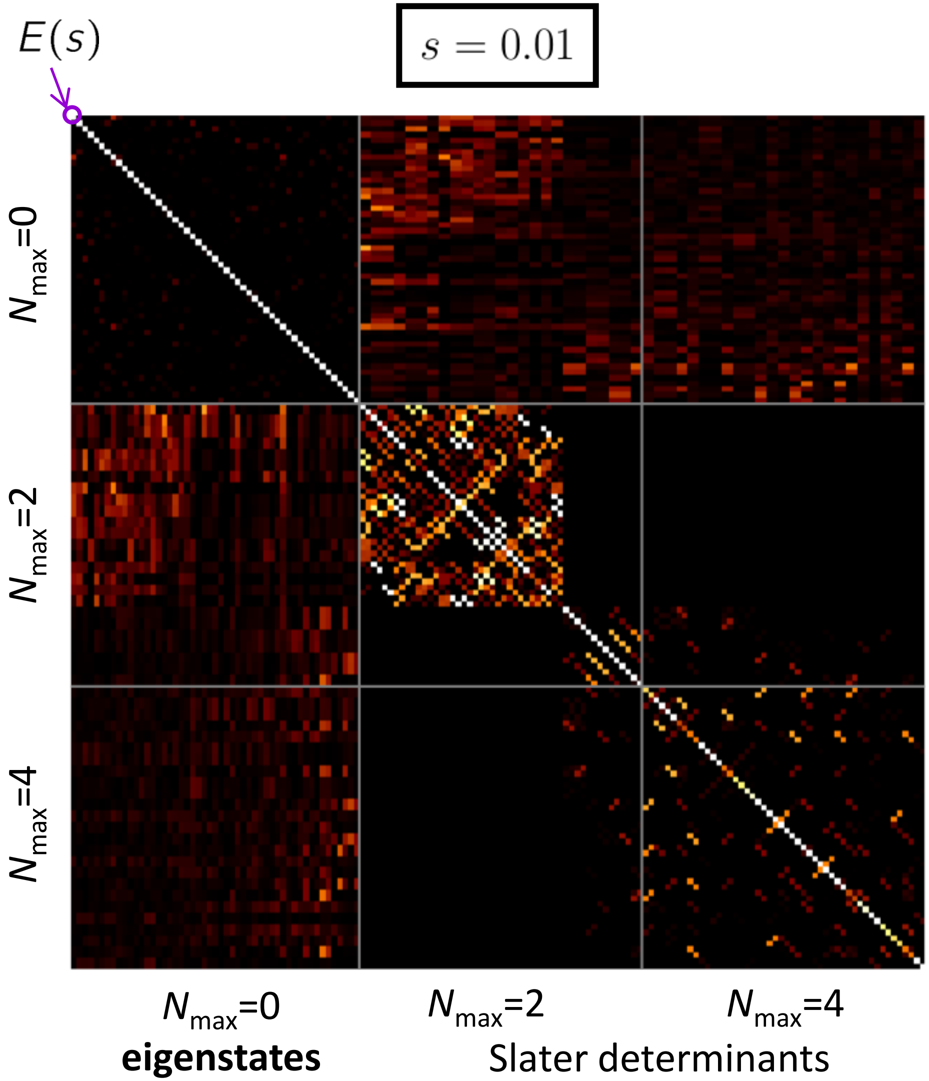

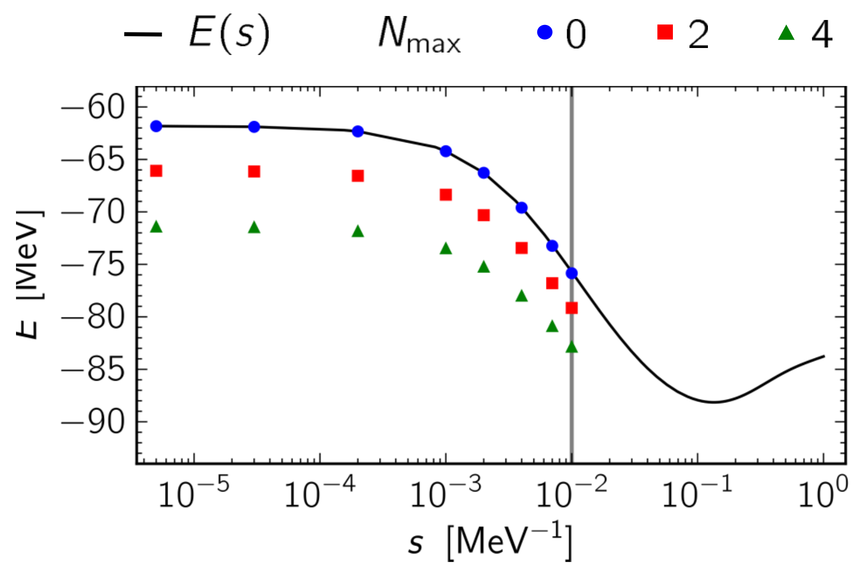

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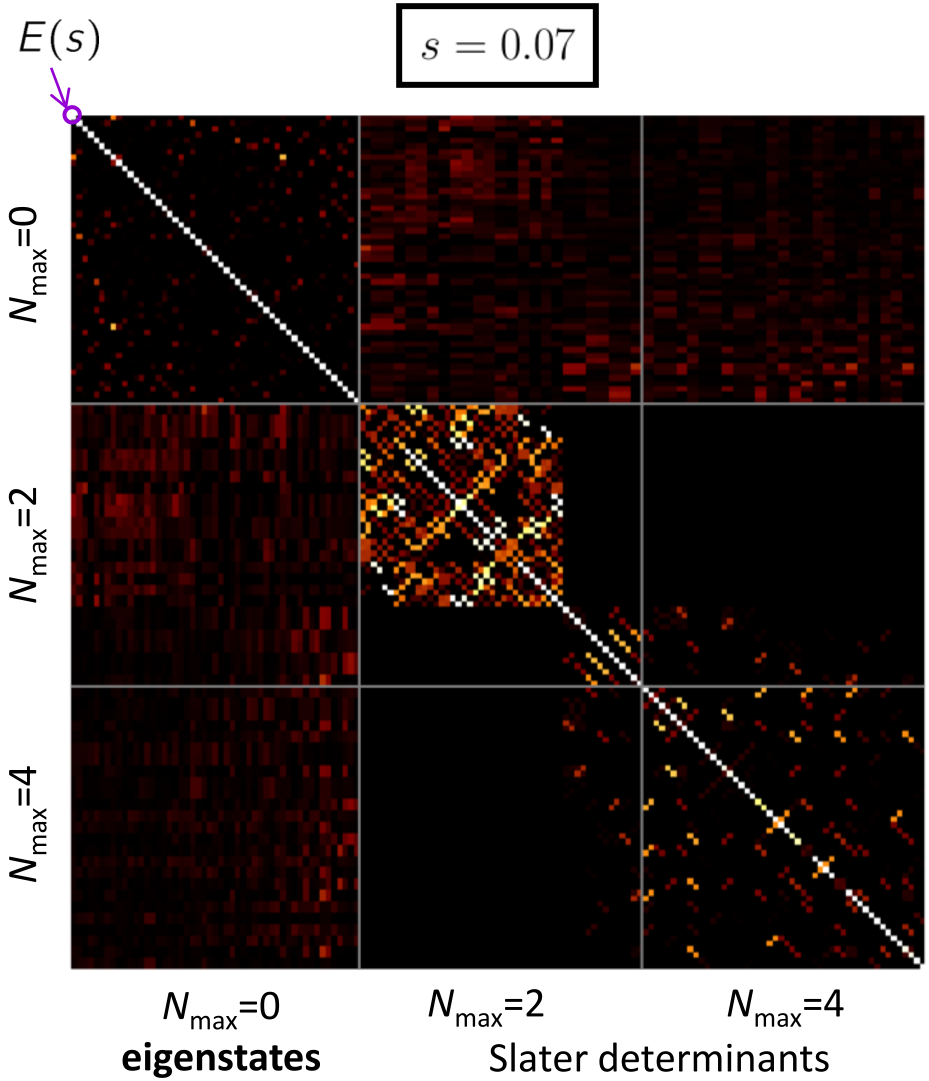

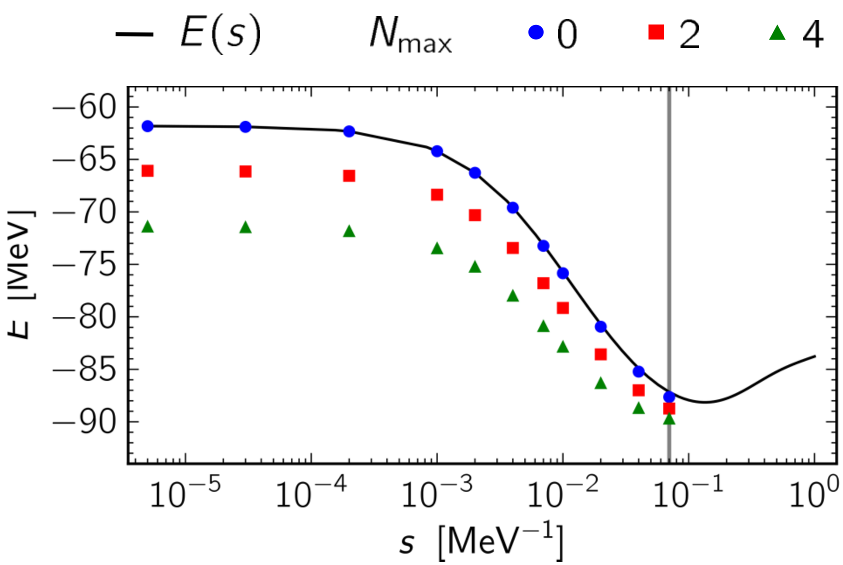

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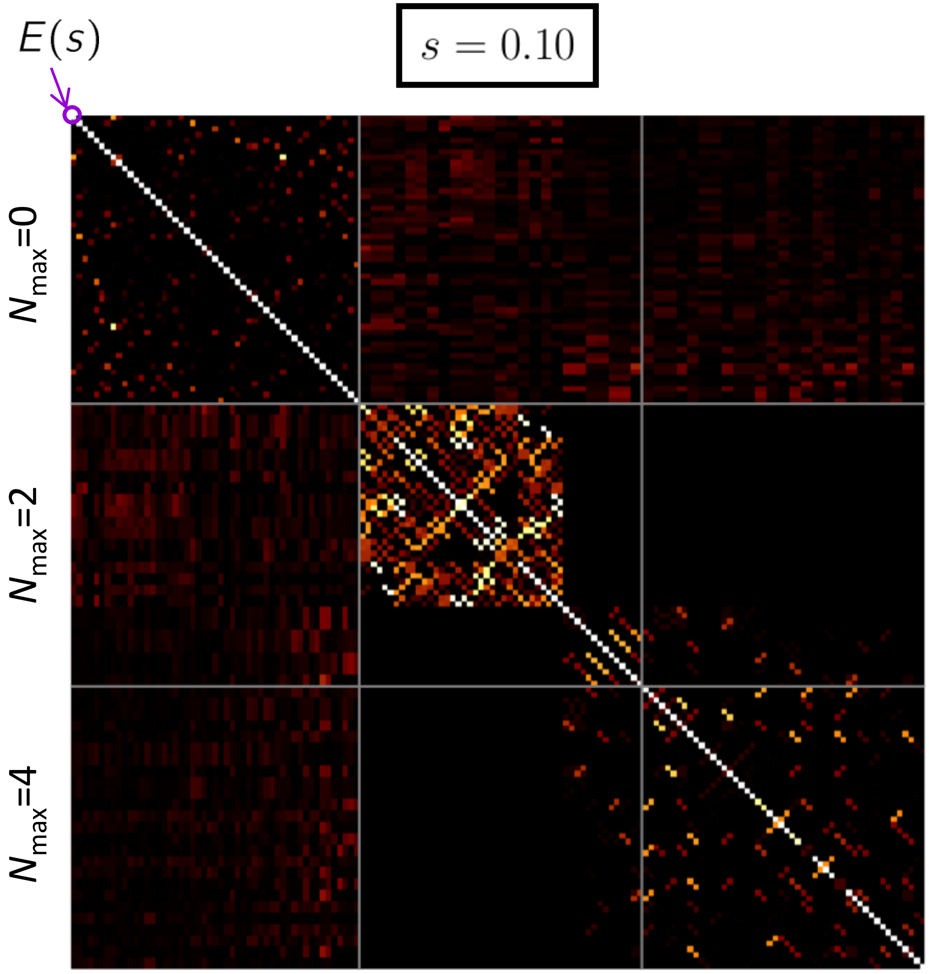
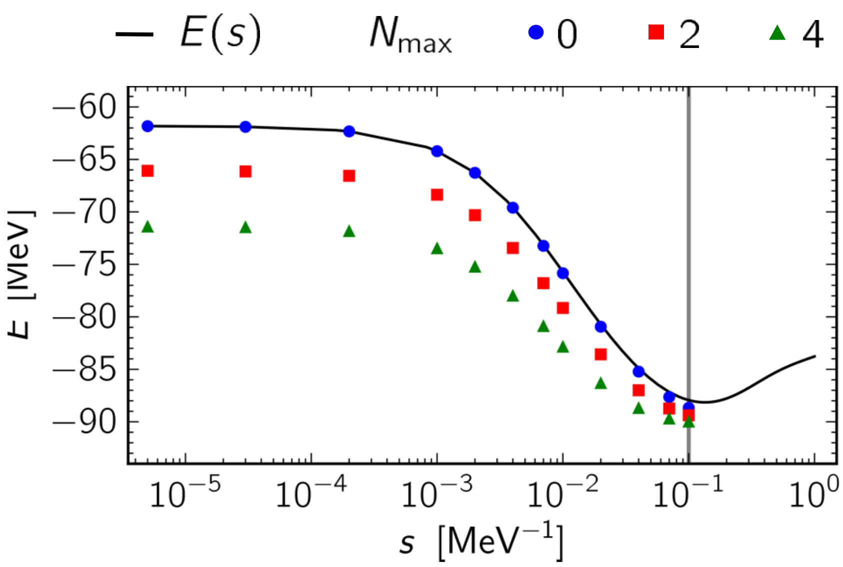
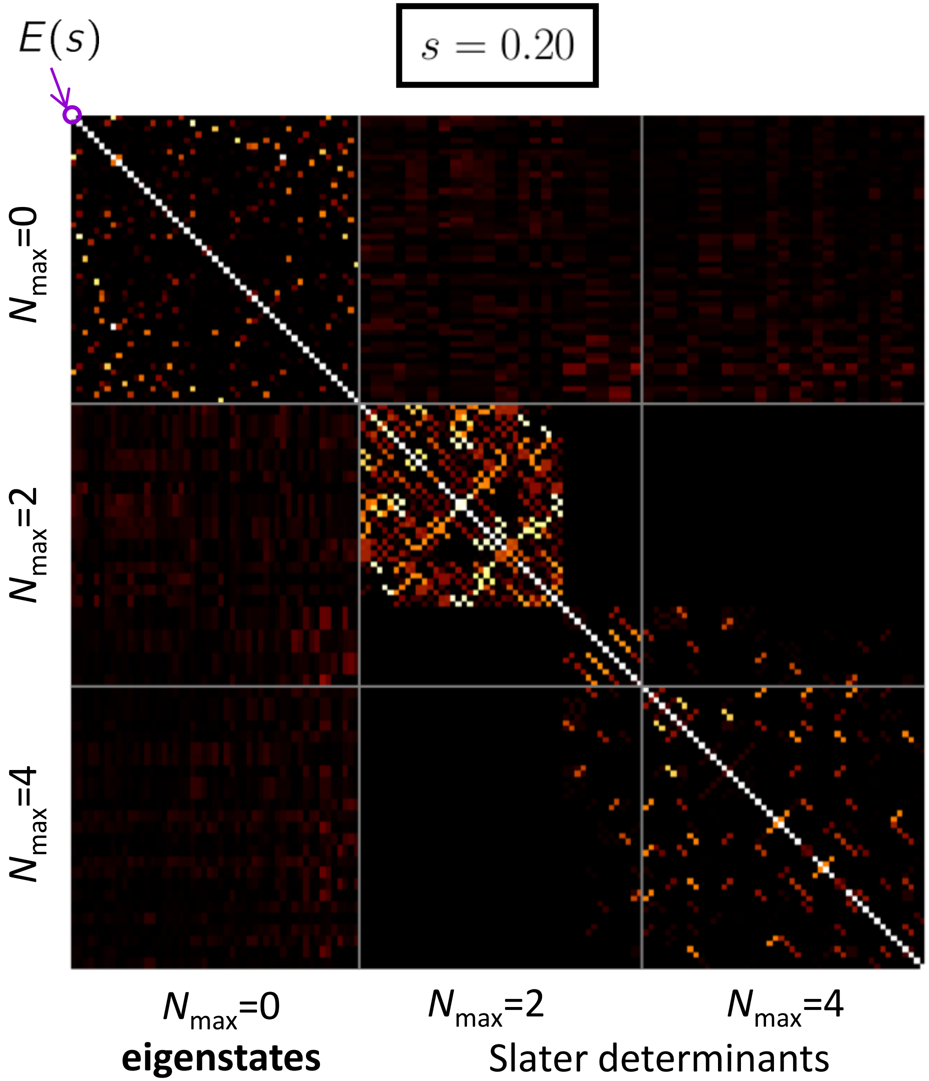
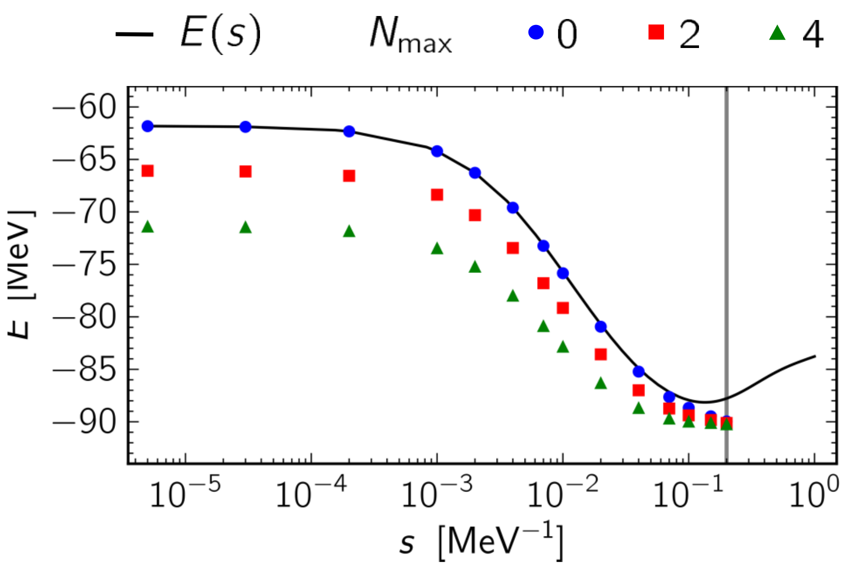




N_{max}=0 **eigenstates** | N_{max}=2 | N_{max}=4 Slater determinants

Novel Approach: IM-NCSM
Hamiltonian Matrix in A-Body Basis: ^{12}C





Novel Approach: IM-NCSM
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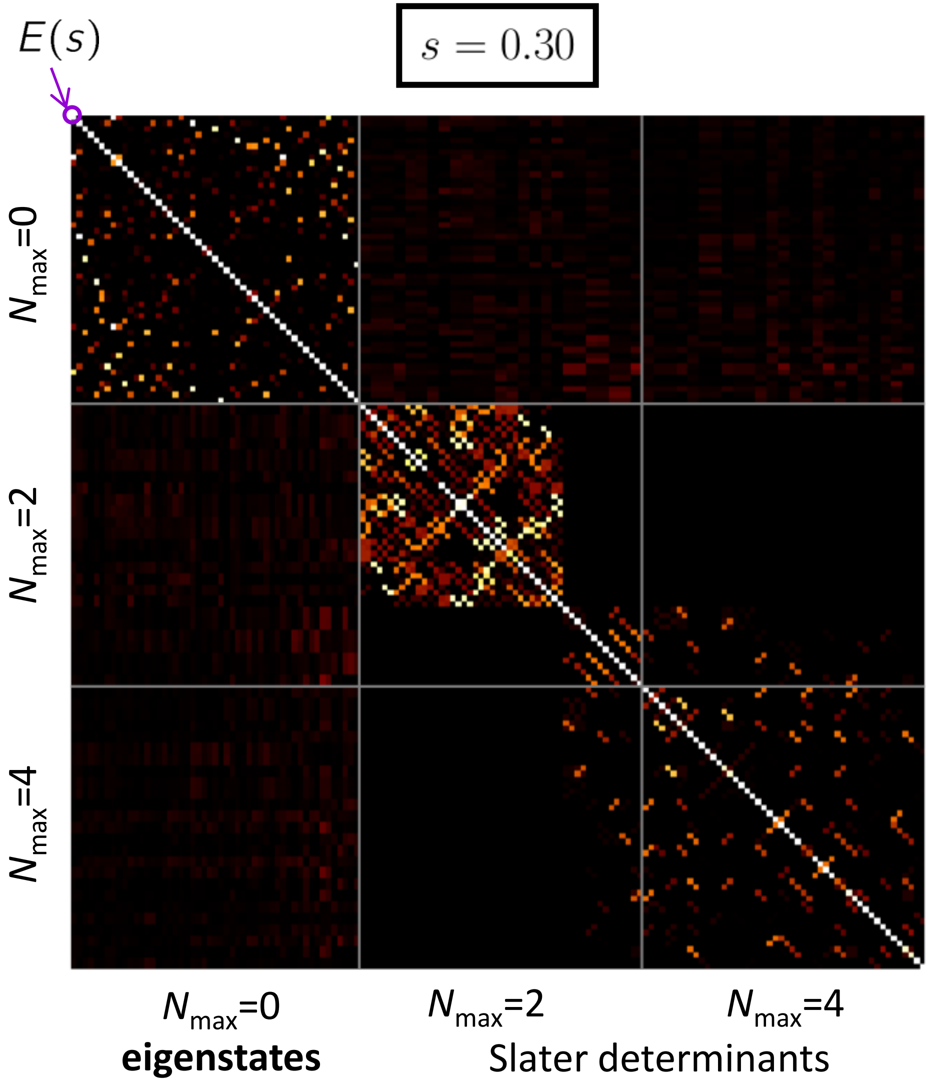

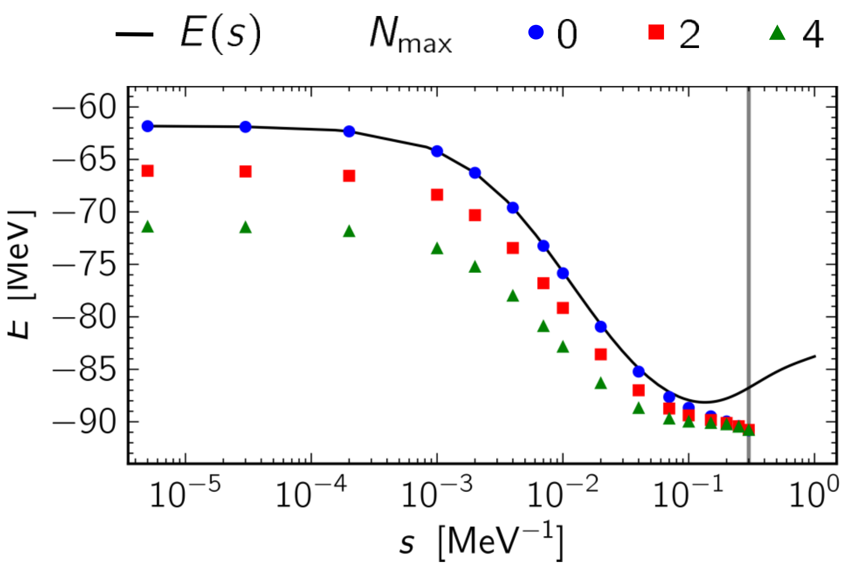

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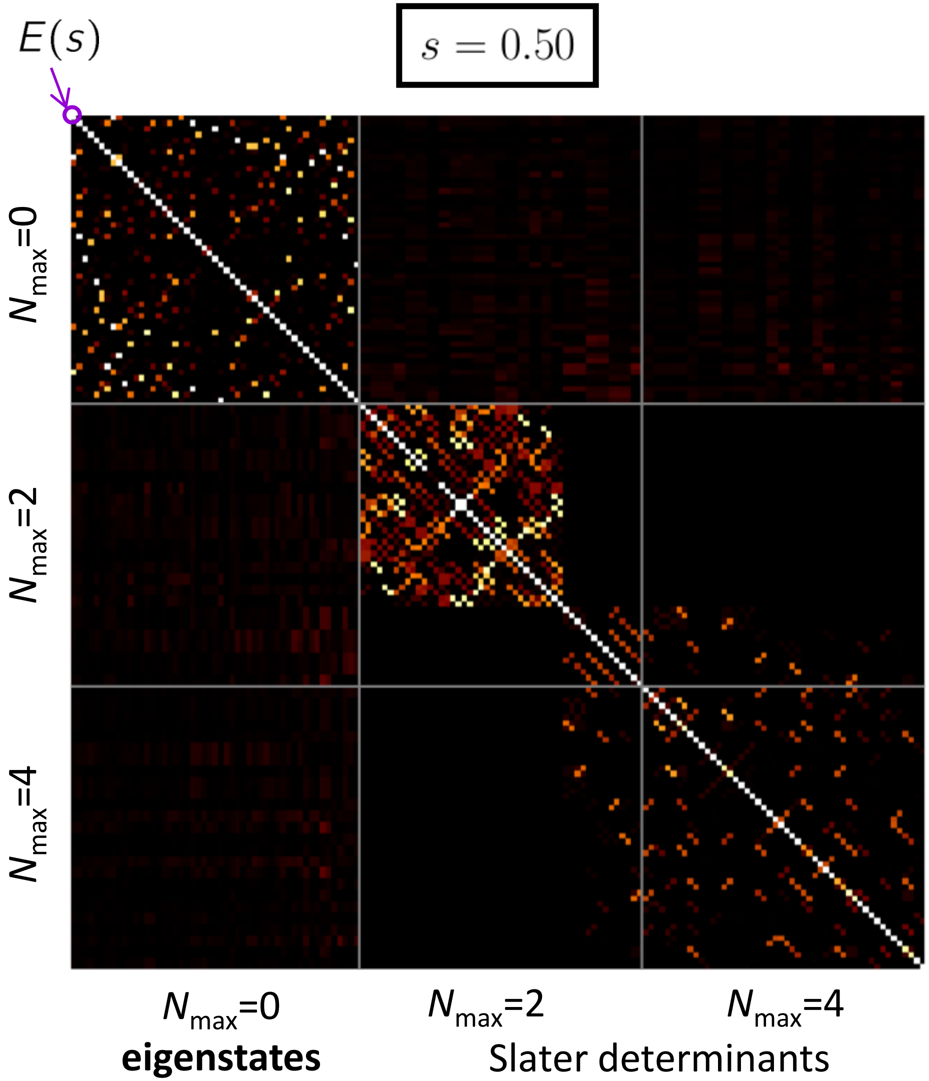

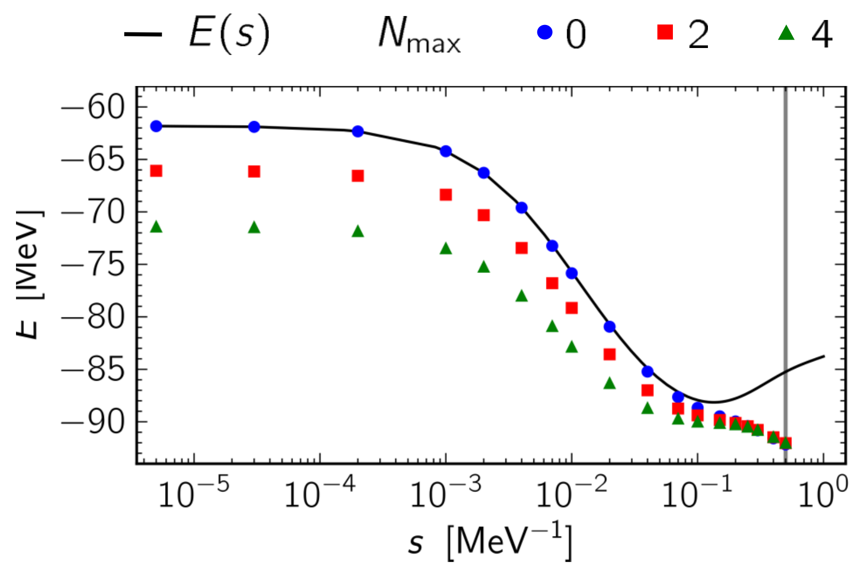

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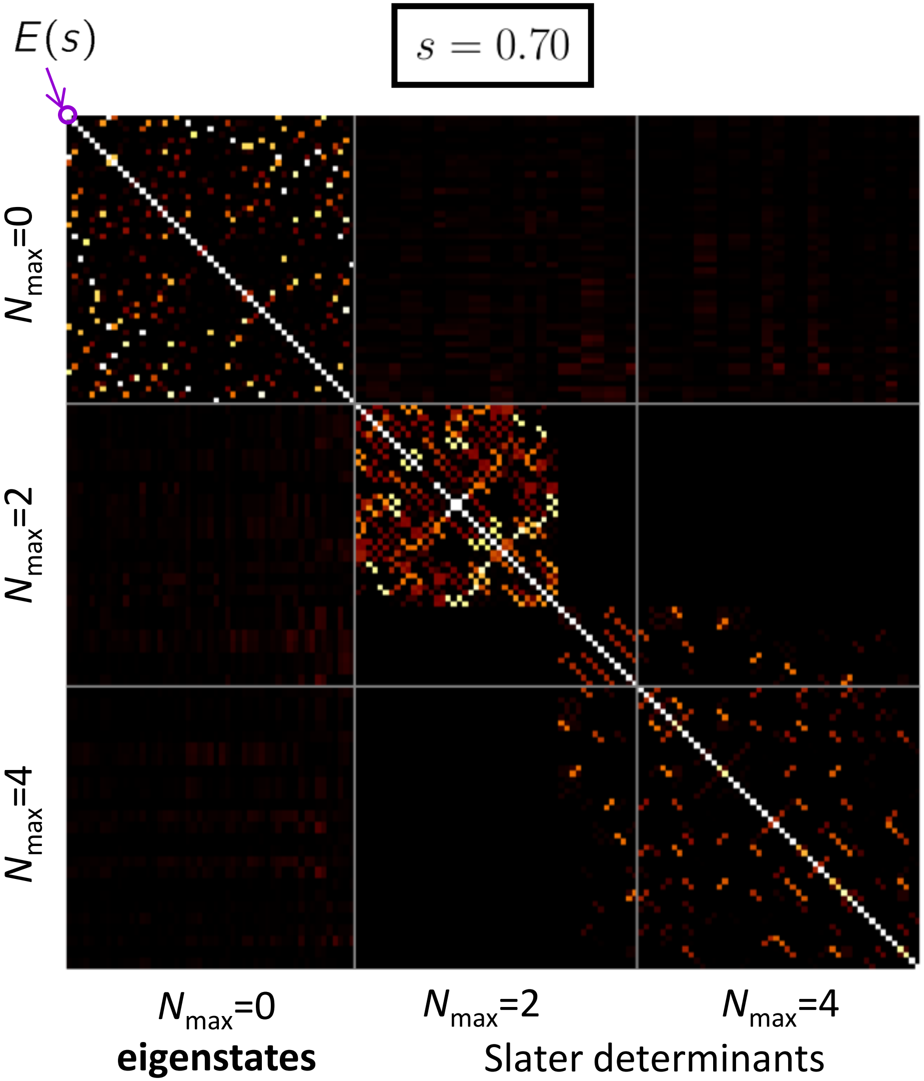
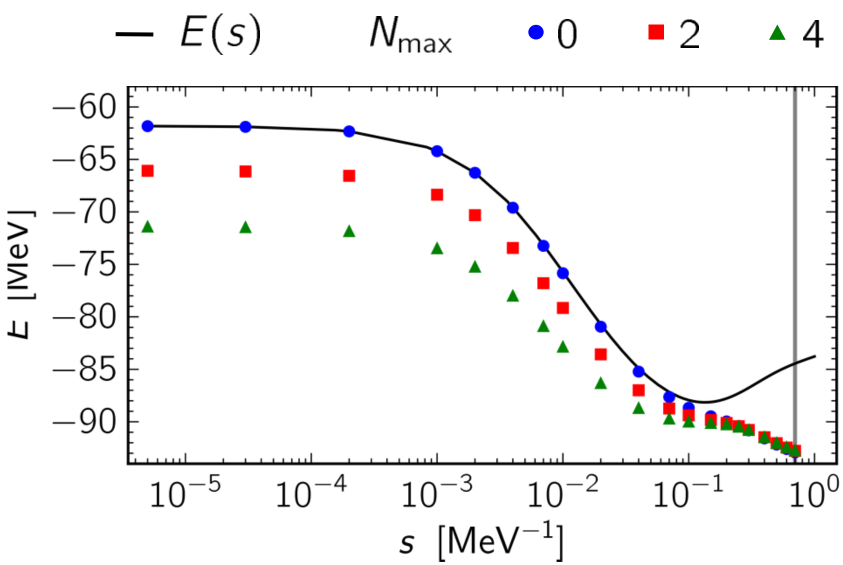
Hamiltonian Matrix in *A*-Body Basis: ^{12}C





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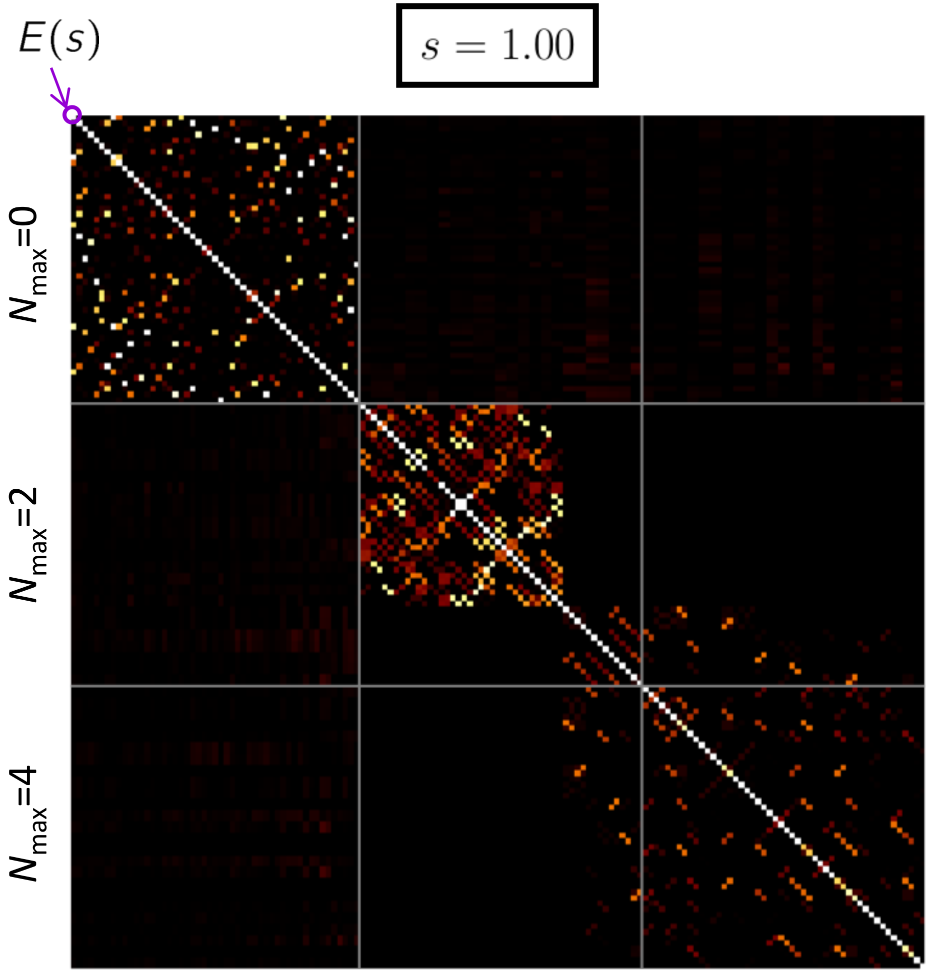
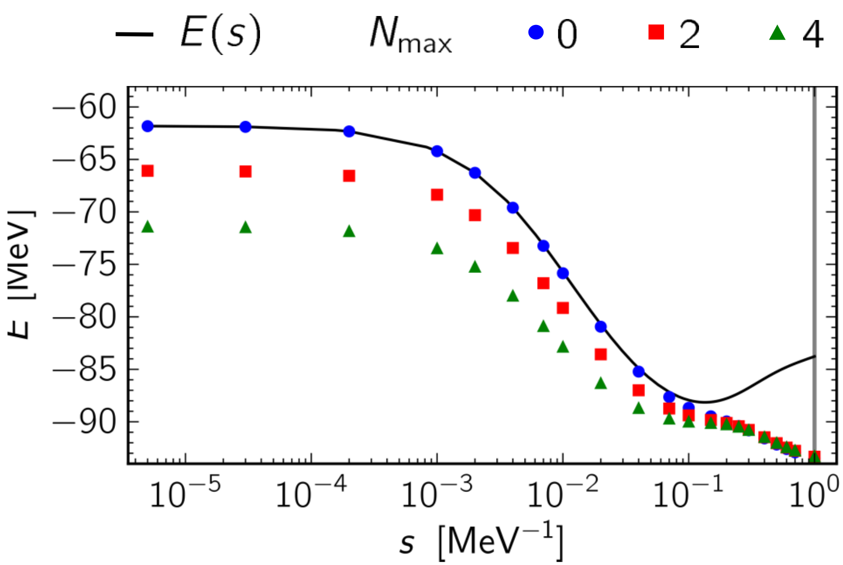


N_{max}=0 **eigenstates** | N_{max}=2 | N_{max}=4 Slater determinants



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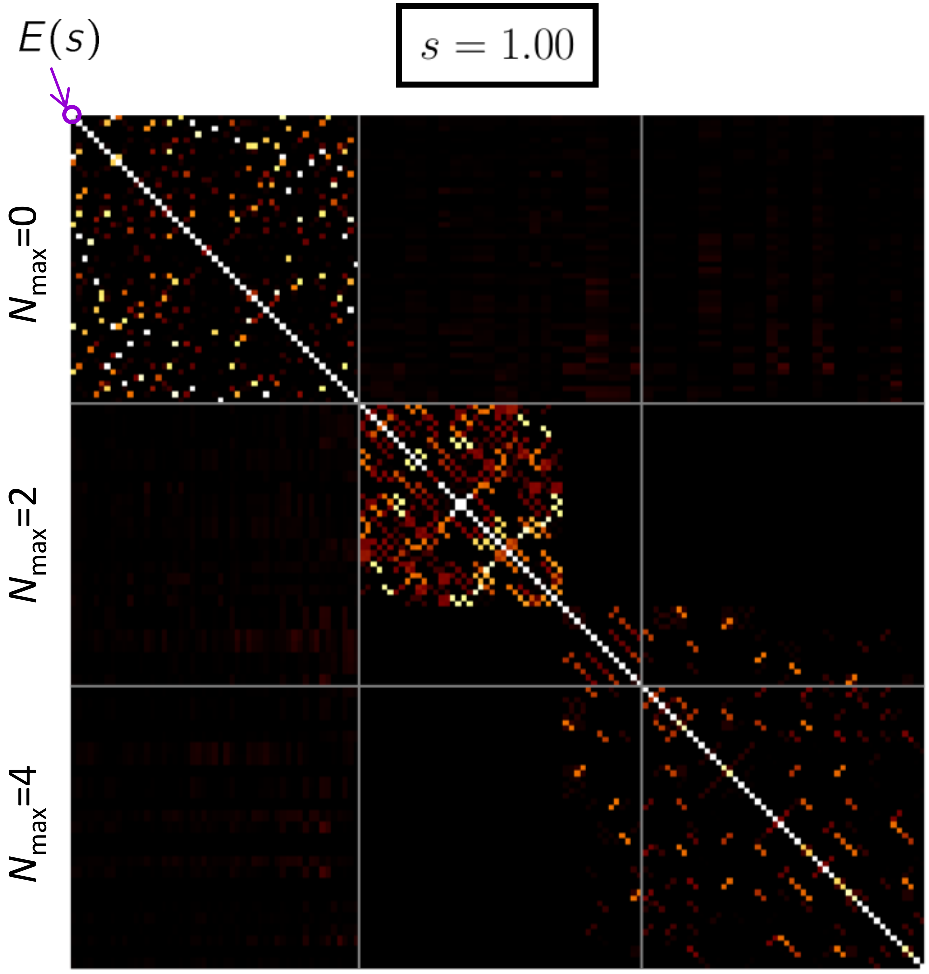

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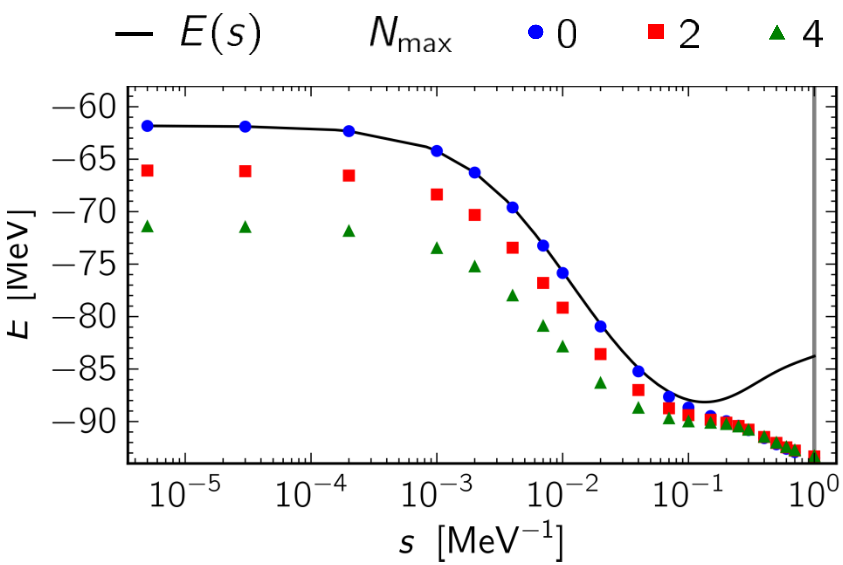

for sufficiently large flow parameter eigenvalues in N_{max}=0, 2 and 4 equal

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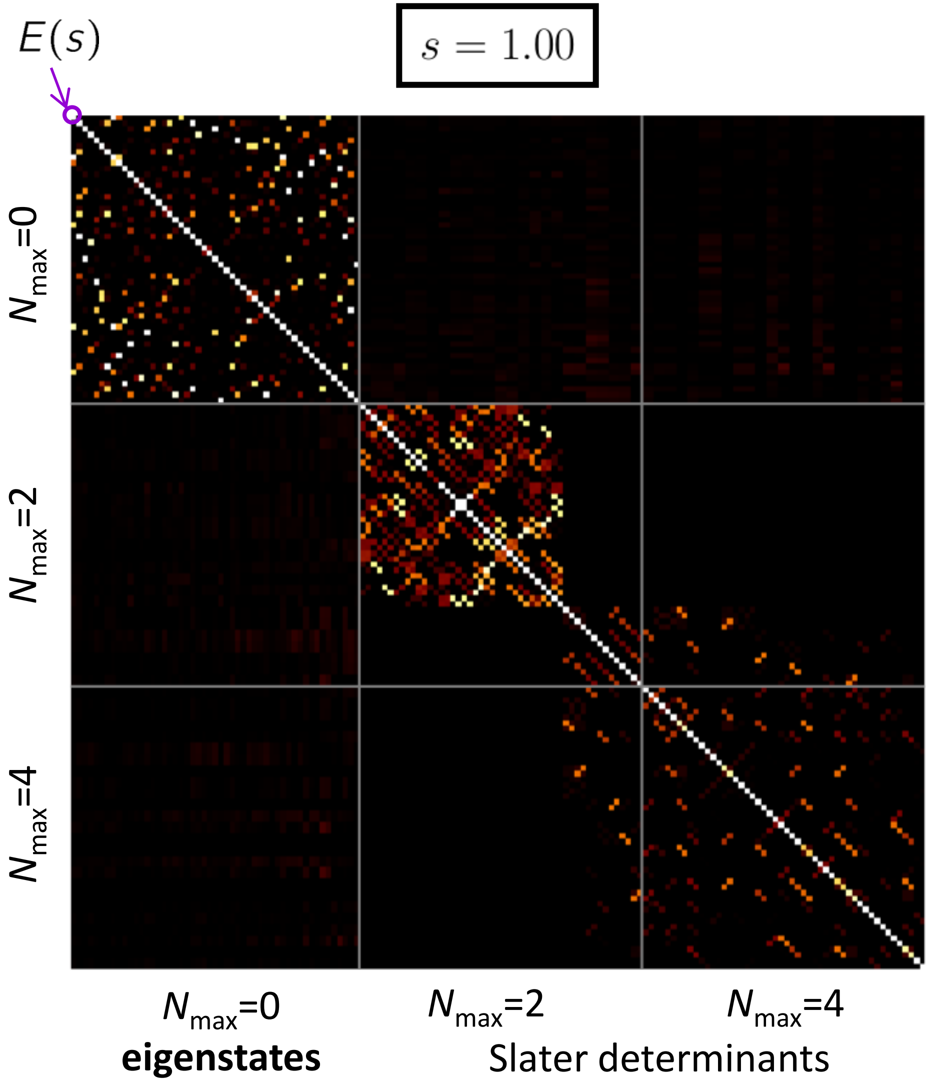

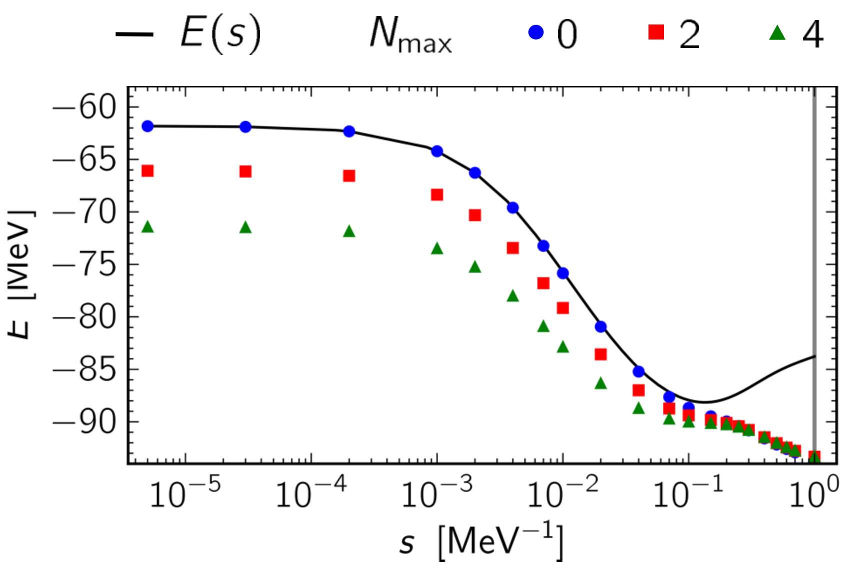

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IM-SRG decouples reference state from N_{max} =2 and 4 spaces

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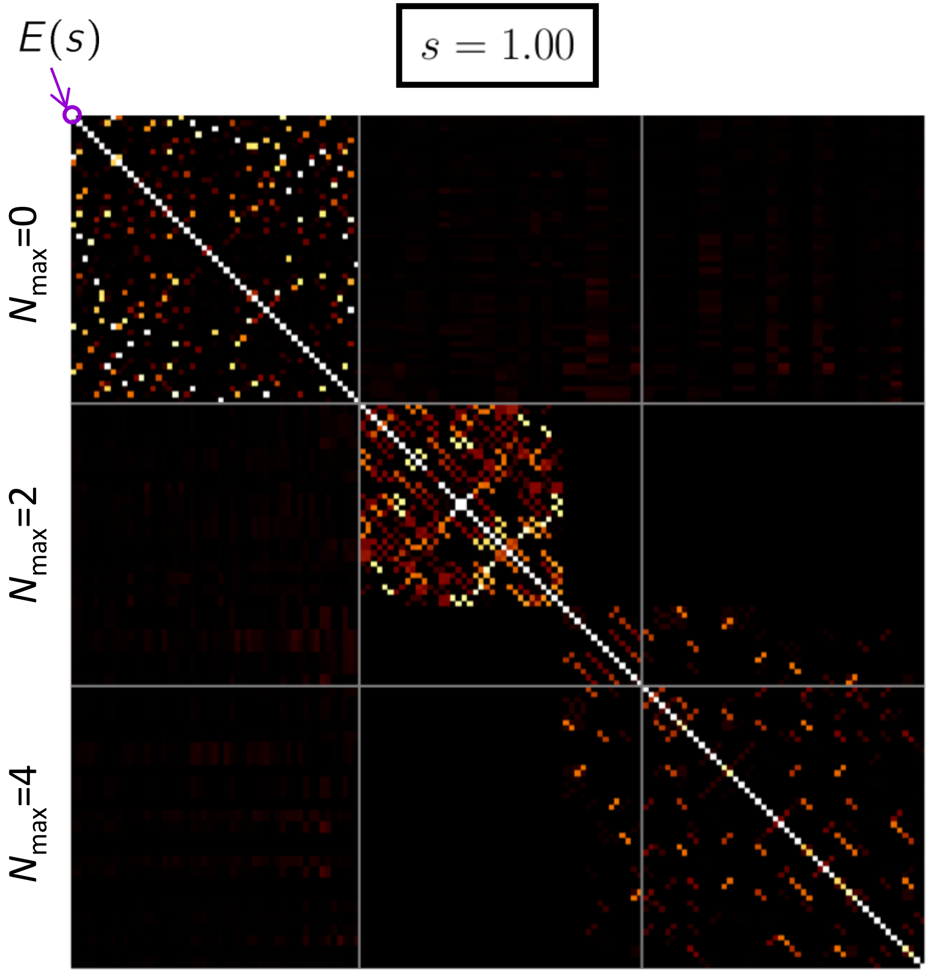

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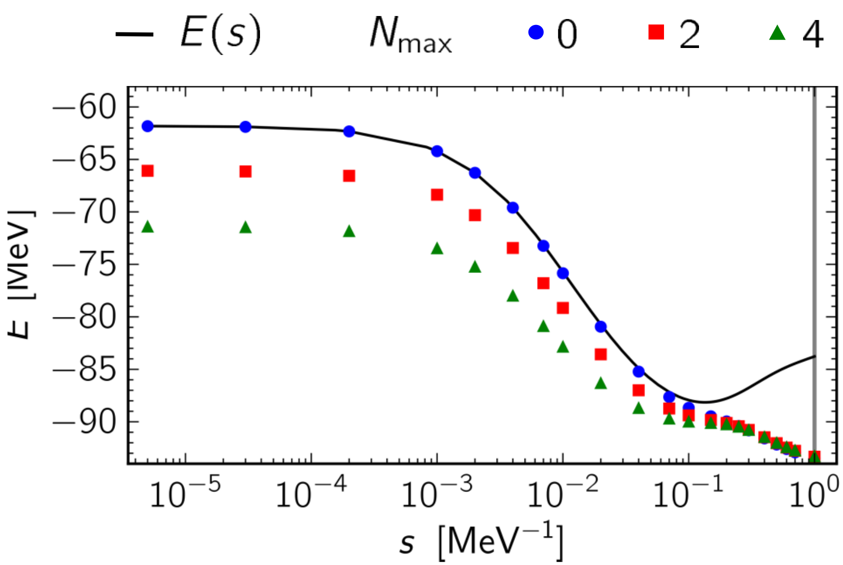

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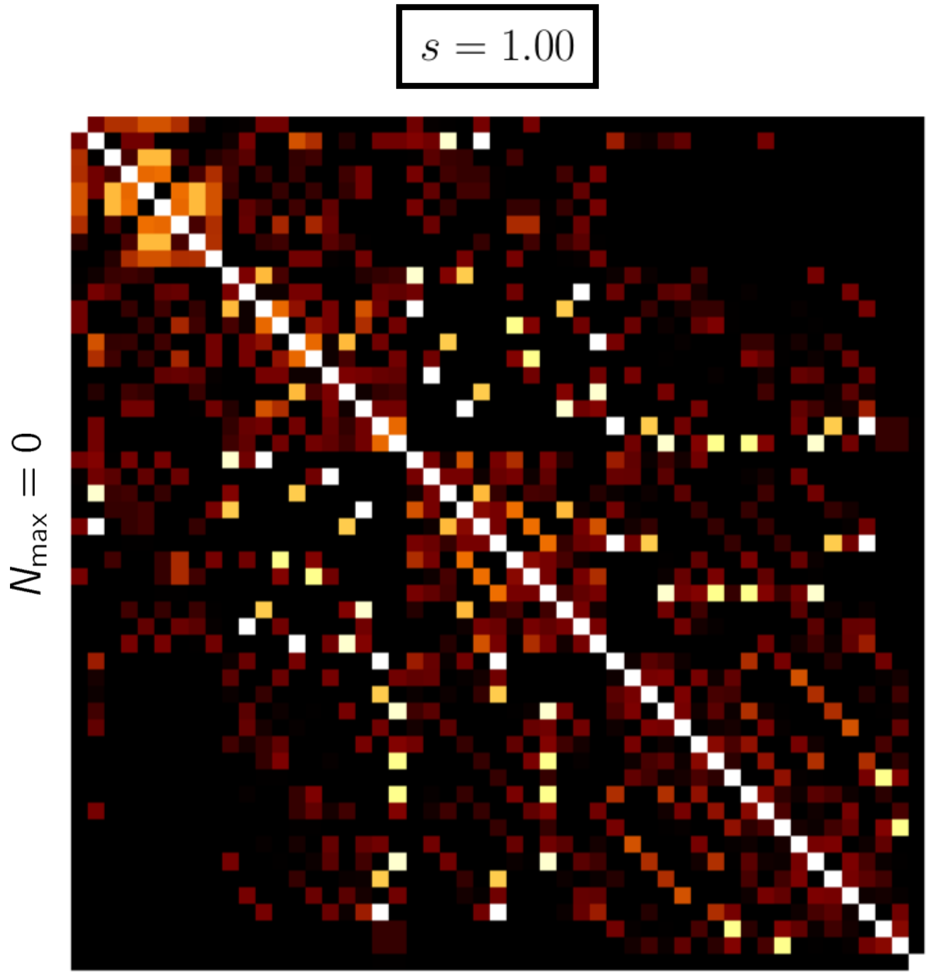
IM-SRG decouples reference state from N_{max} =2 and 4 spaces

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

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



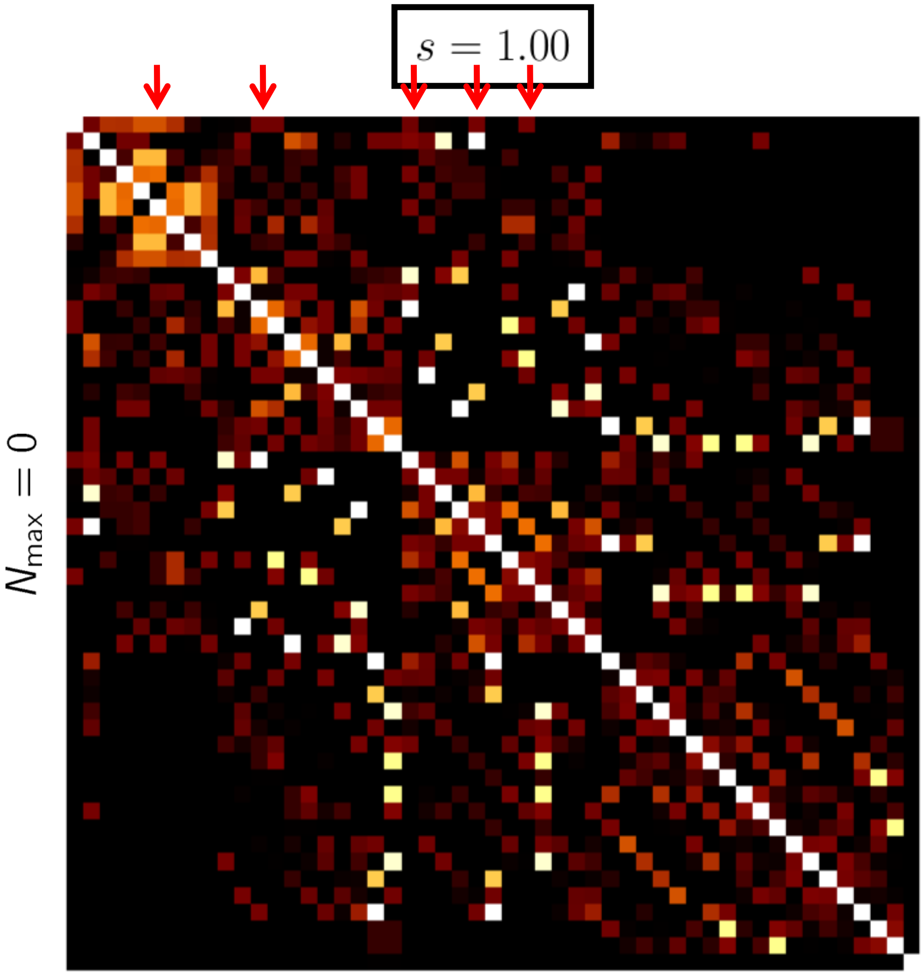
N_{max}=0
eigenstates

← first basis state = reference state

- N_{max}=0 states couple to reference state $|\Phi_{ref}\rangle$

Novel Approach: IM-NCSM

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



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N_{max}=0 eigenstates

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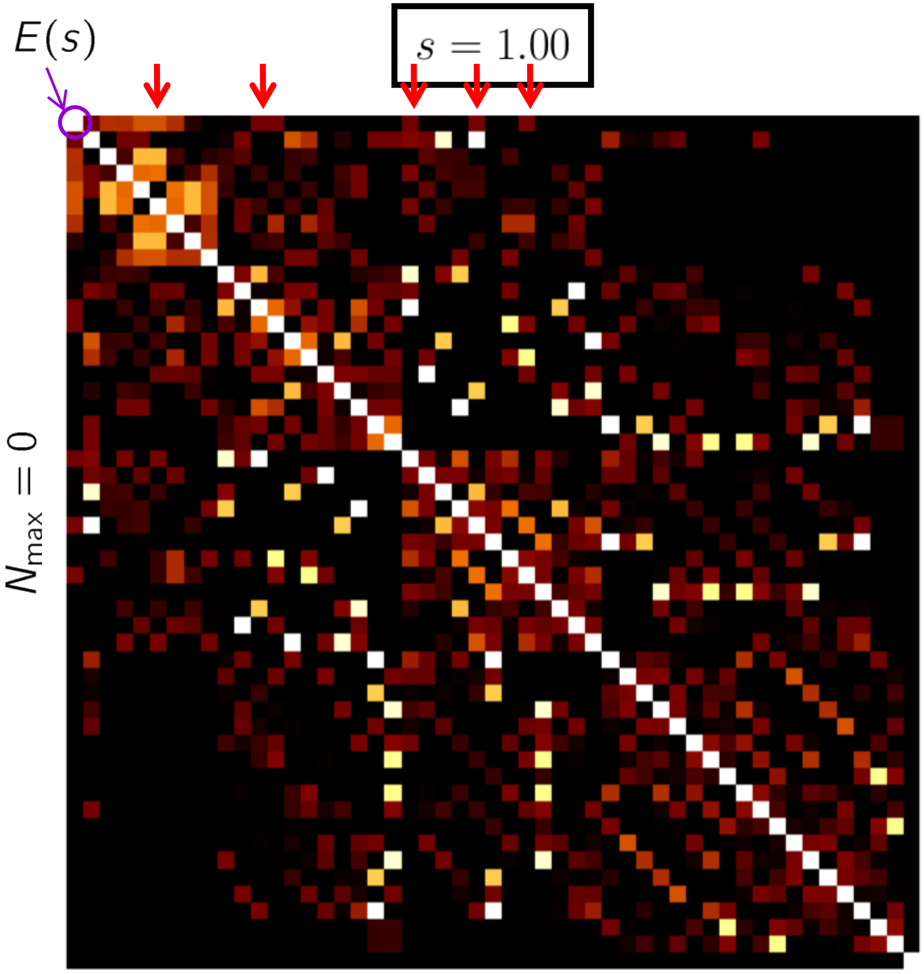
Hamilton Matrix in *A*-Body Basis: ^{12}C

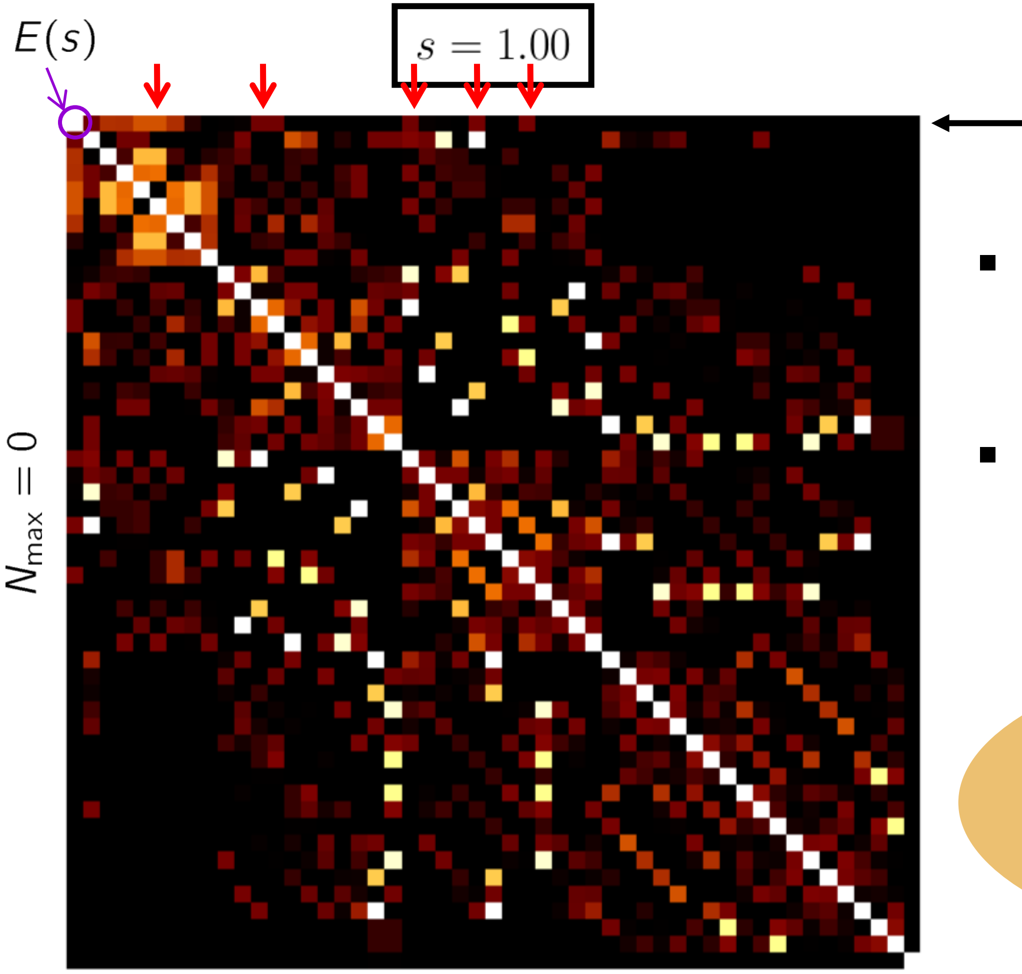


N_{max}=0 eigenstates

first basis state = reference state

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

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



first basis state = reference state

N_{max} eigenstates

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- $E(s)$ and N_{max}=0 eigenvalue cannot be identical

diagonalization of evolved Hamiltonian necessary

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Evolution of Ground-State Energy

chiral NN+$3N_{NO2B}$

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

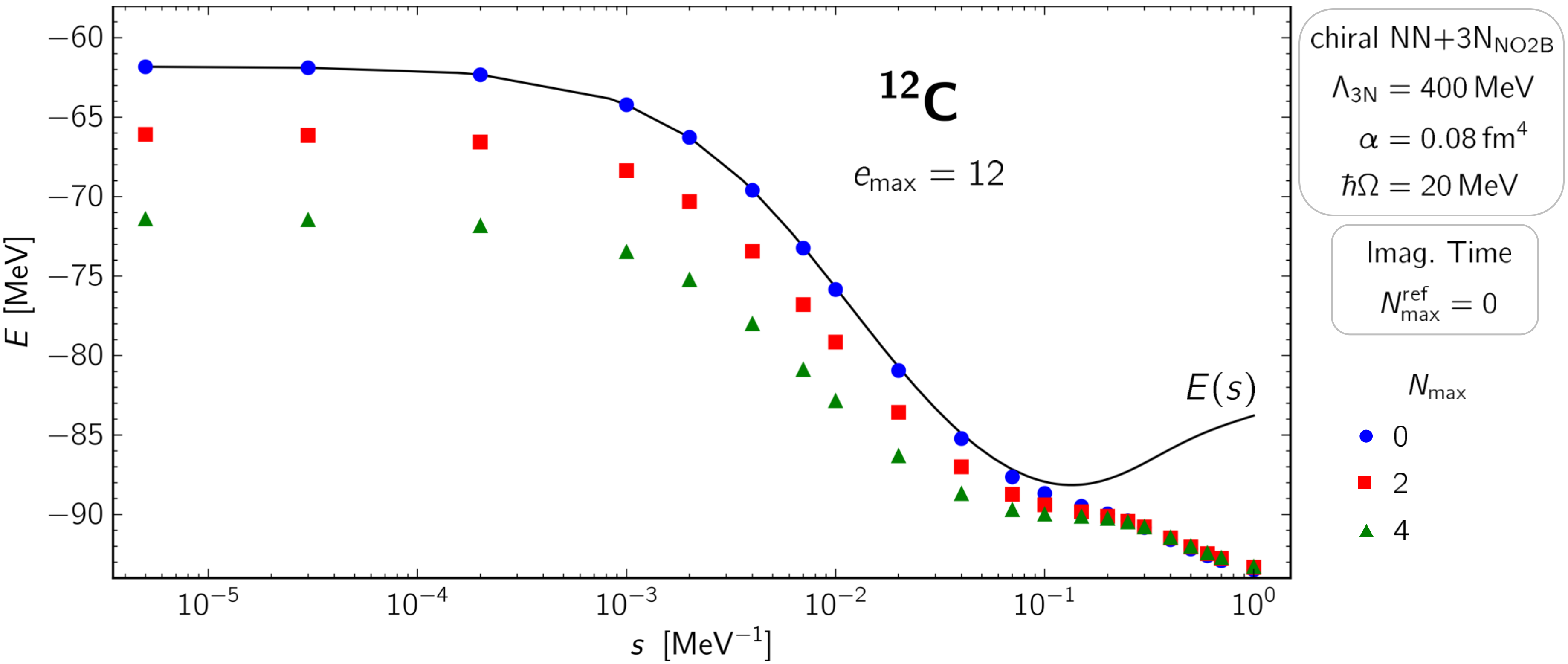
$\alpha = 0.08\,\text{fm}^4$

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

Imag. Time

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

Evolution of Ground-State Energy



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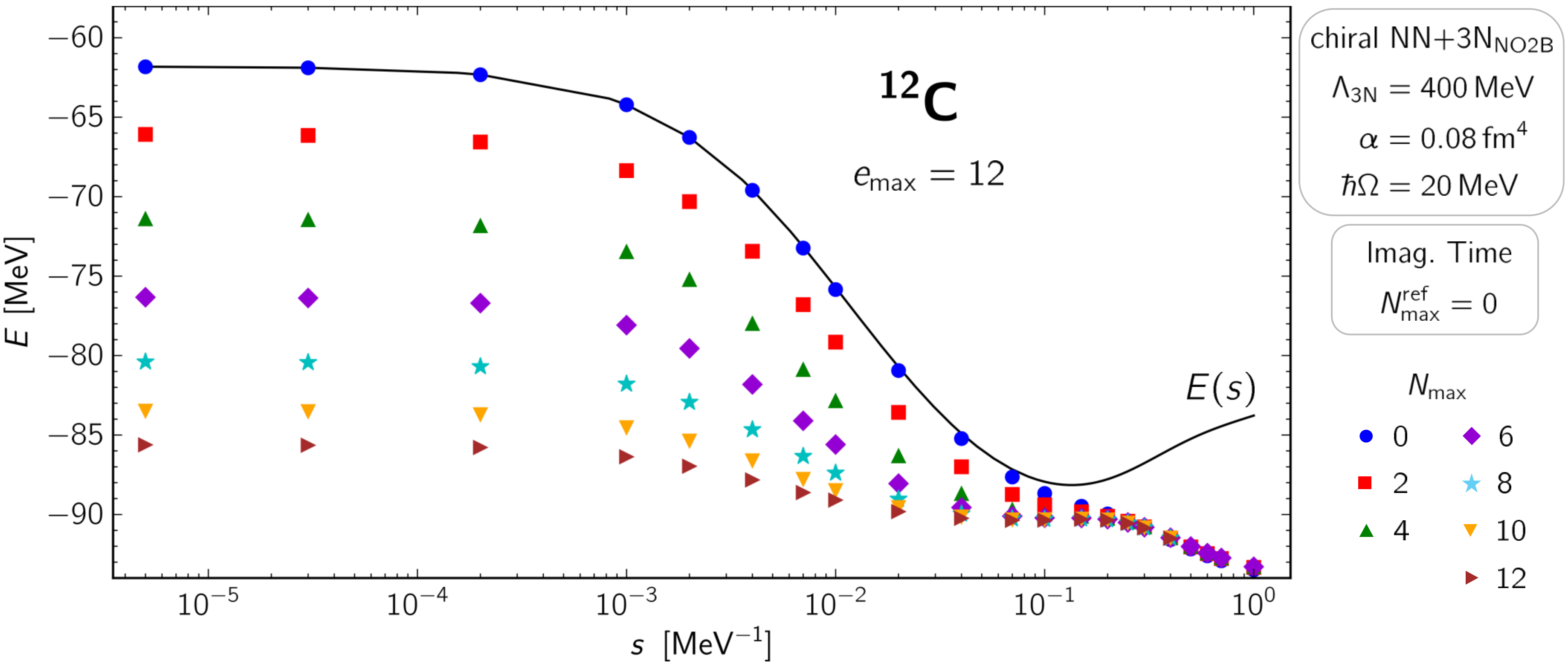
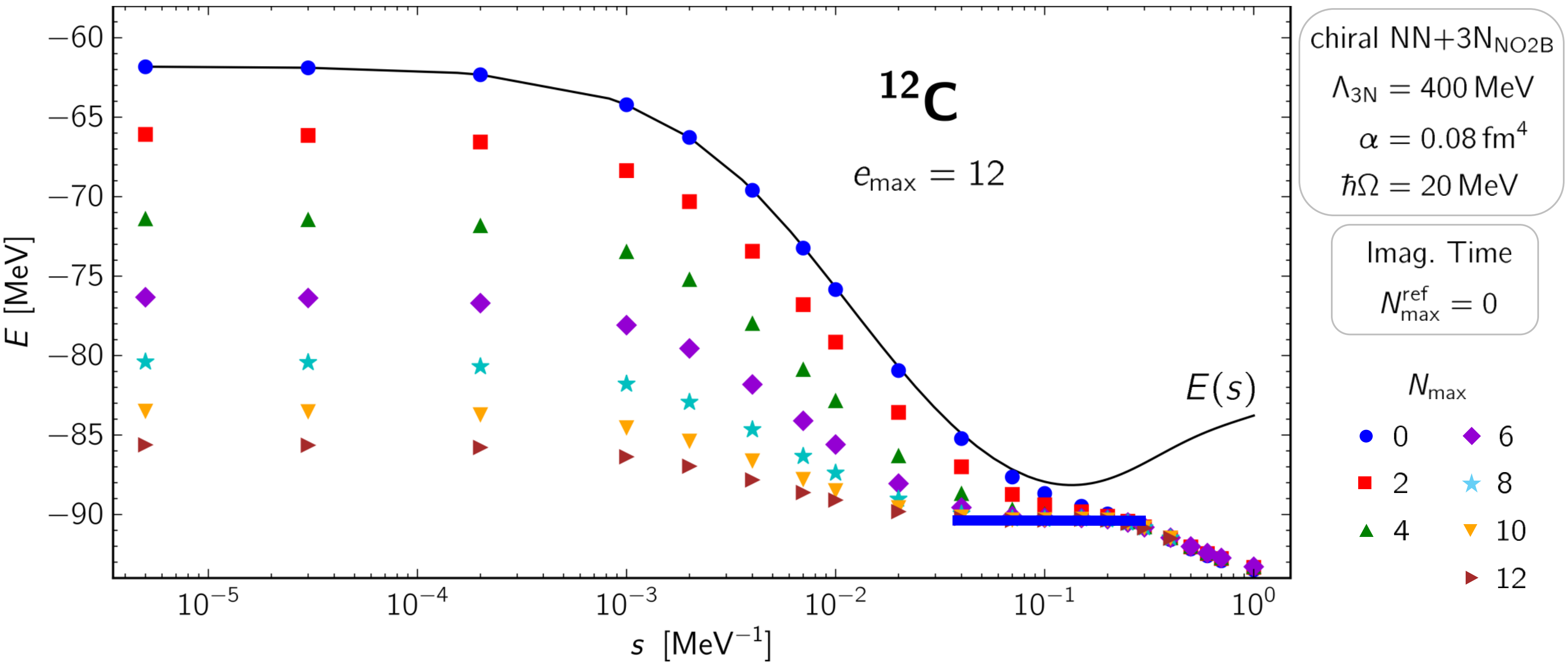


- drastically enhanced model-space convergence for IM-NCSM

Results

Evolution of Ground-State Energy



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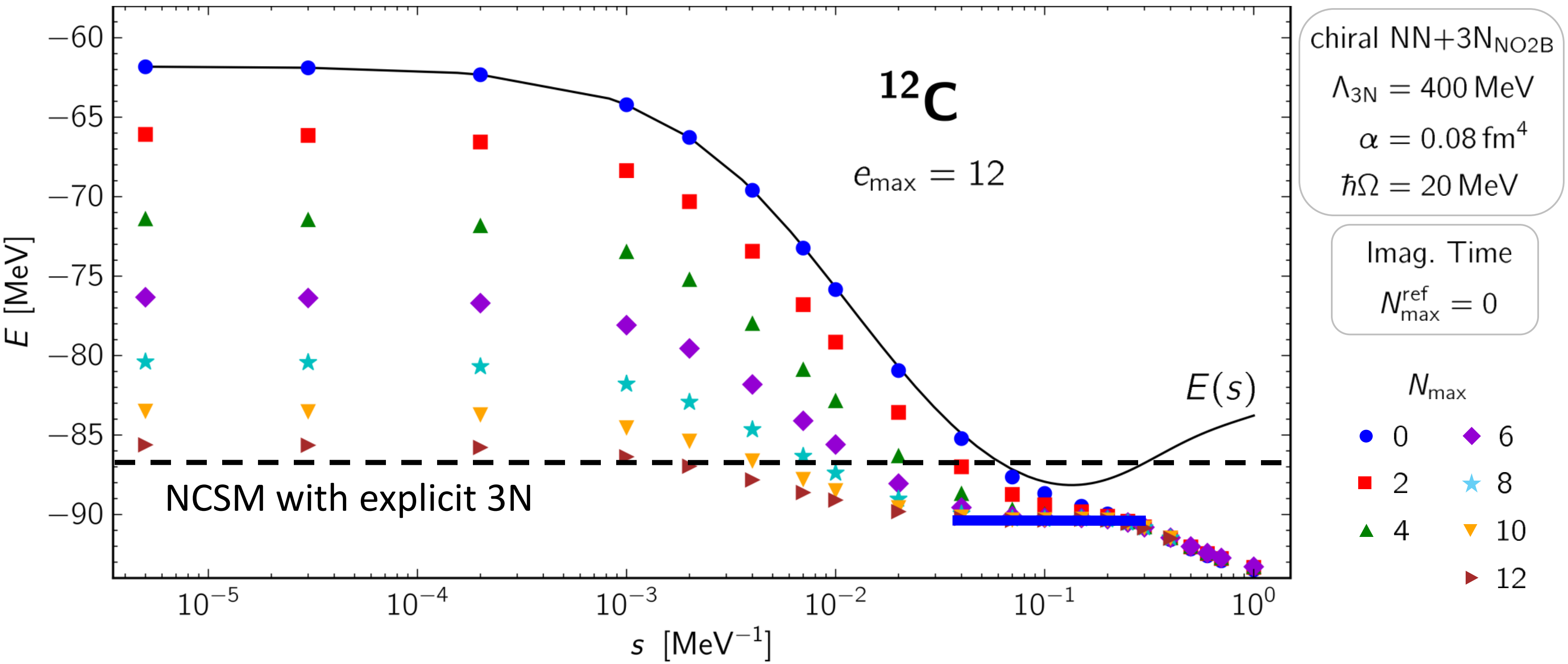

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Evolution of Ground-State Energy

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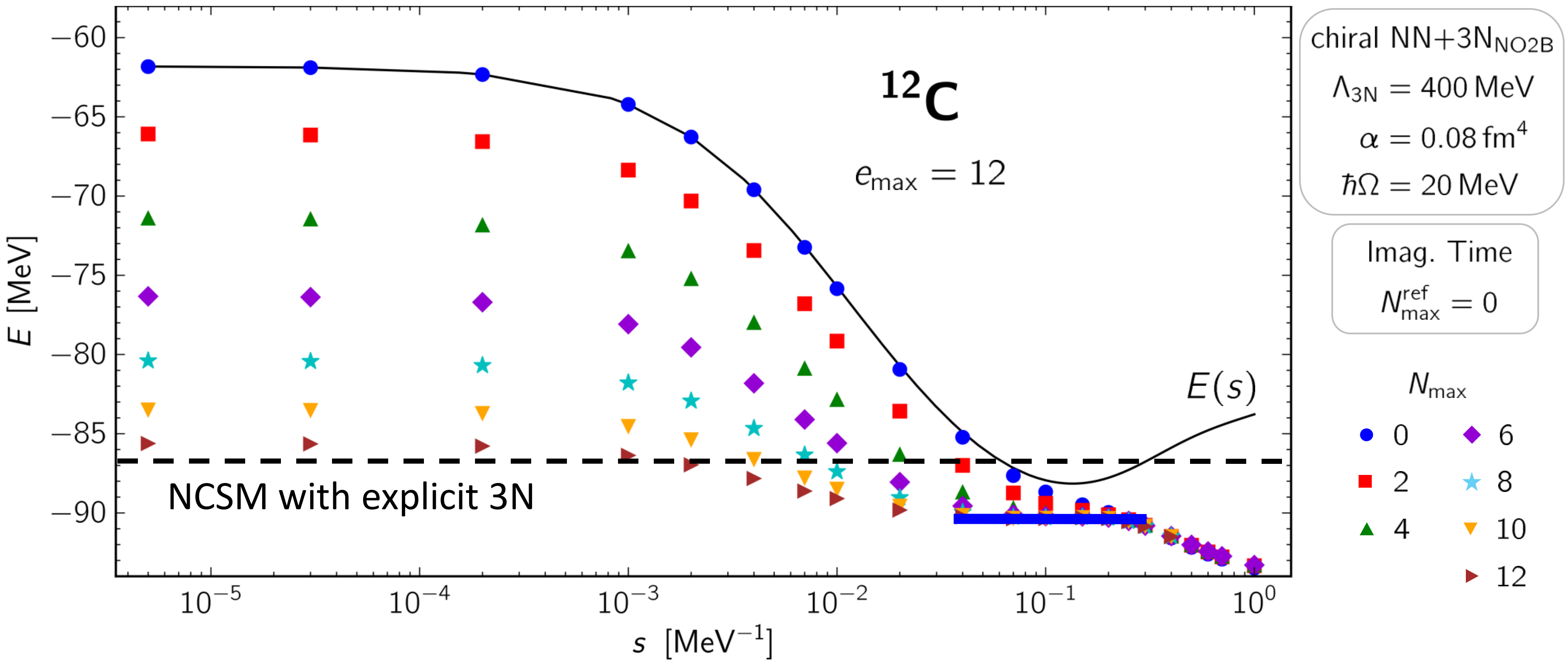

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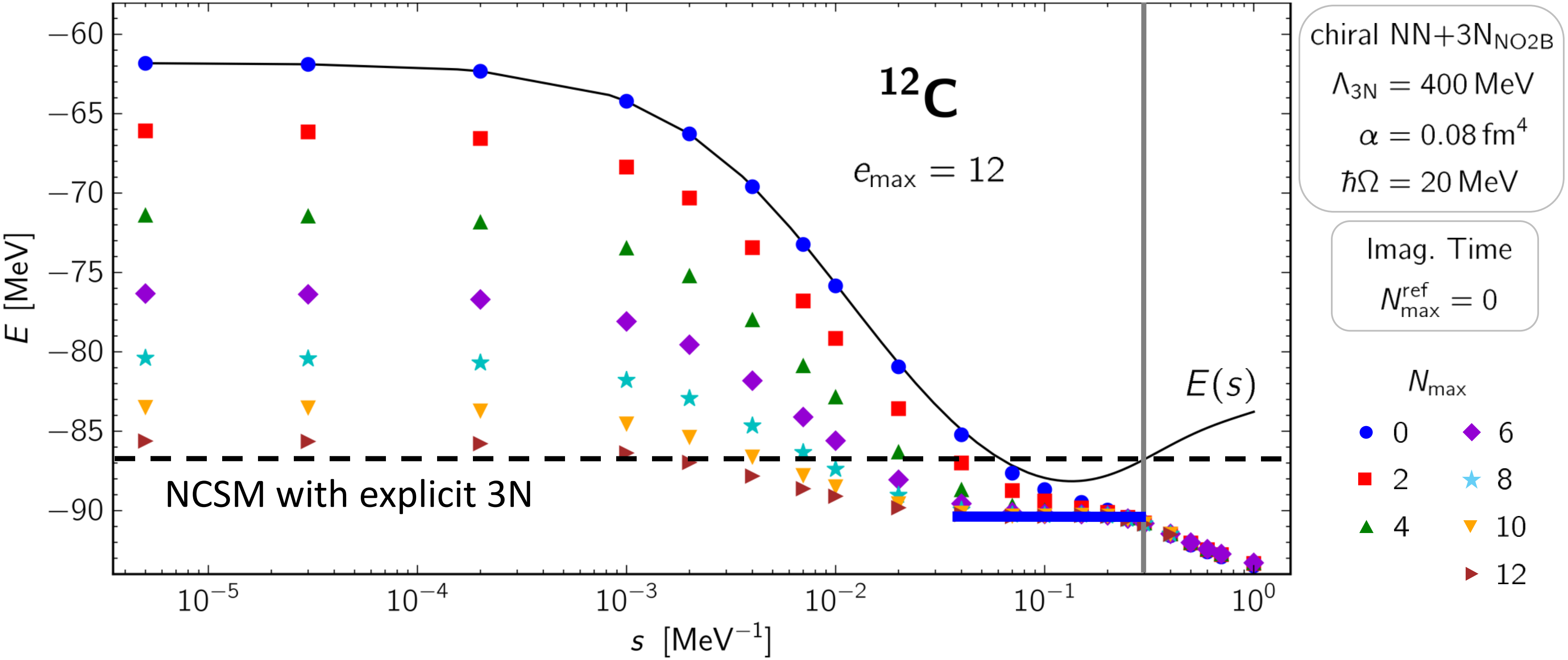

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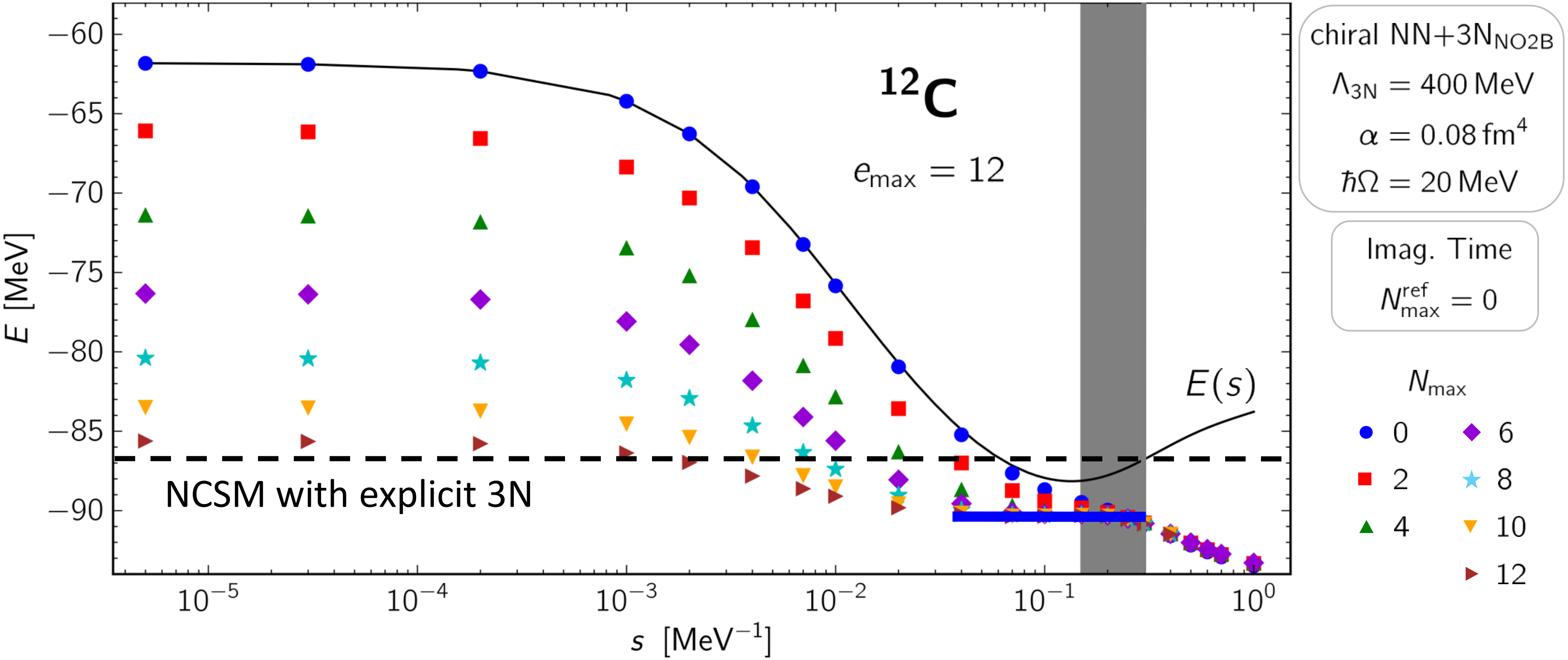

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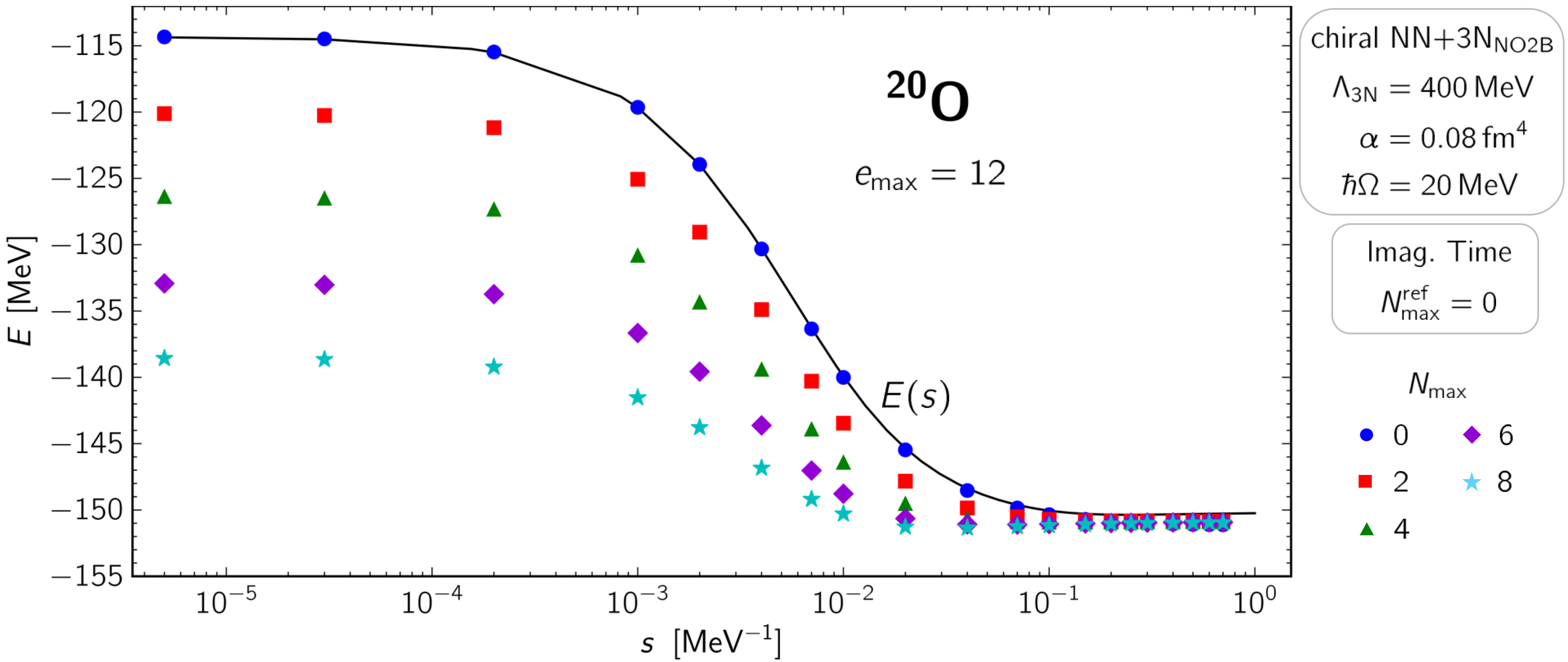

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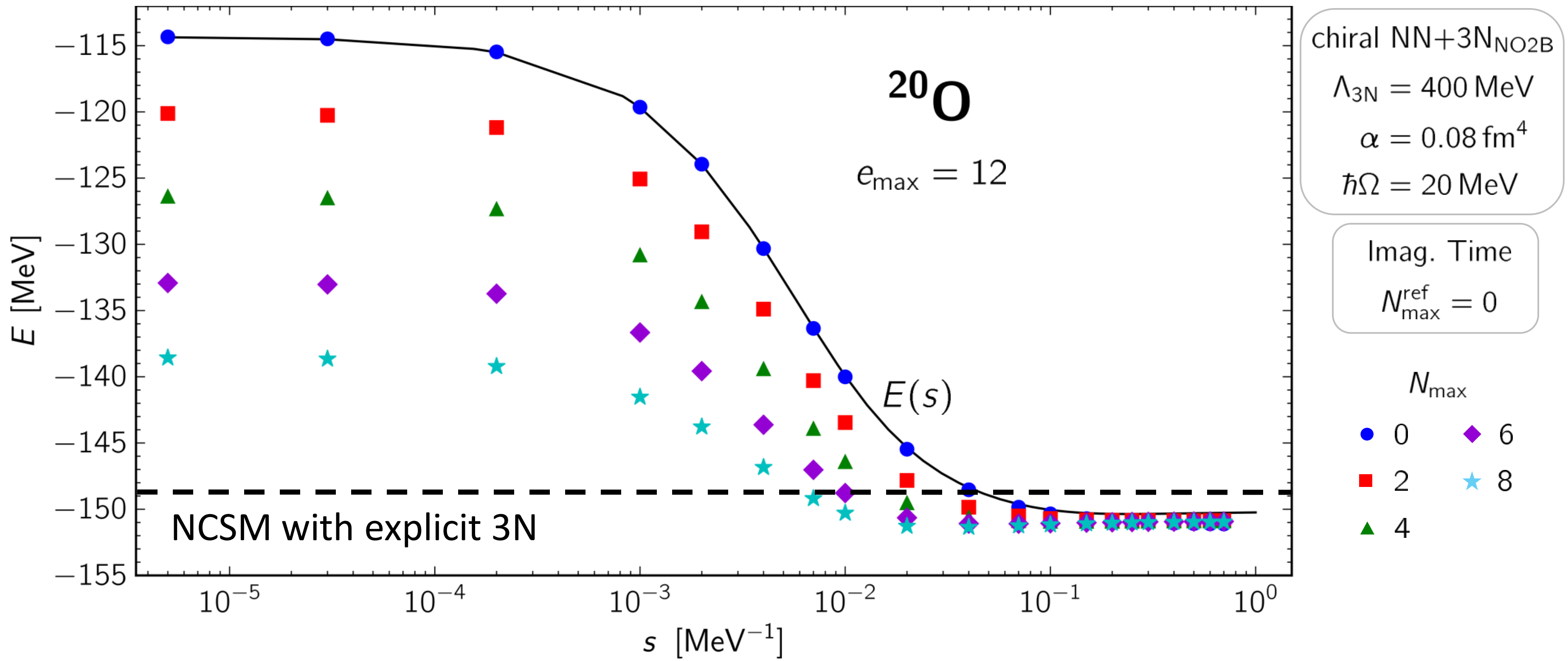

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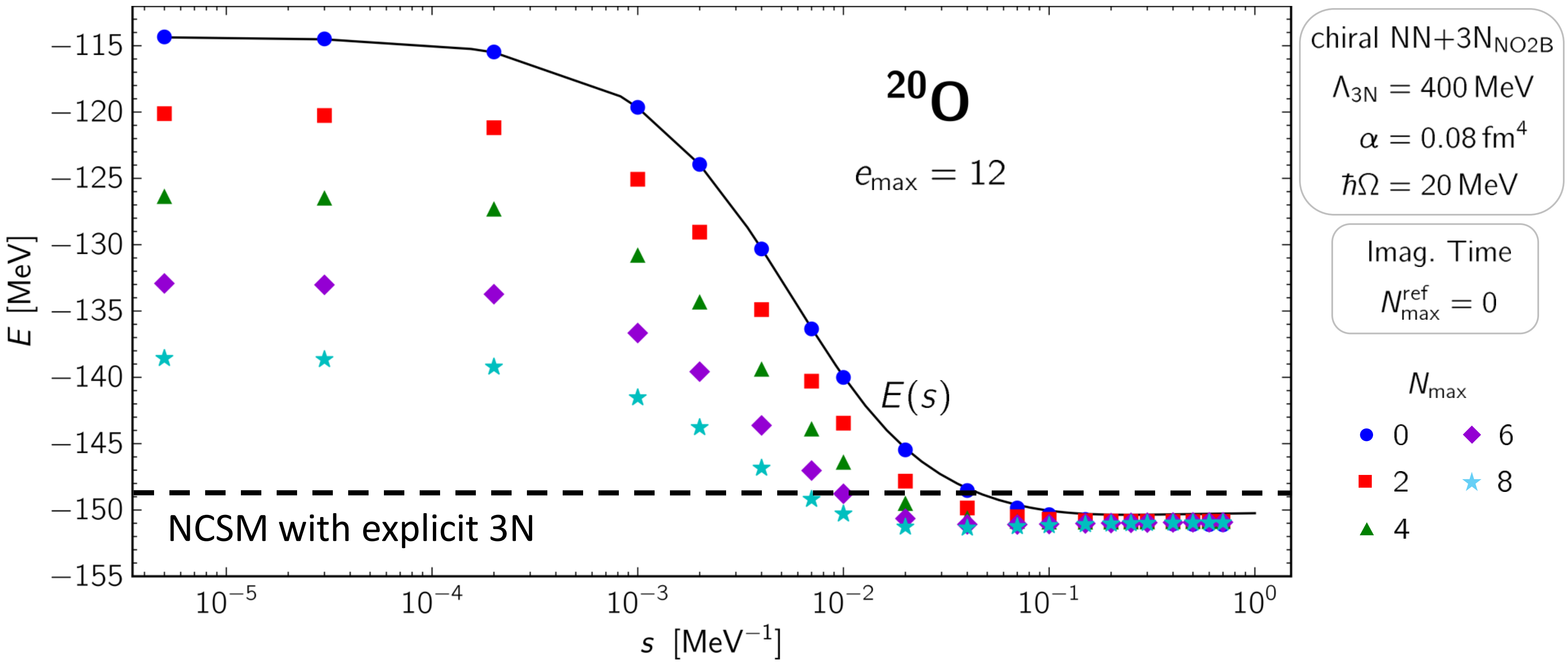

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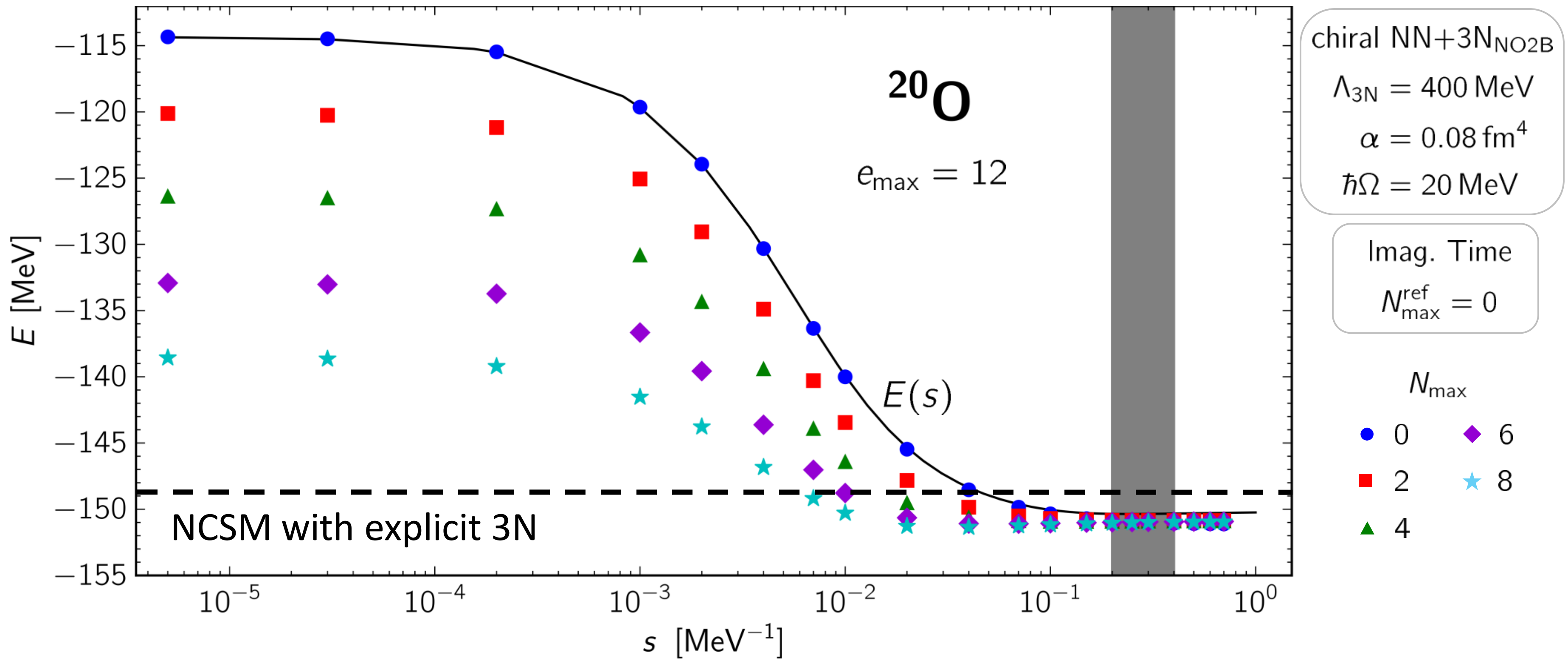

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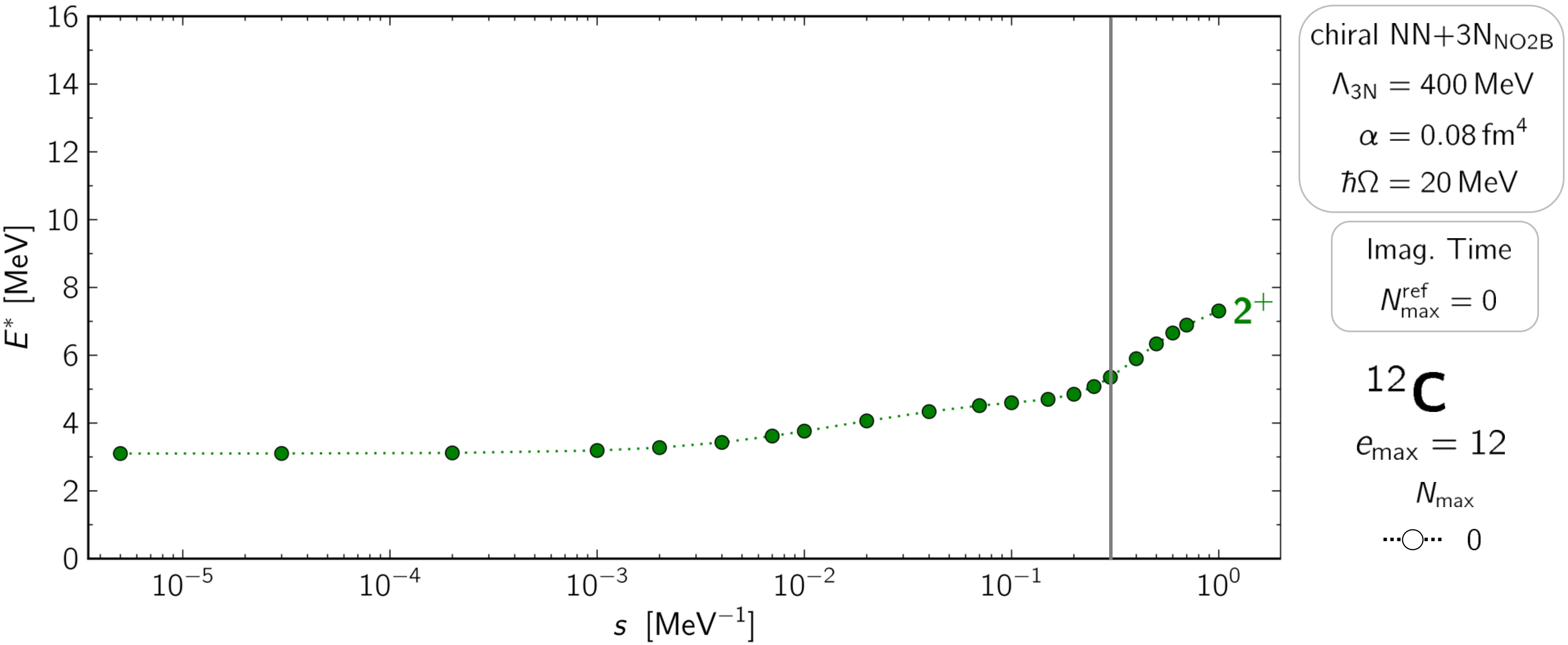

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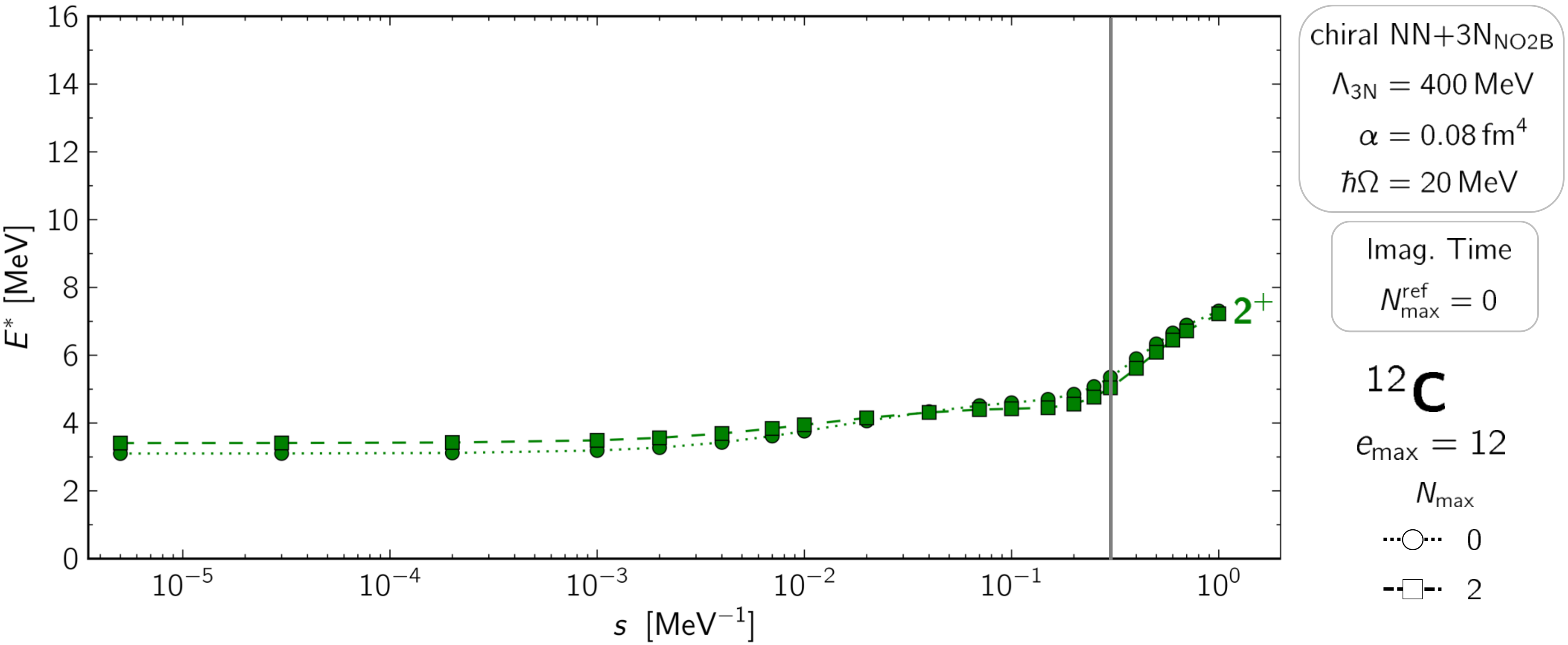

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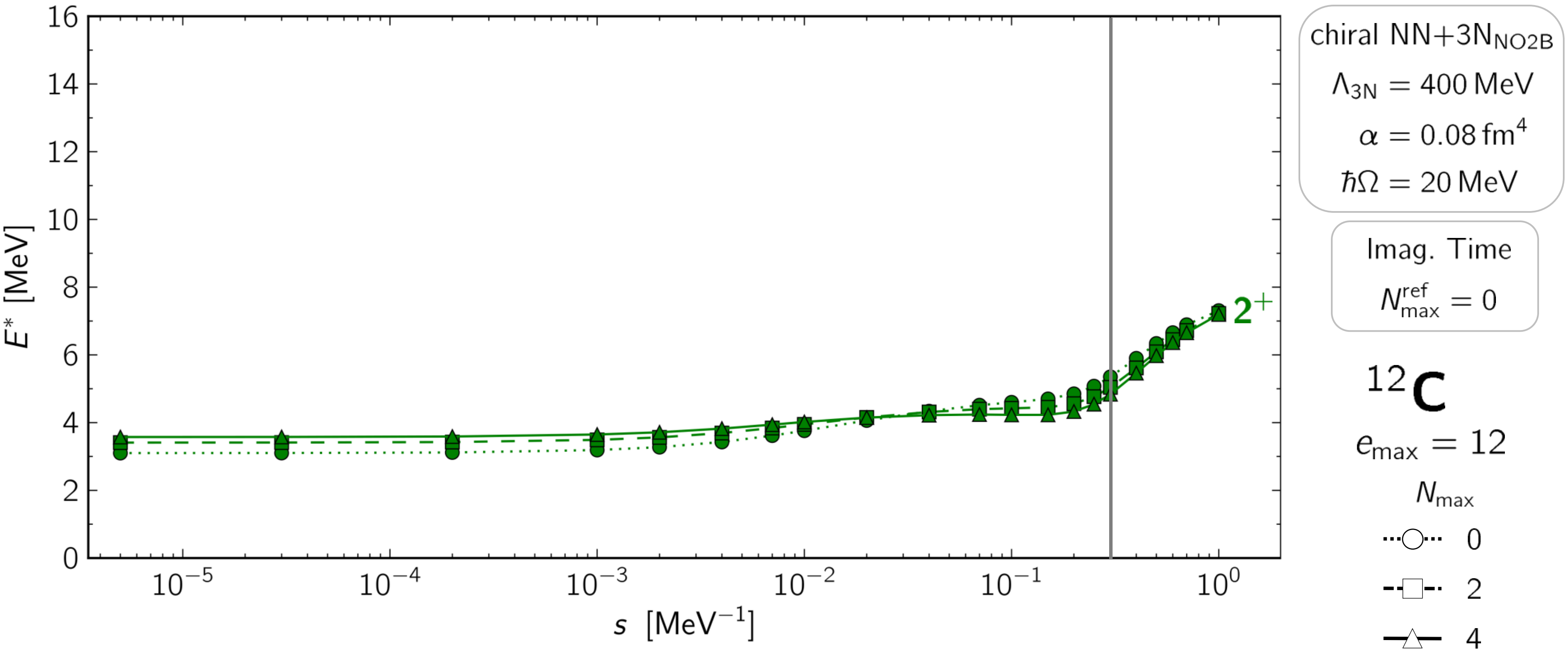
Evolution of Excitation Energies



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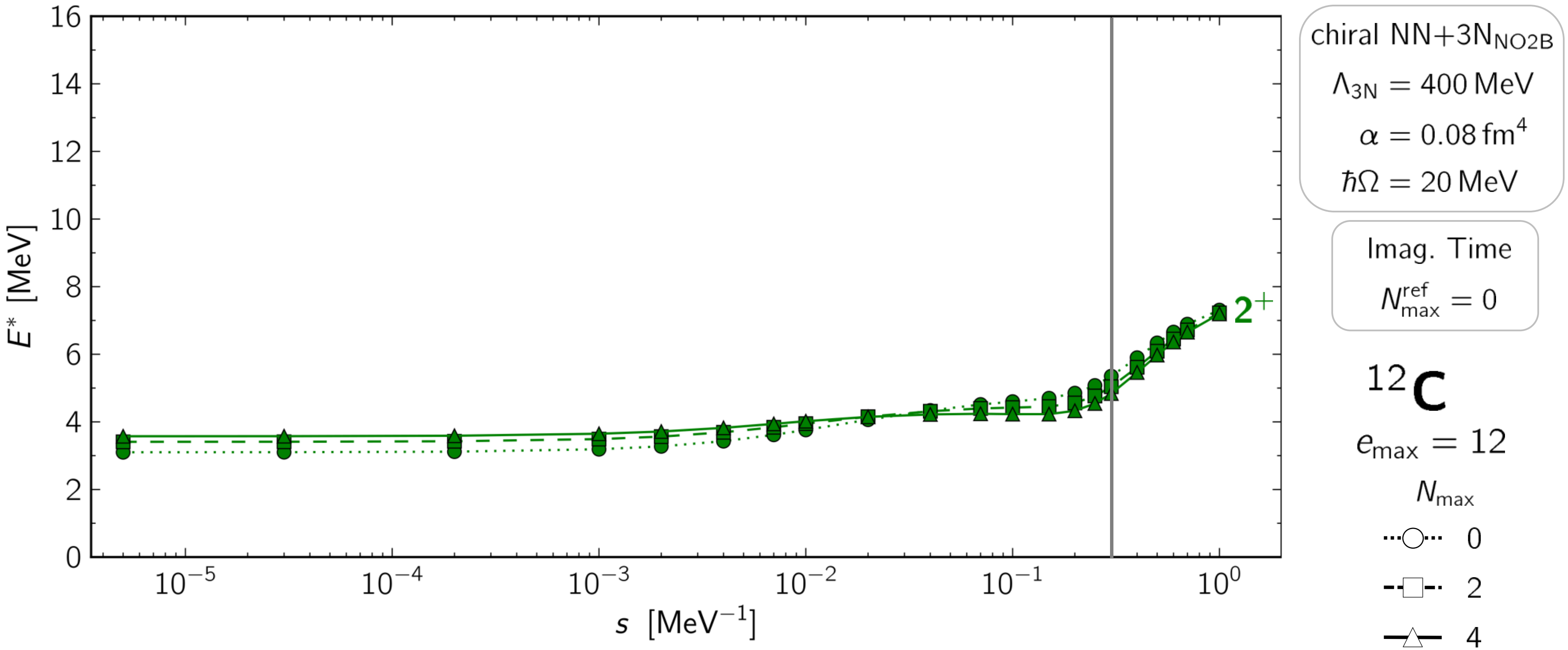

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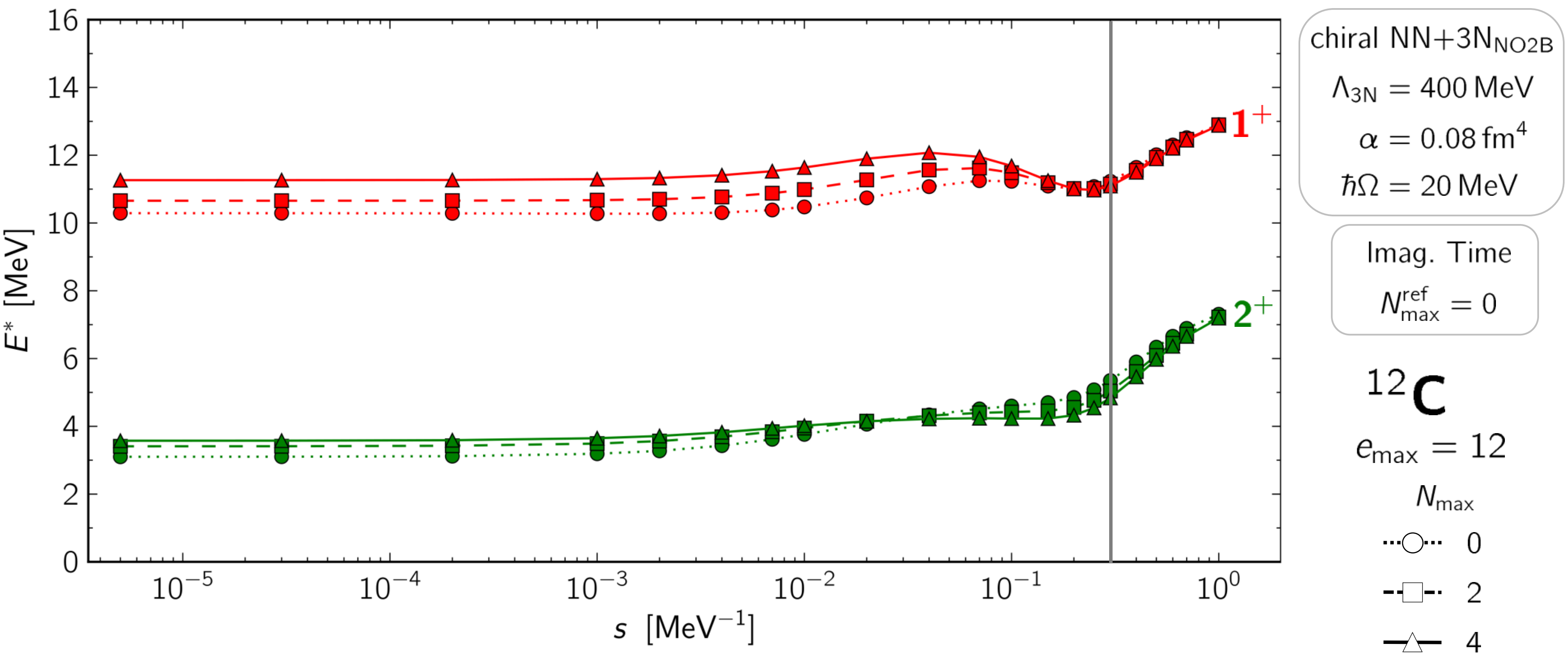

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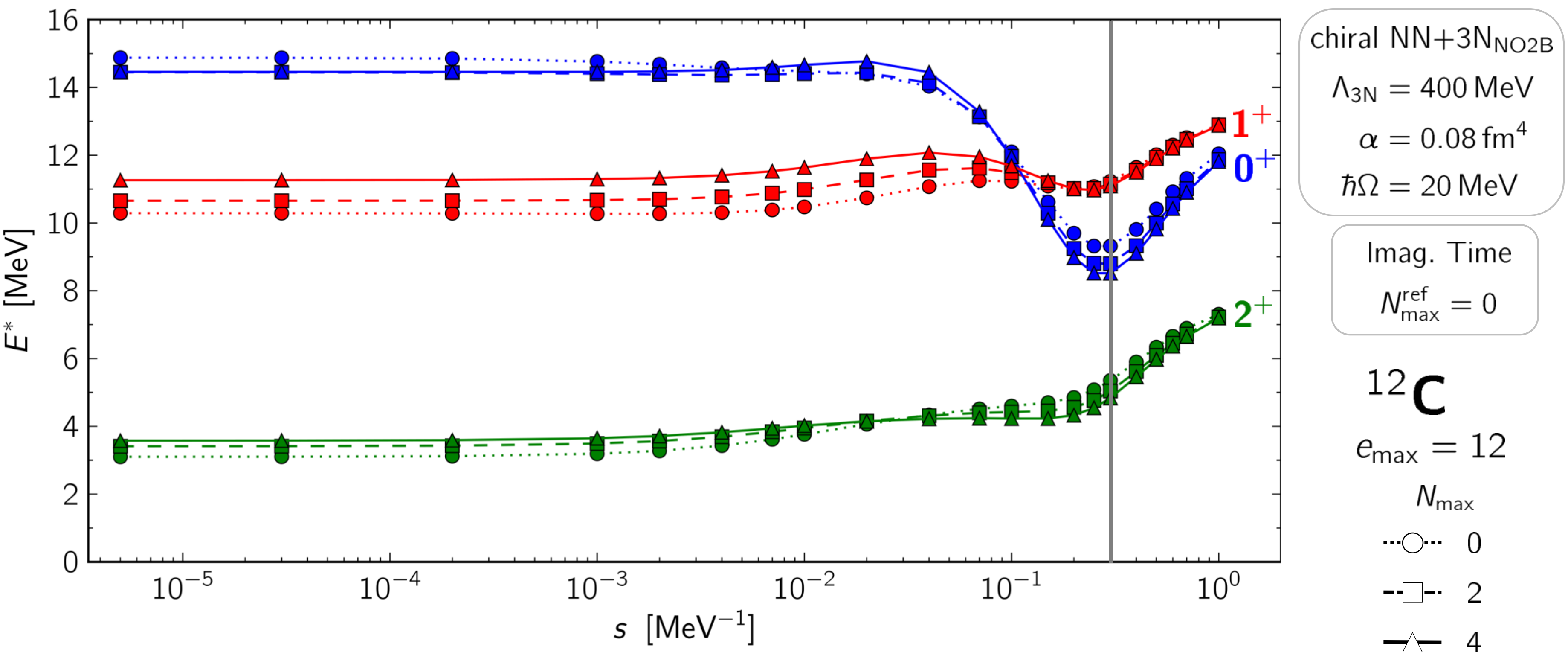

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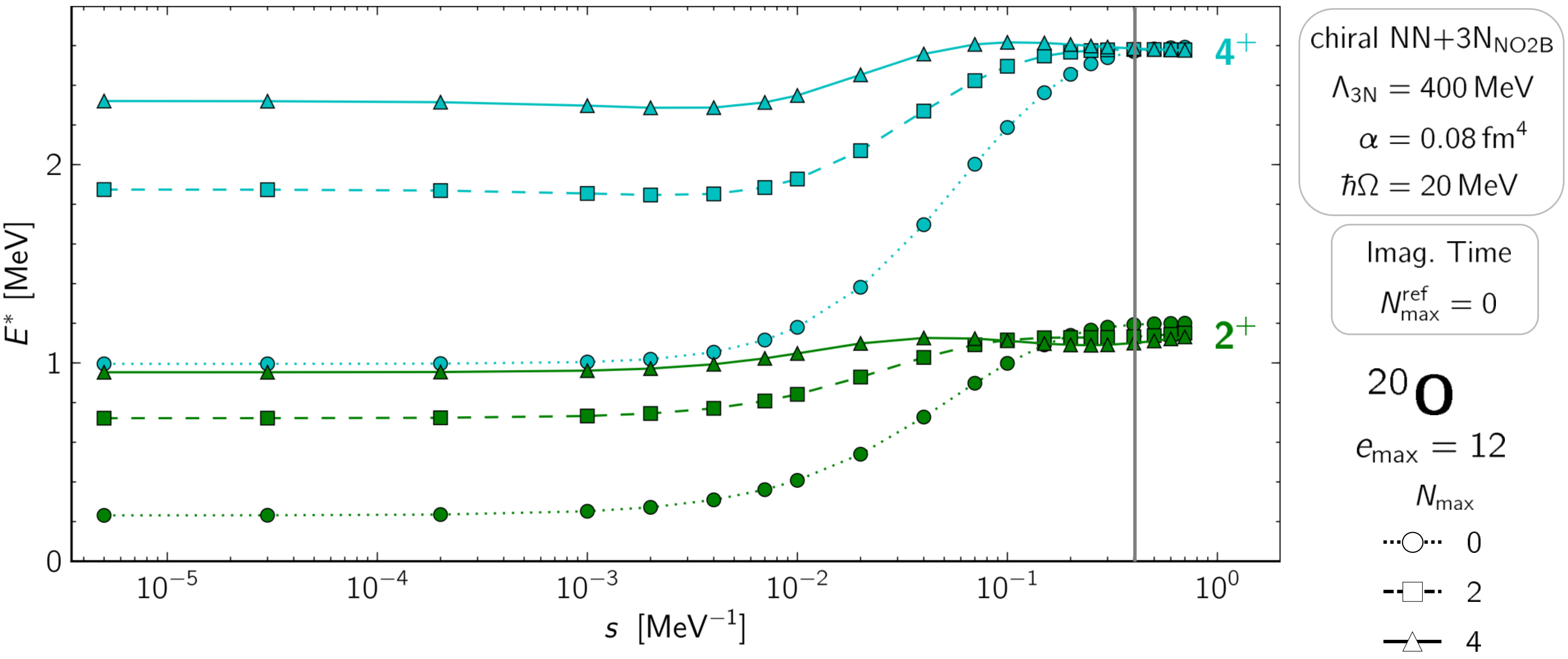
- first excited 0^+ very sensitive to flow parameter → **Hoyle state?**

Evolution of Excitation Energies



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

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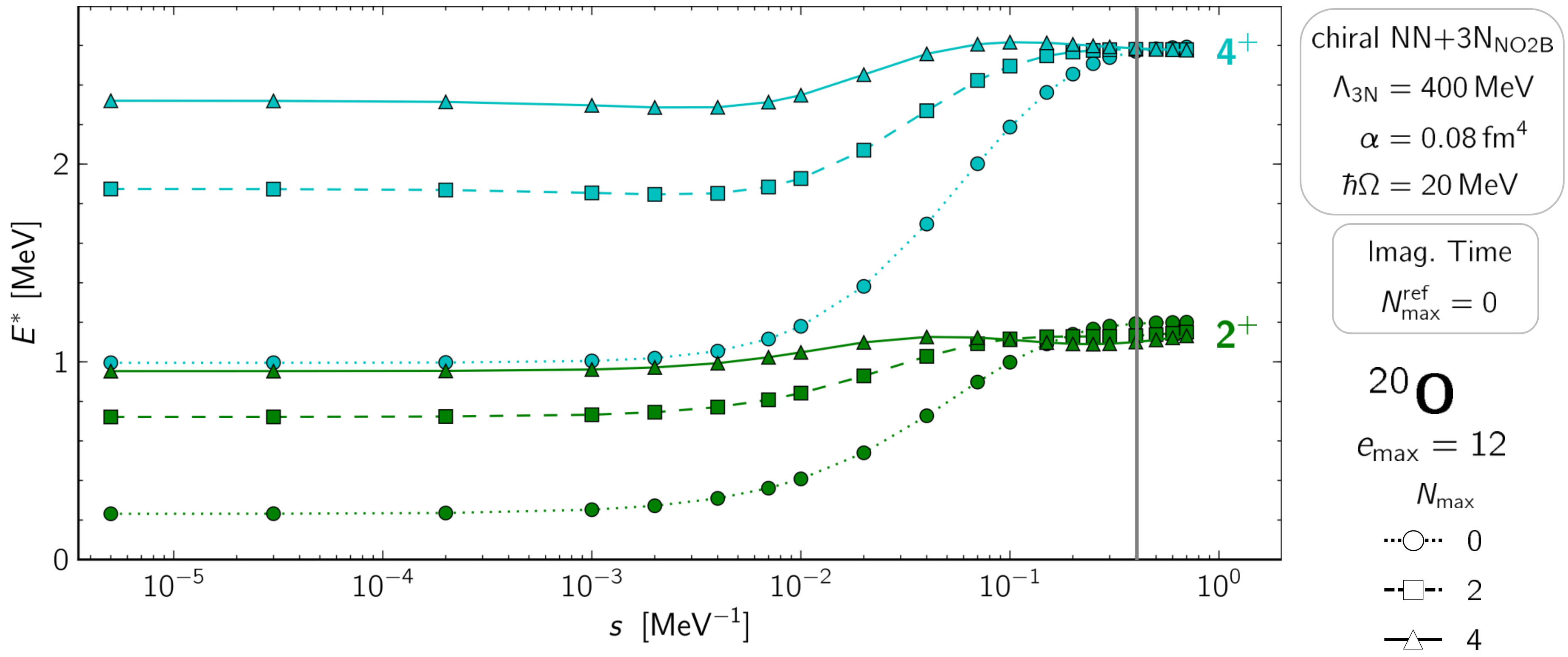

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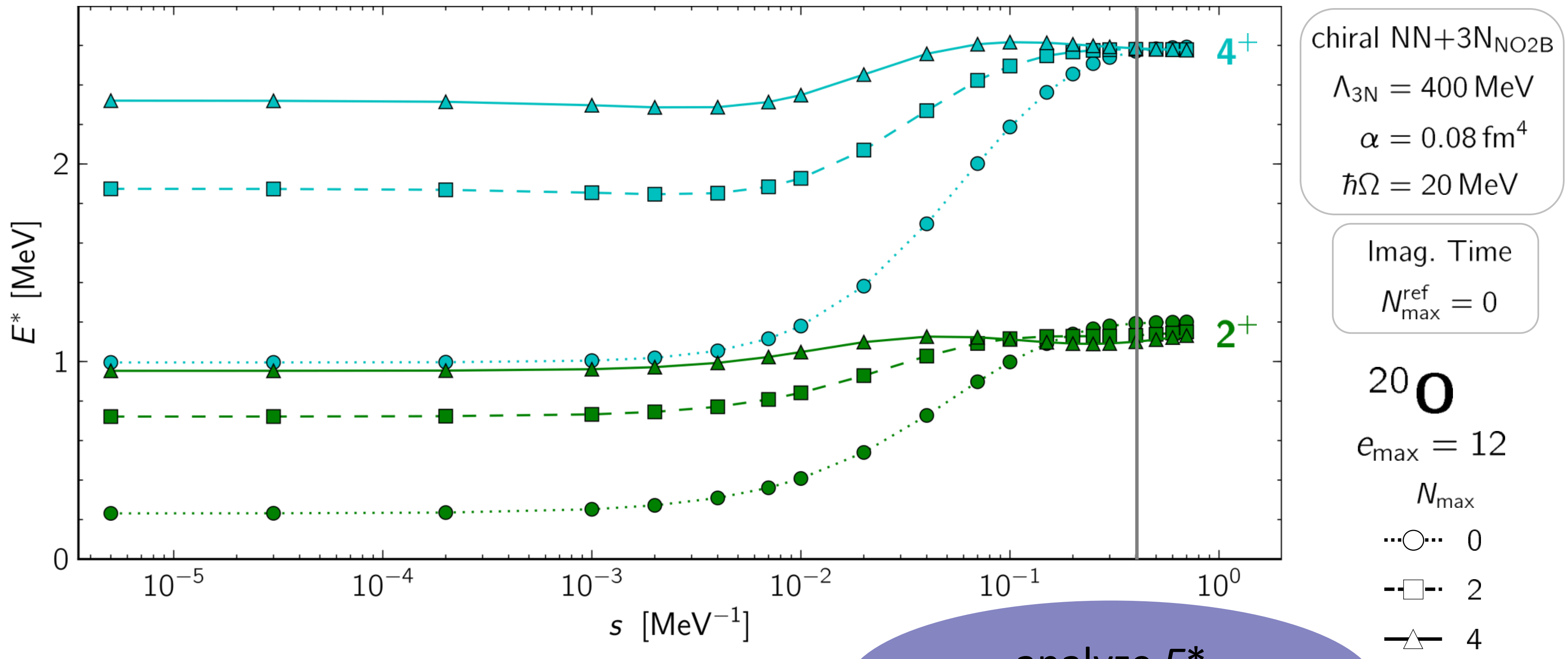

analyze E^* as function of N_{max}

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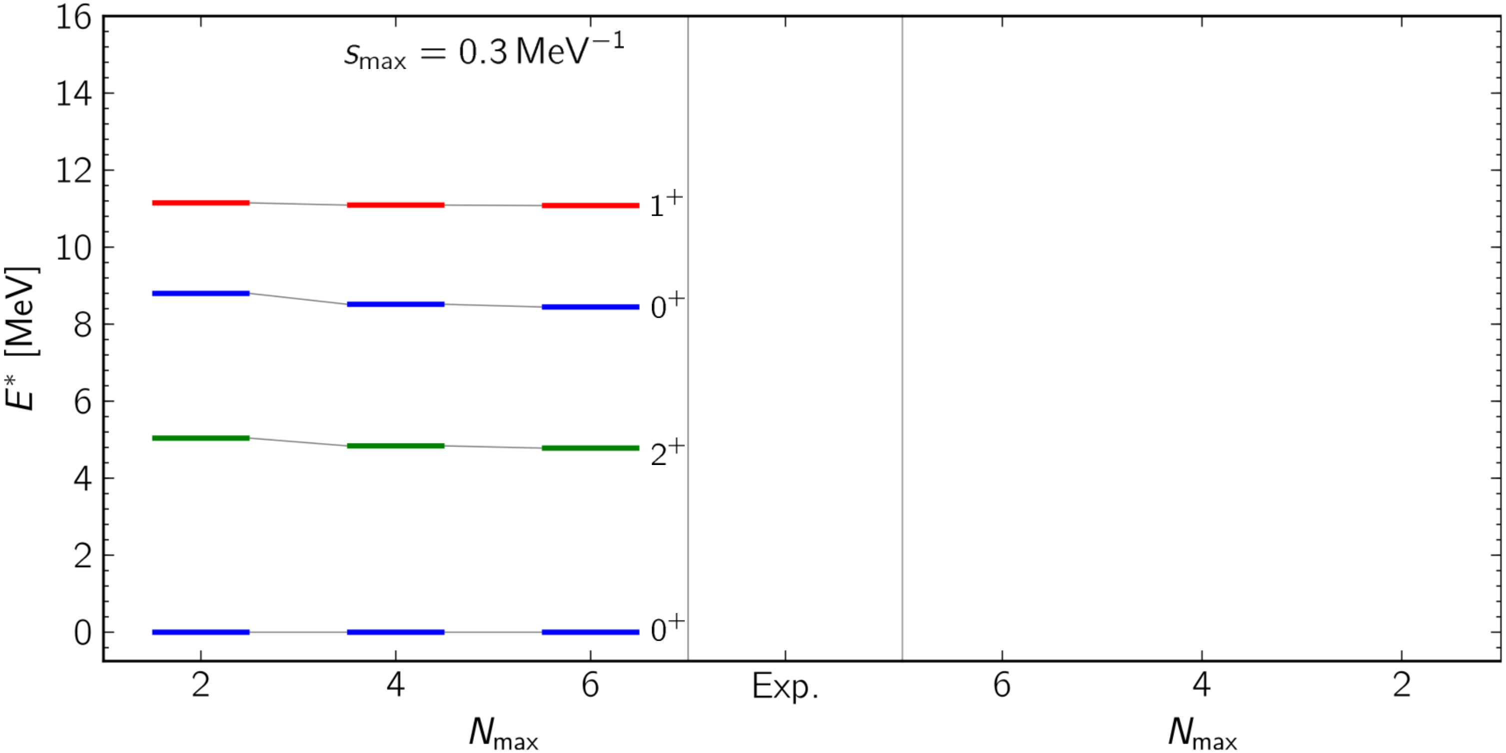
Spectra

IM-NCSM



chiral NN+3N$_{NO2B}$

$\Lambda_{3N} = 400$ MeV

$\alpha = 0.08$ fm^4

$\hbar\Omega = 20$ MeV

Imag. Time

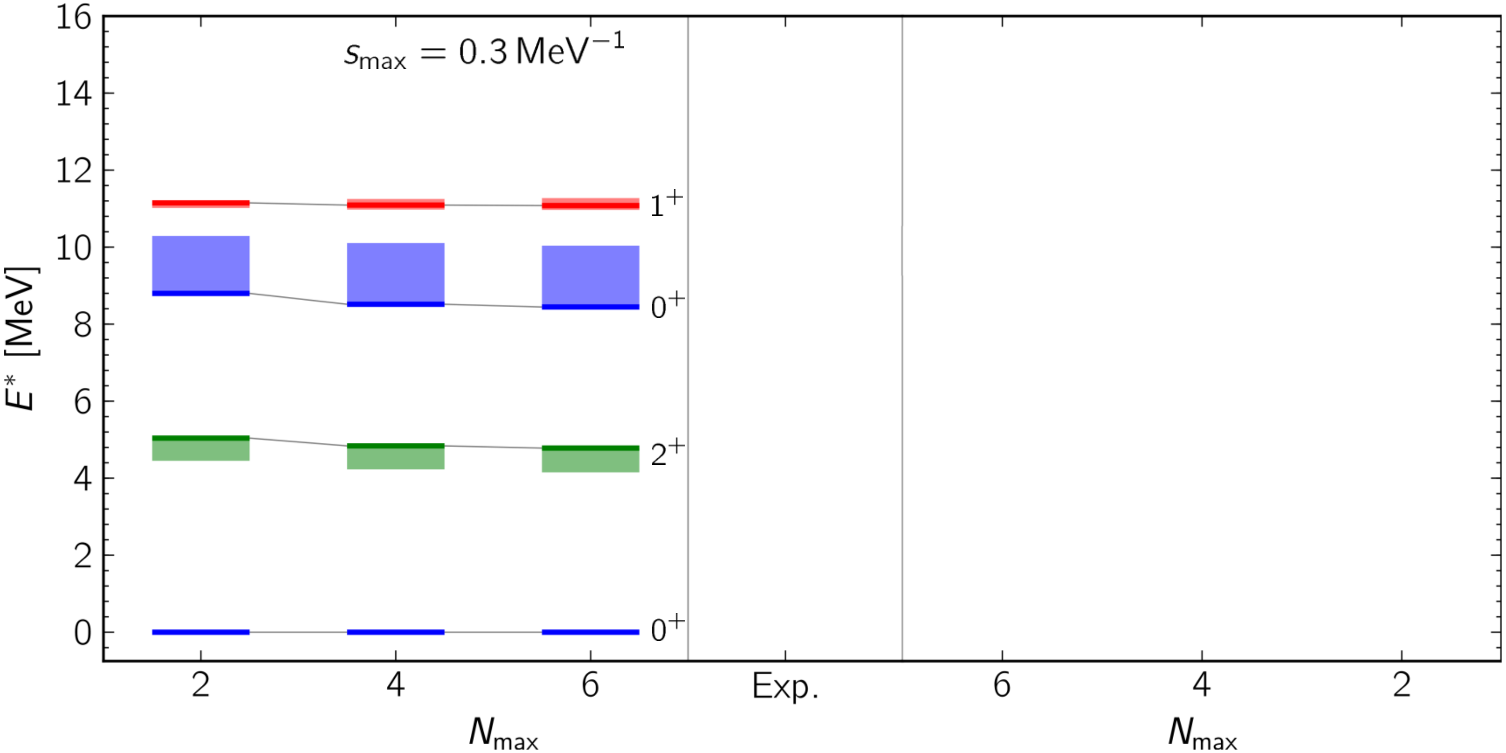
$N_{max}^{ref} = 0$

^{12}**C**

$e_{max} = 12$

Spectra

IM-NCSM



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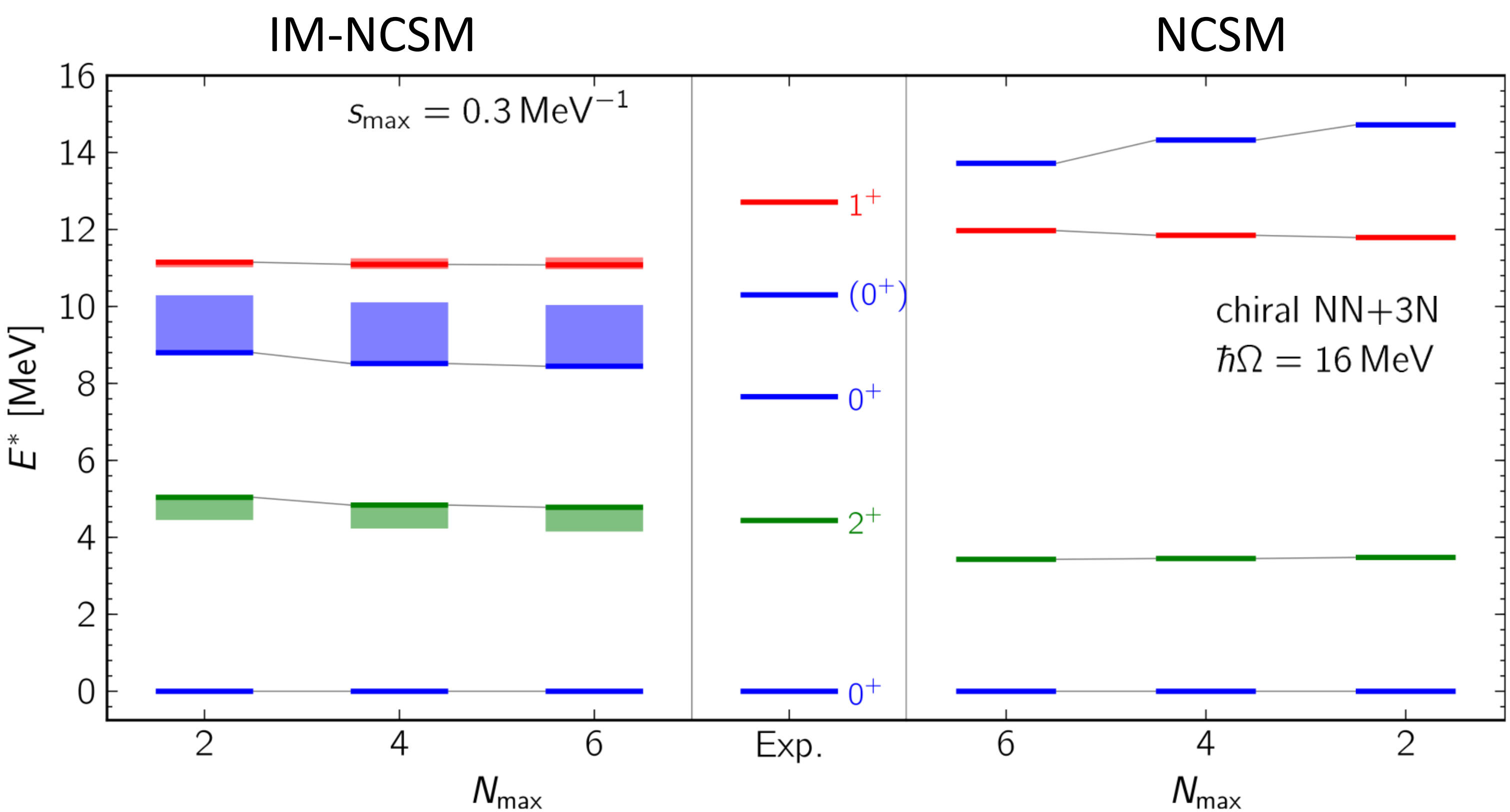
- uncertainty band due to flow-parameter variation between $s_{max}/2$ and s_{max}

Spectra



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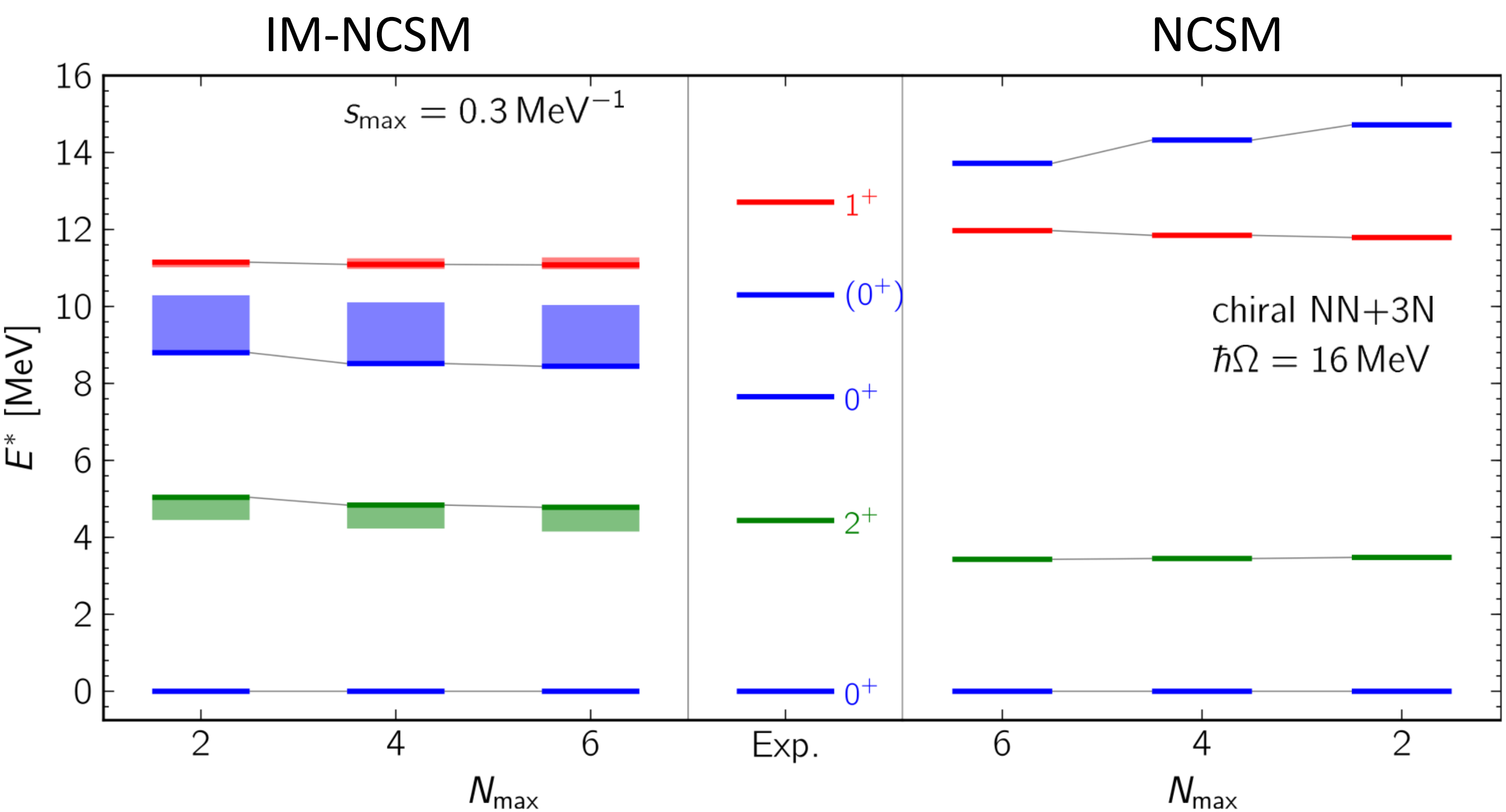

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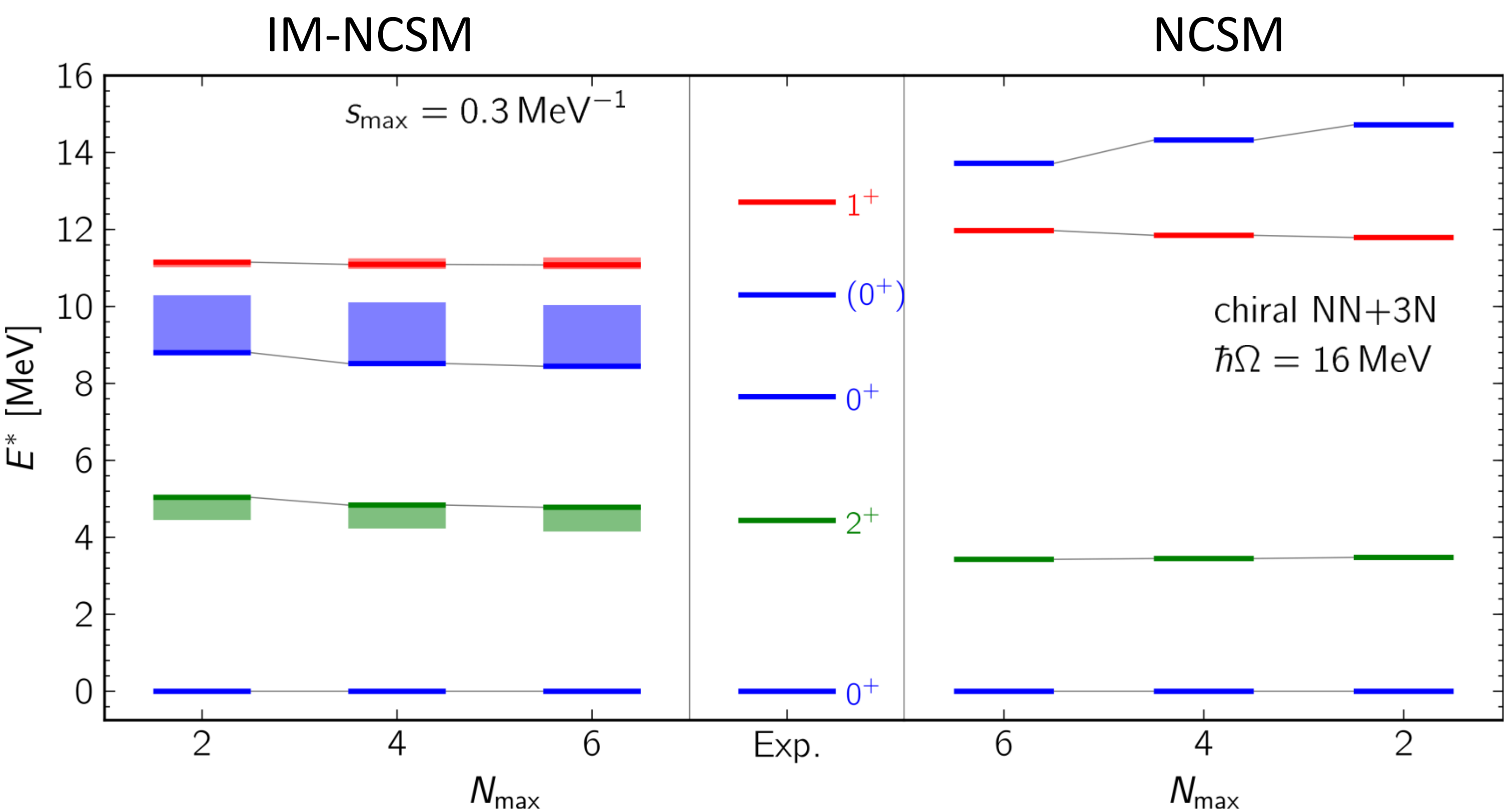

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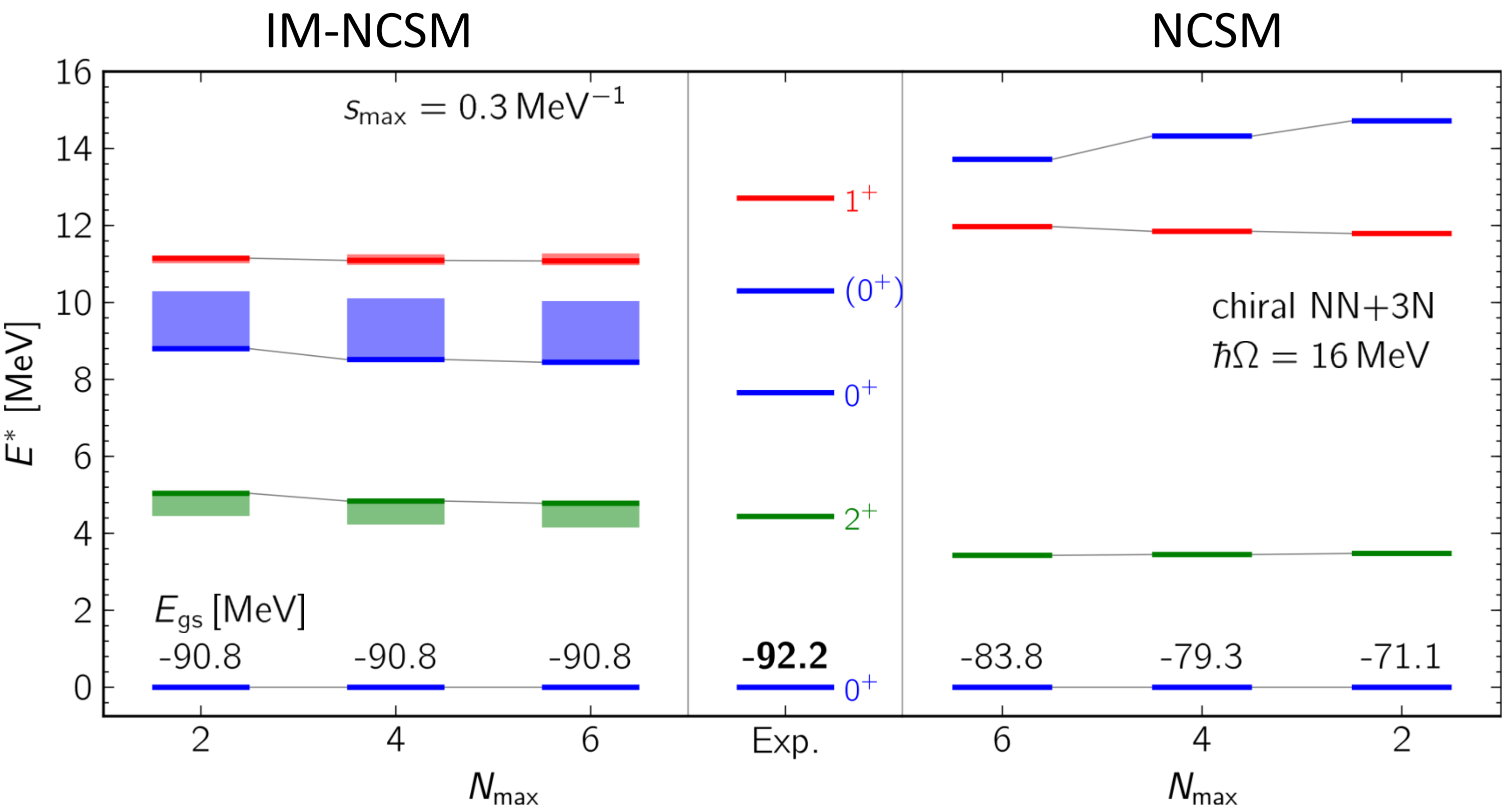

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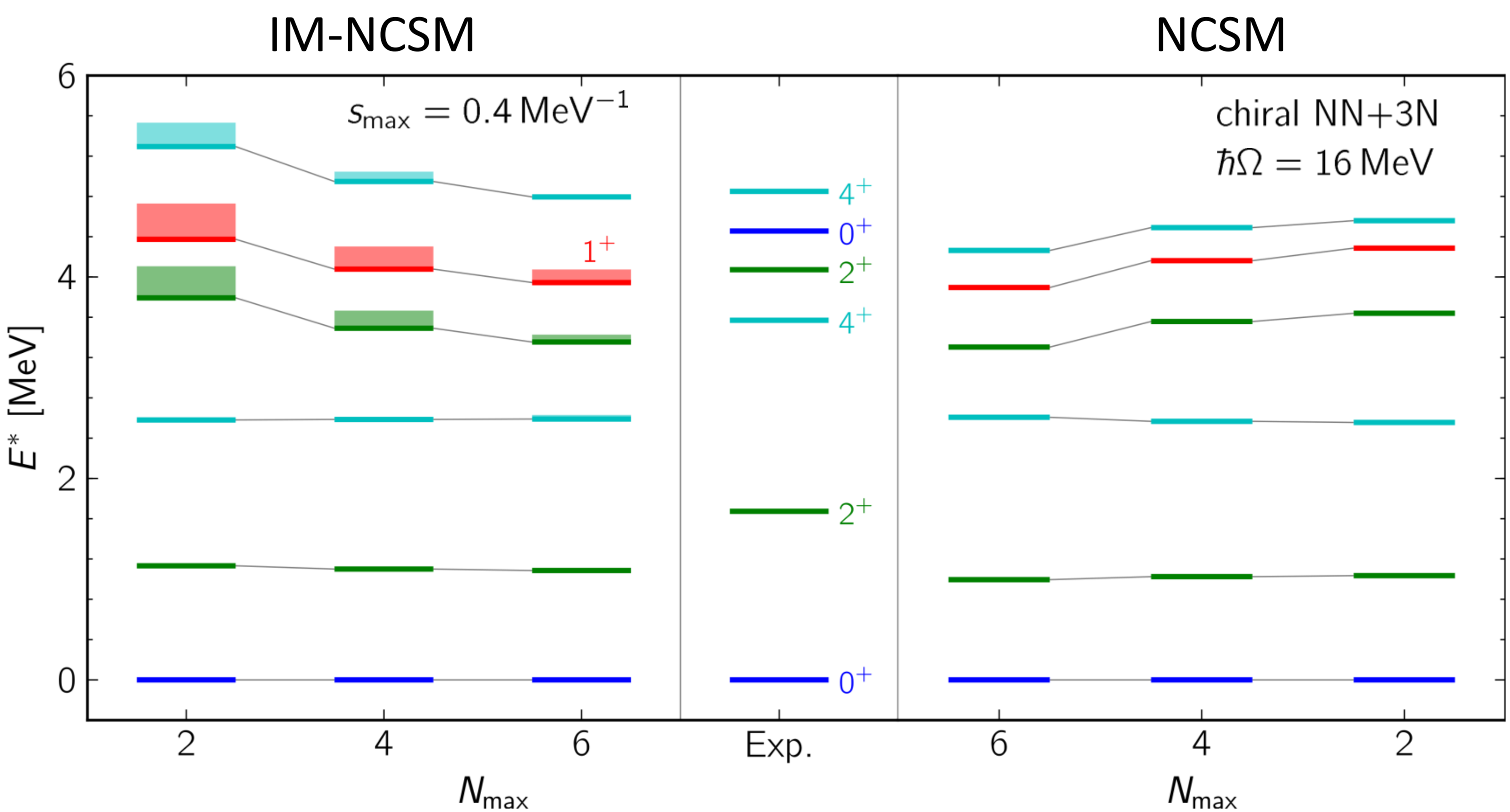
Results
Spectra



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- first 2^+ and 4^+ robust and well converged in IM-NCSM

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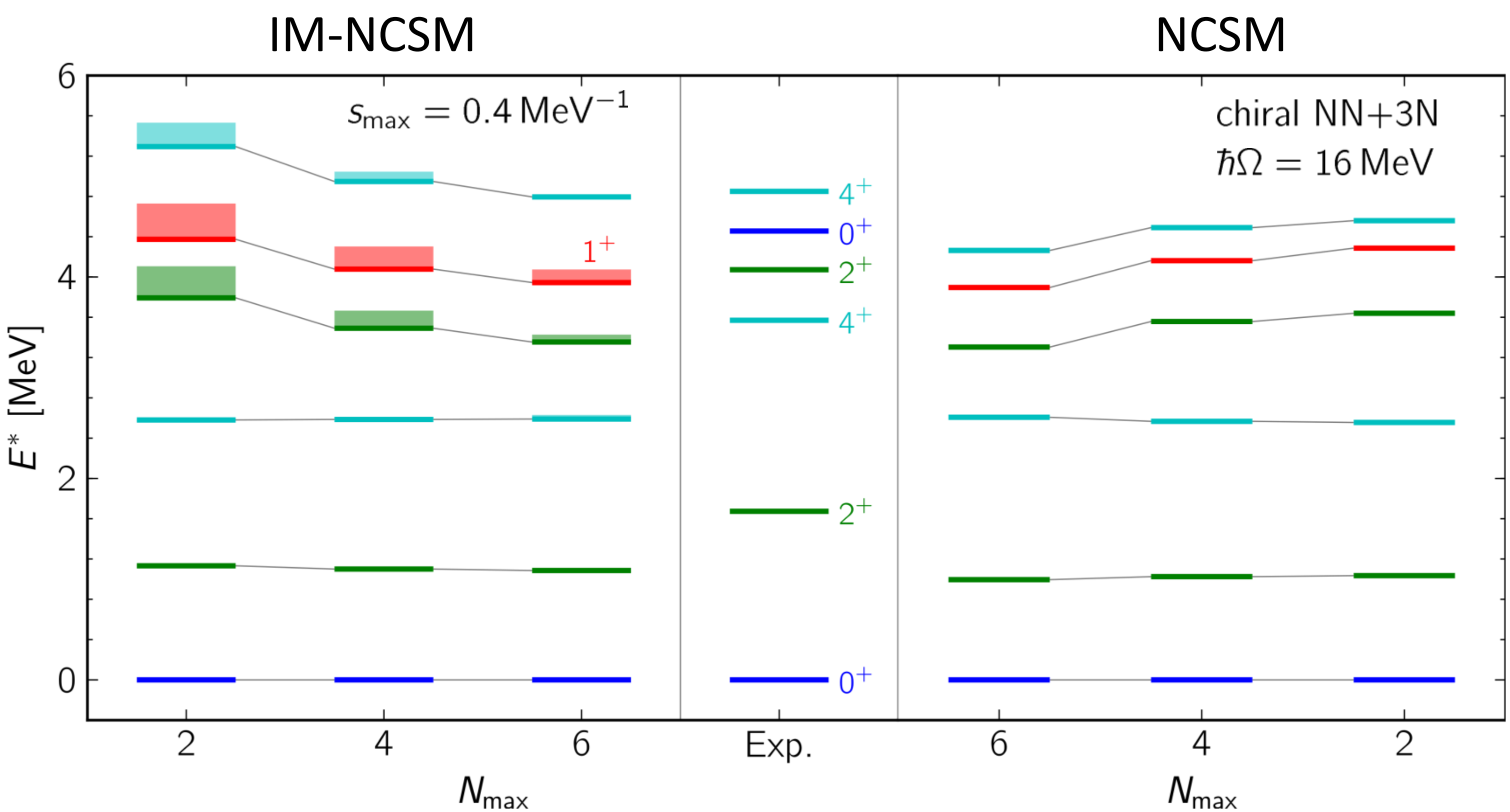

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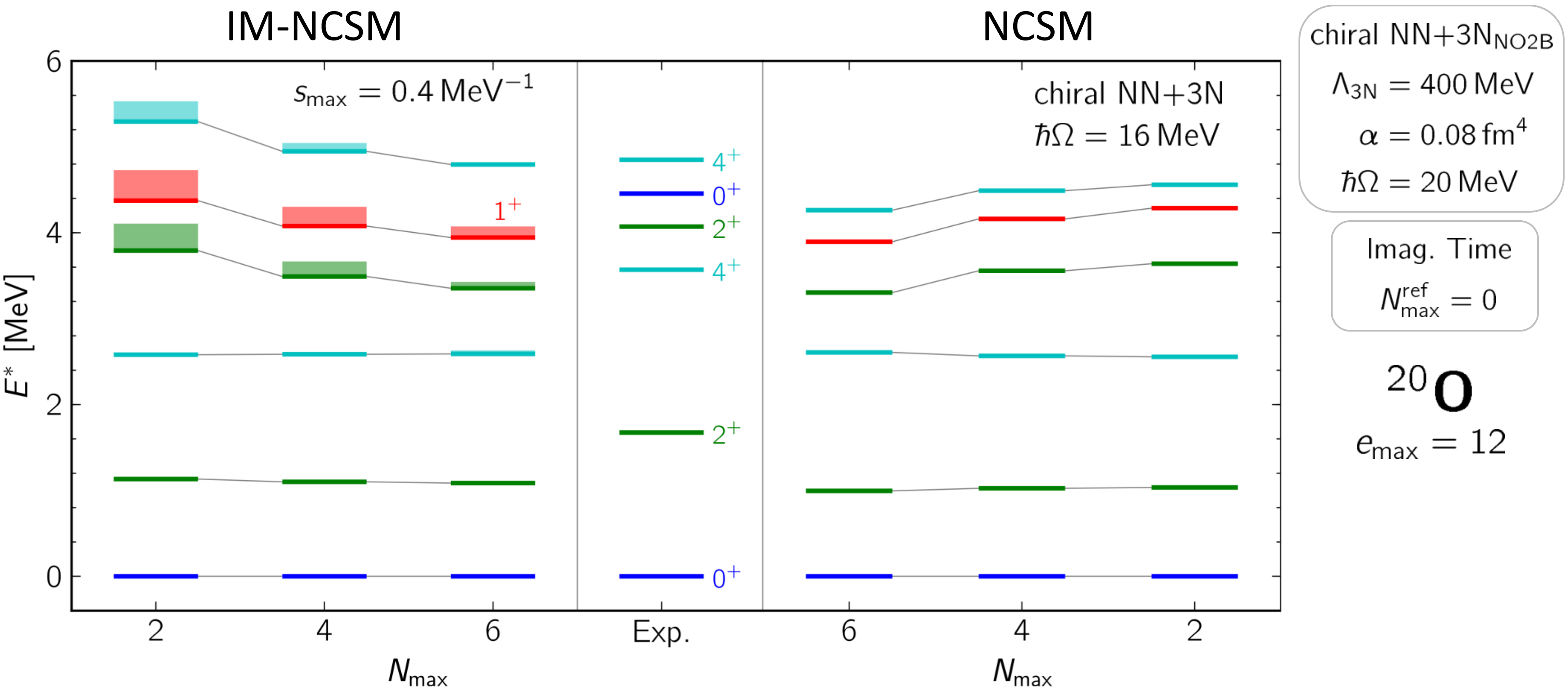

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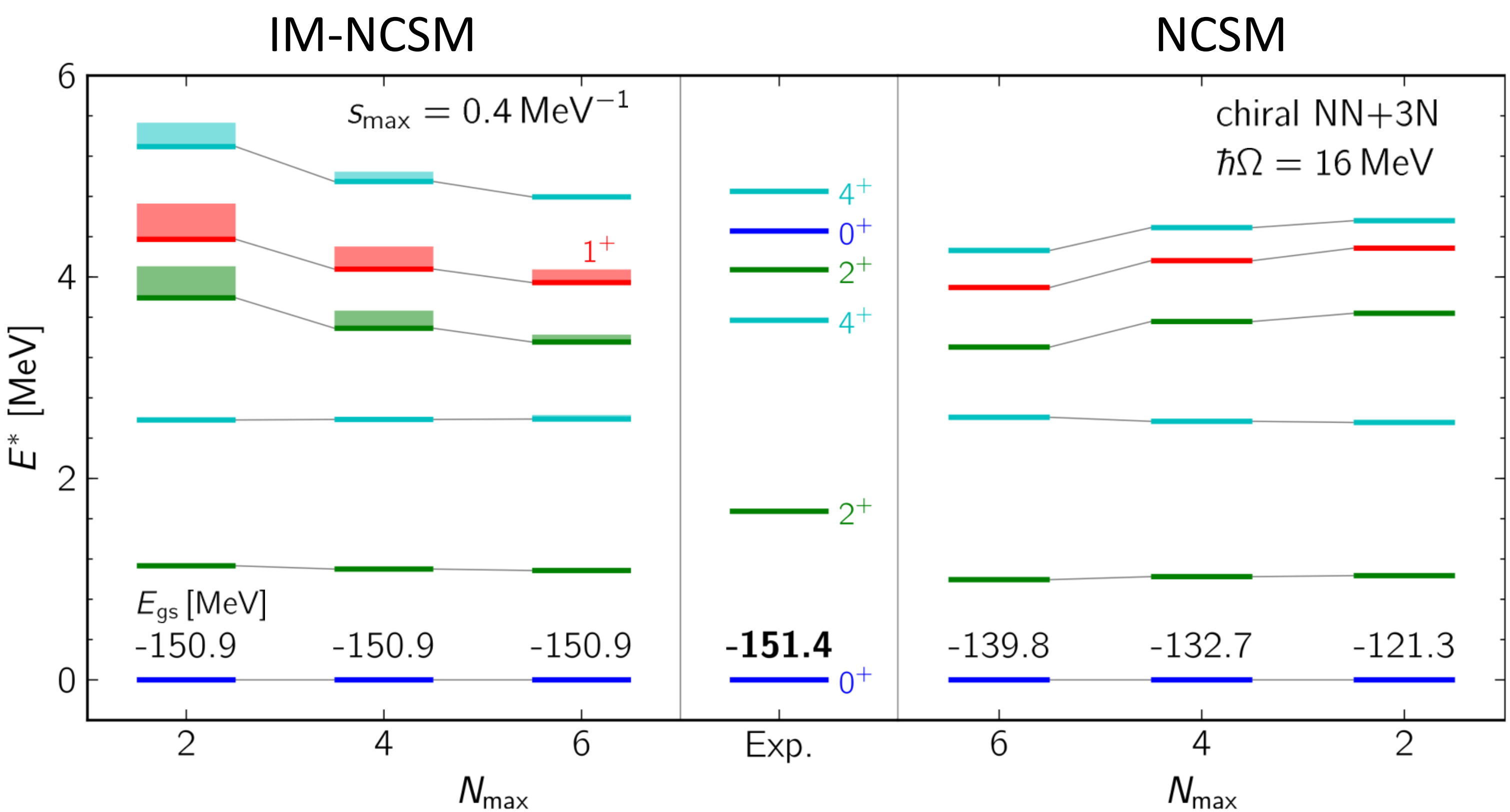

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Summary

TECHNISCHE UNIVERSITÄT DARMSTADT

- ✓ introduced new many-body technique **IM-NCSM** = IM-SRG + NCSM
- ✓ exploits the advantages of both approaches

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- ✓ exploits the advantages of both approaches
- ✓ 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

Outlook

- variation of several parameters: generator, $N_{\text{max}}^{\text{ref}}, \hbar\Omega, \ldots$
- consistent evolution radius, electromagnetic, … operators
- detailed analysis of the Hoyle state in ^{12}C

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TECHNISCHE UNIVERSITÄT DARMSTADT

- variation of several parameters: generator, $N_{\text{max}}^{\text{ref}}$, $\hbar\Omega$, …
- consistent evolution radius, electromagnetic, … operators
- detailed analysis of the Hoyle state in ^{12}C
- extend applicability of IM-NCSM to odd nuclei

  using particle-attached particle-removed formalism
- include three-body operators in IM-SRG

Thank You For Your Attention

TECHNISCHE UNIVERSITÄT DARMSTADT

Thanks to my group & collaborator

- S. Alexa, S. Dentinger, T. Hüther, L. Kreher, L. Mertes, S. Ruppert, **R. Roth**, S. Schulz, H. Spiess, H. Spielvogel, C. Stumpf, A. Tichai, R. Trippel, **K. Vobig**, R. Wirth
  Institut für Kernphysik, TU Darmstadt
- **H. Hergert**
  NSCL/FRIB, Michigan State University

Bundesministerium für Bildung und Forschung

LOEWE
Exzellente Forschung für Hessens Zukunft

Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

HELMHOLTZ GEMEINSCHAFT

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

COMPUTING TIME

TECHNISCHE
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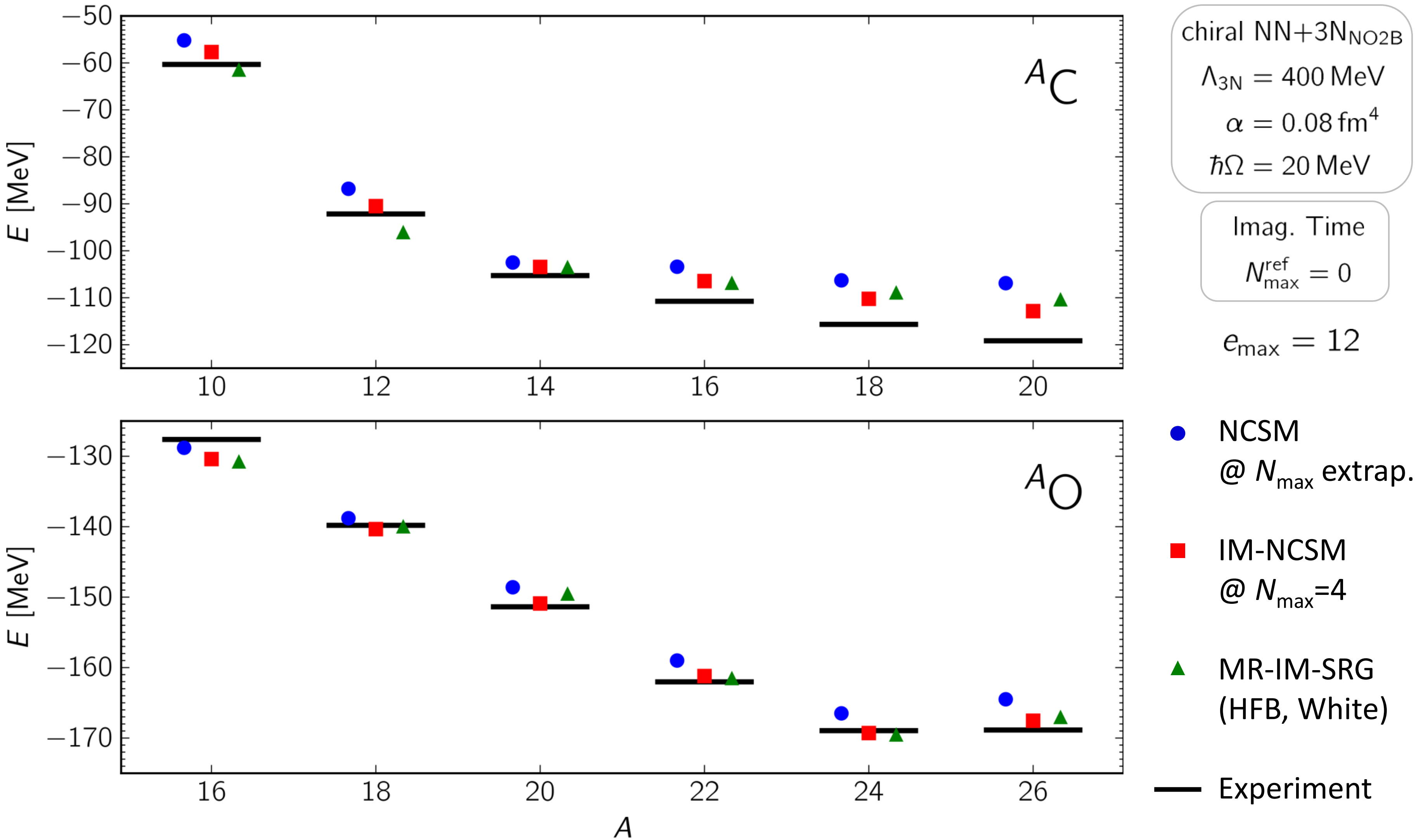
DARMSTADT

Appendix

Results

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



Dependence on Single-Particle Basis

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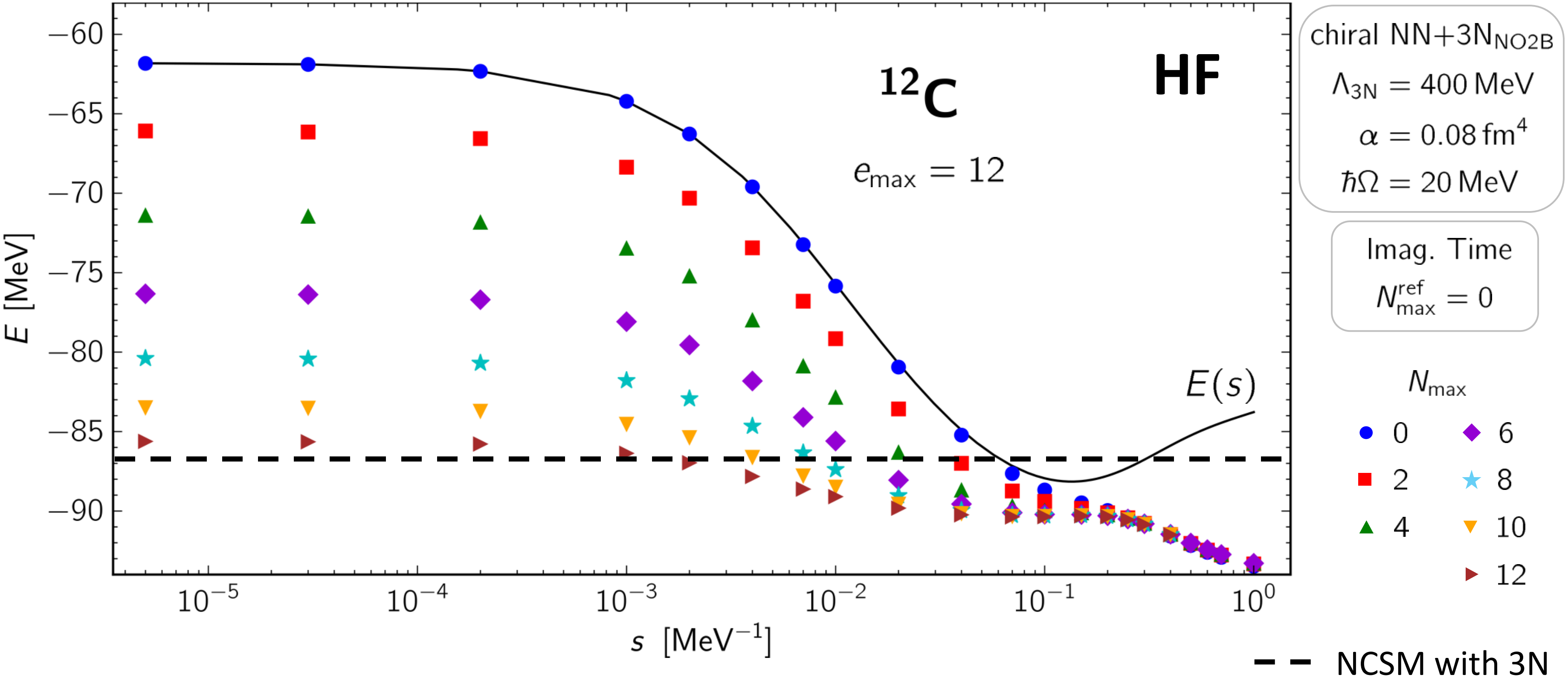

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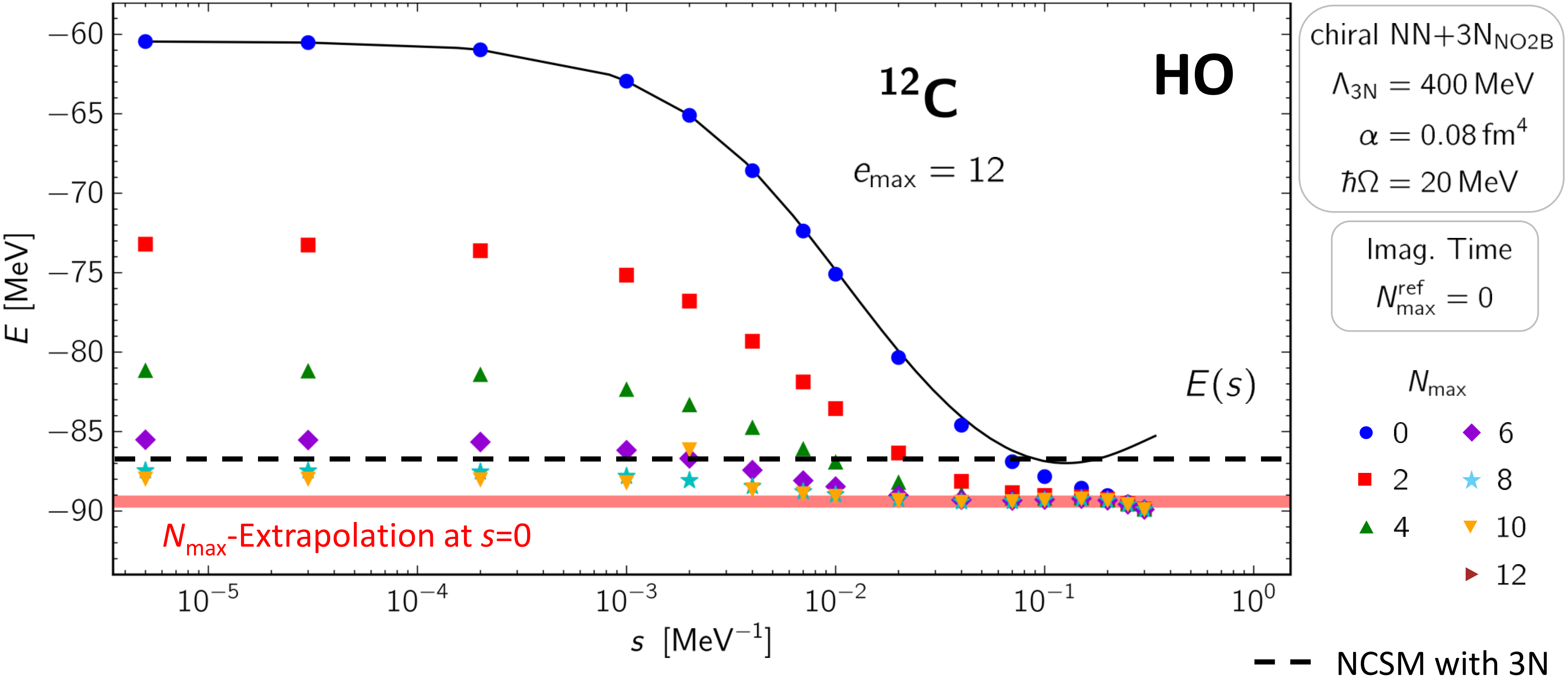

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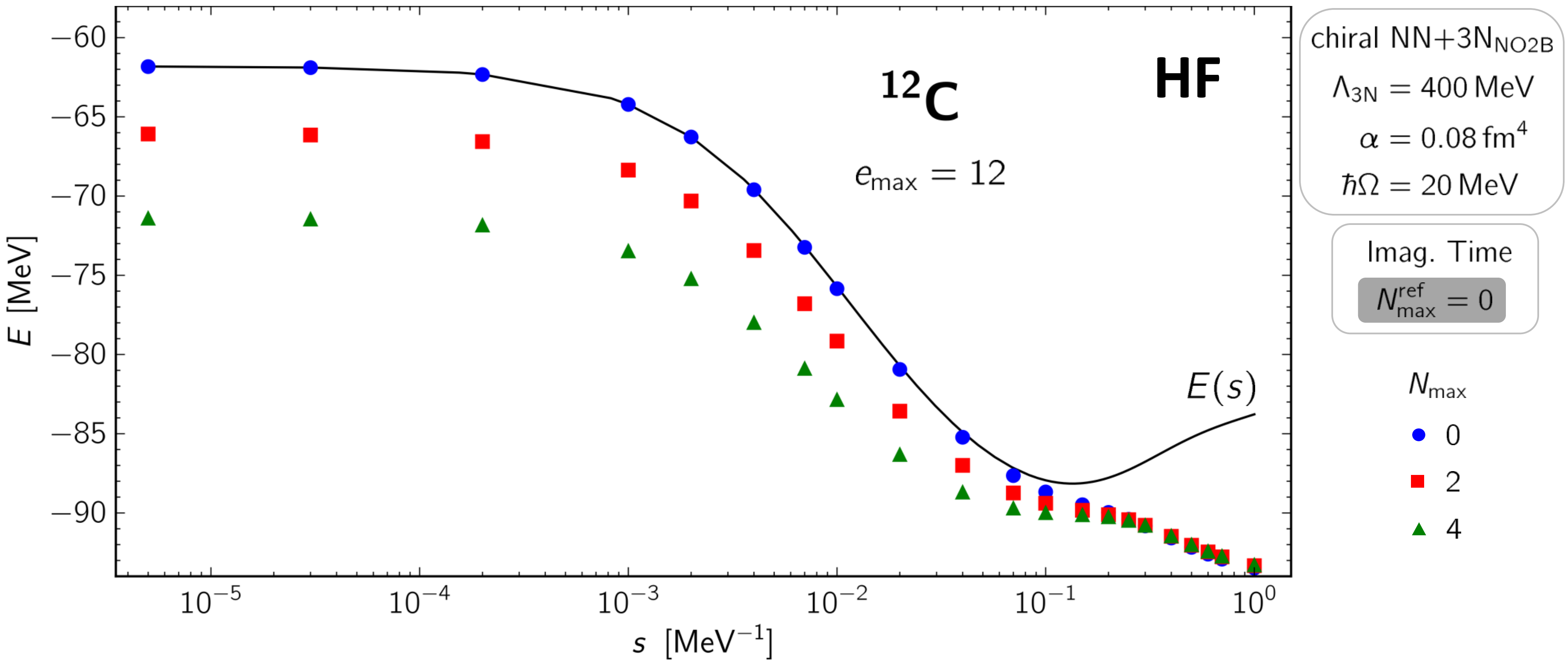
Dependence on N_{max}^{ref}



- quite insensitive on N_{max}^{ref}
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Dependence on N_{max}^{ref}

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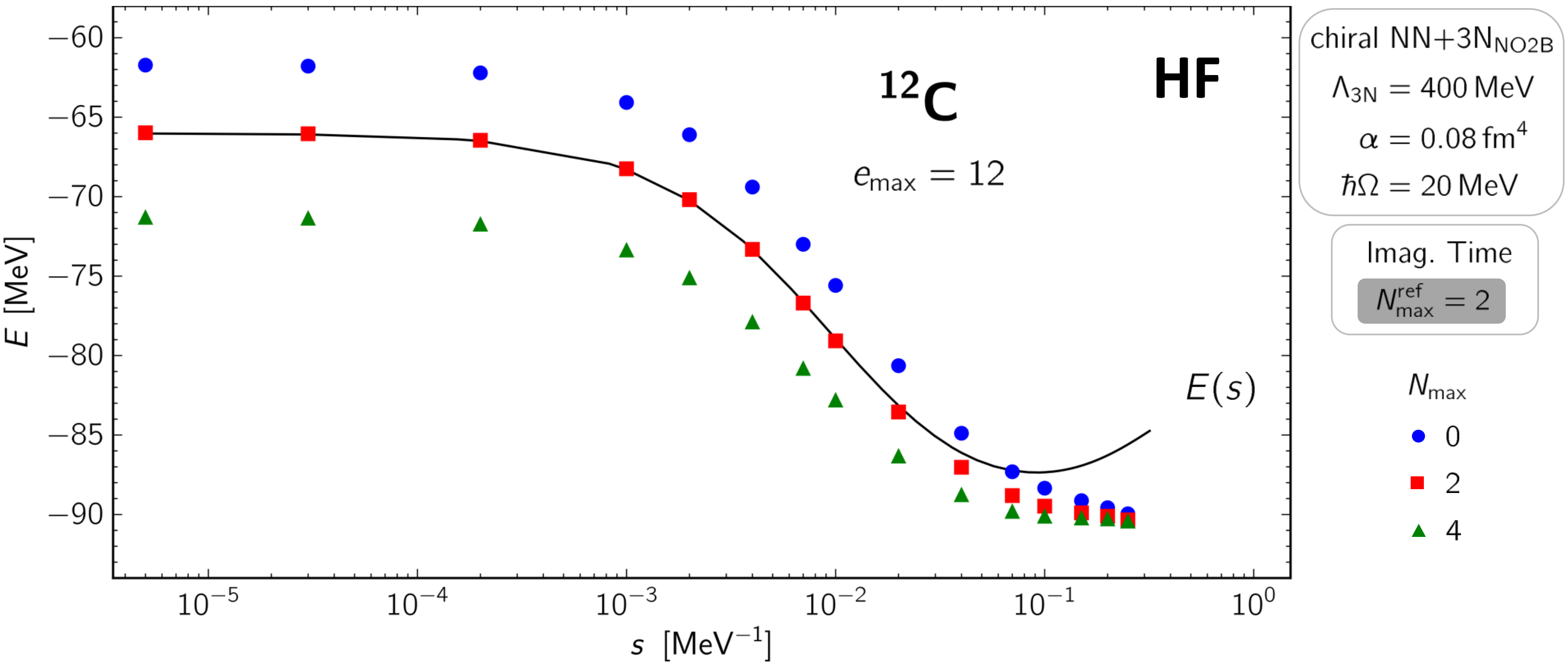

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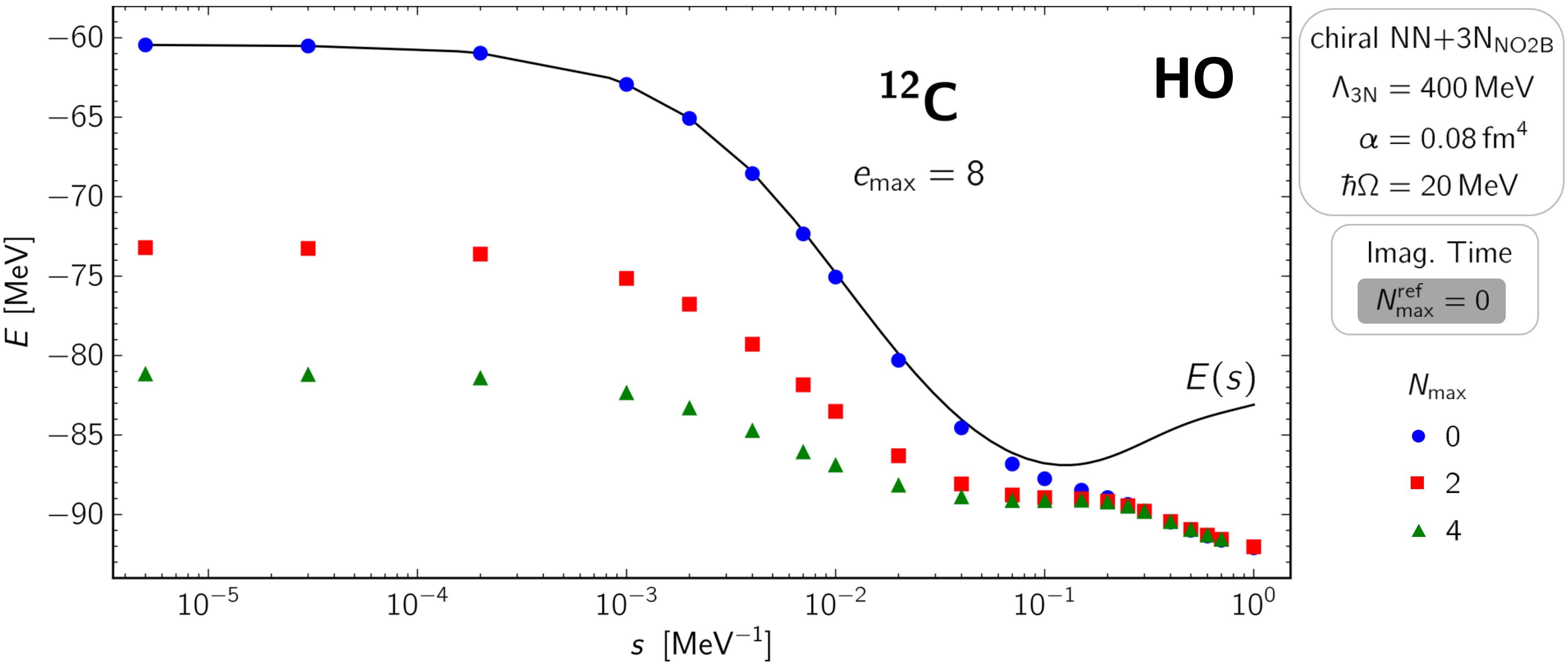

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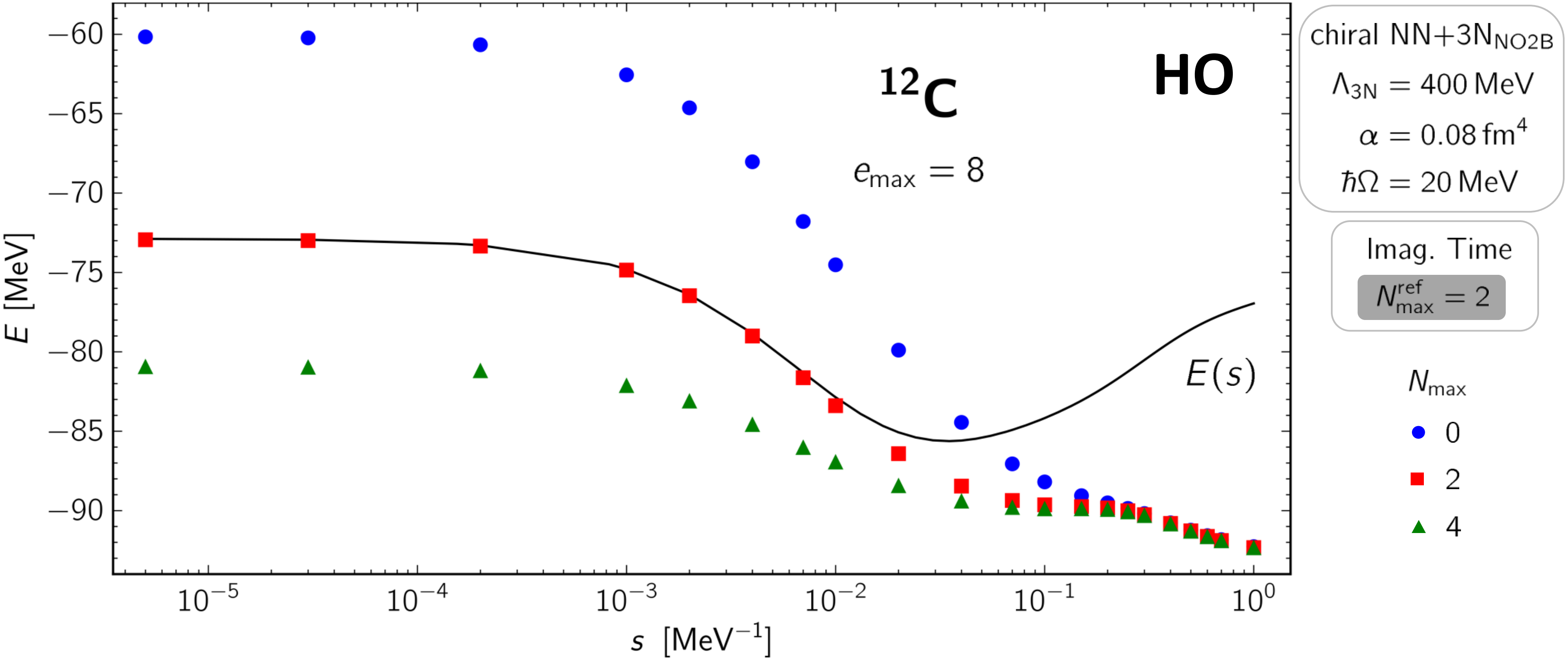

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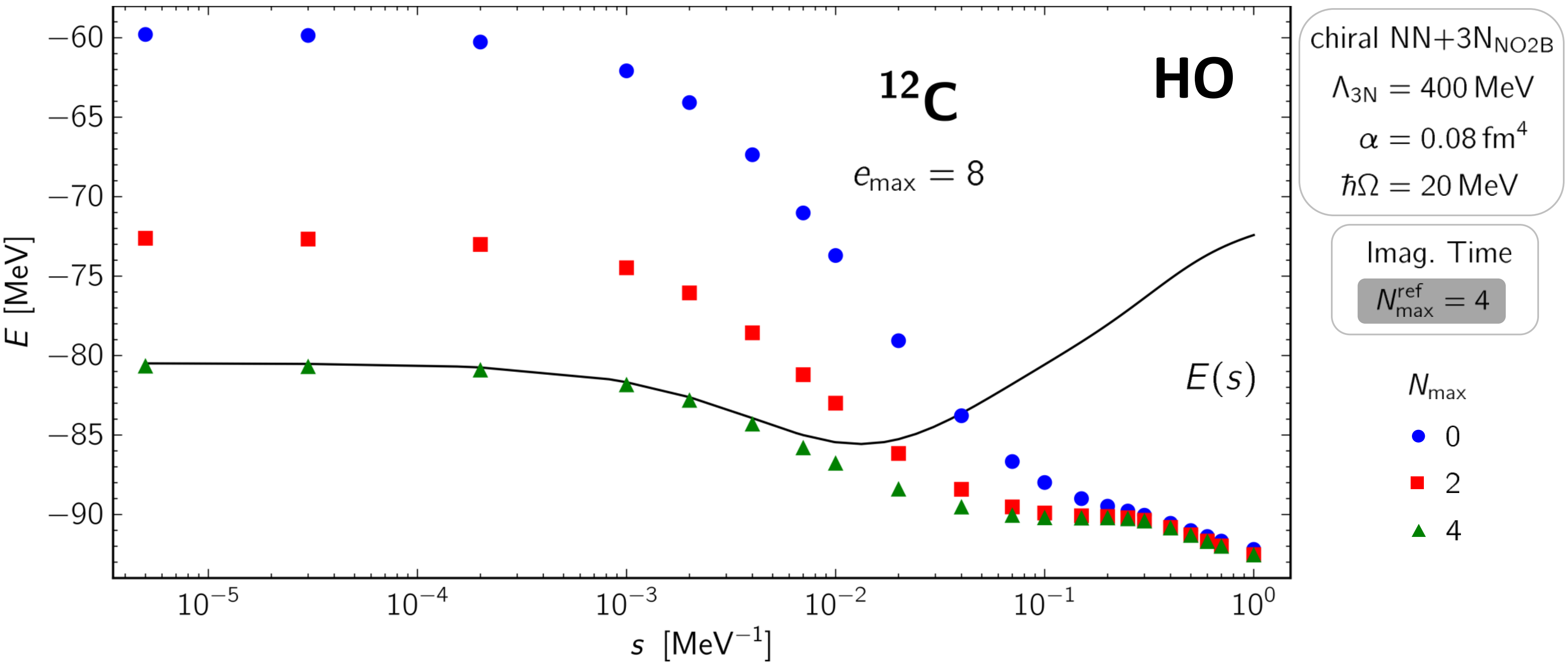

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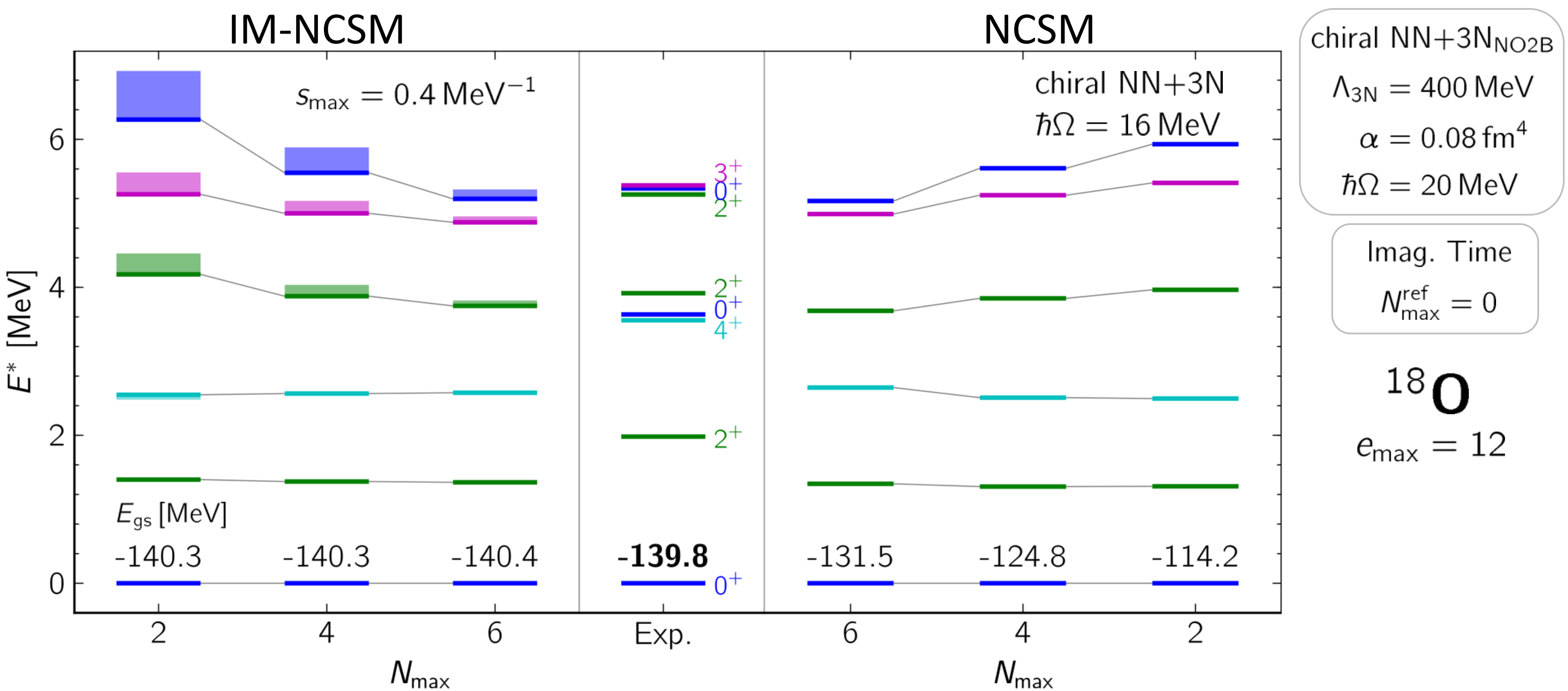

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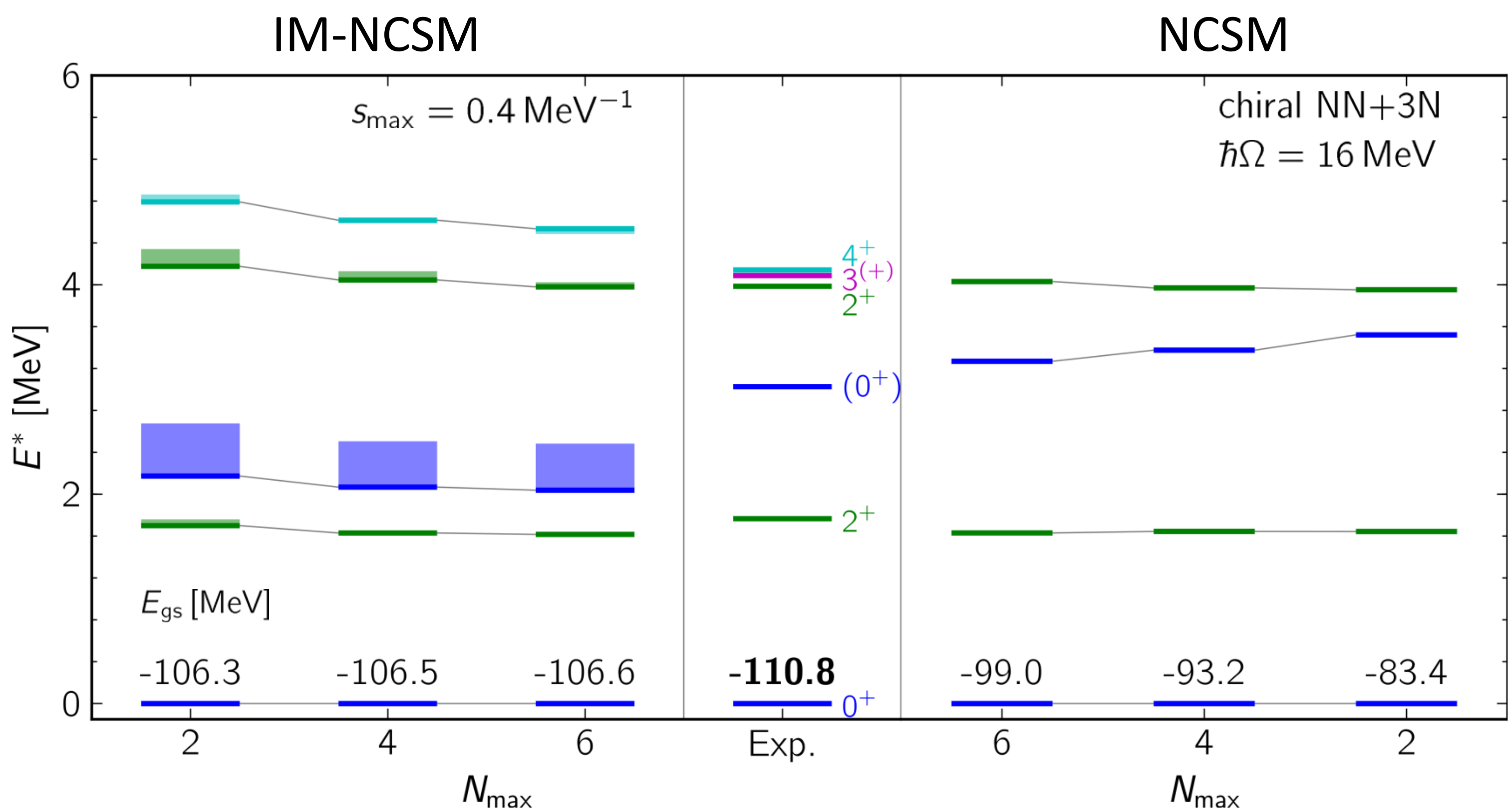

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$\hbar\Omega = 20\,\mathrm{MeV}$

Imag. Time

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

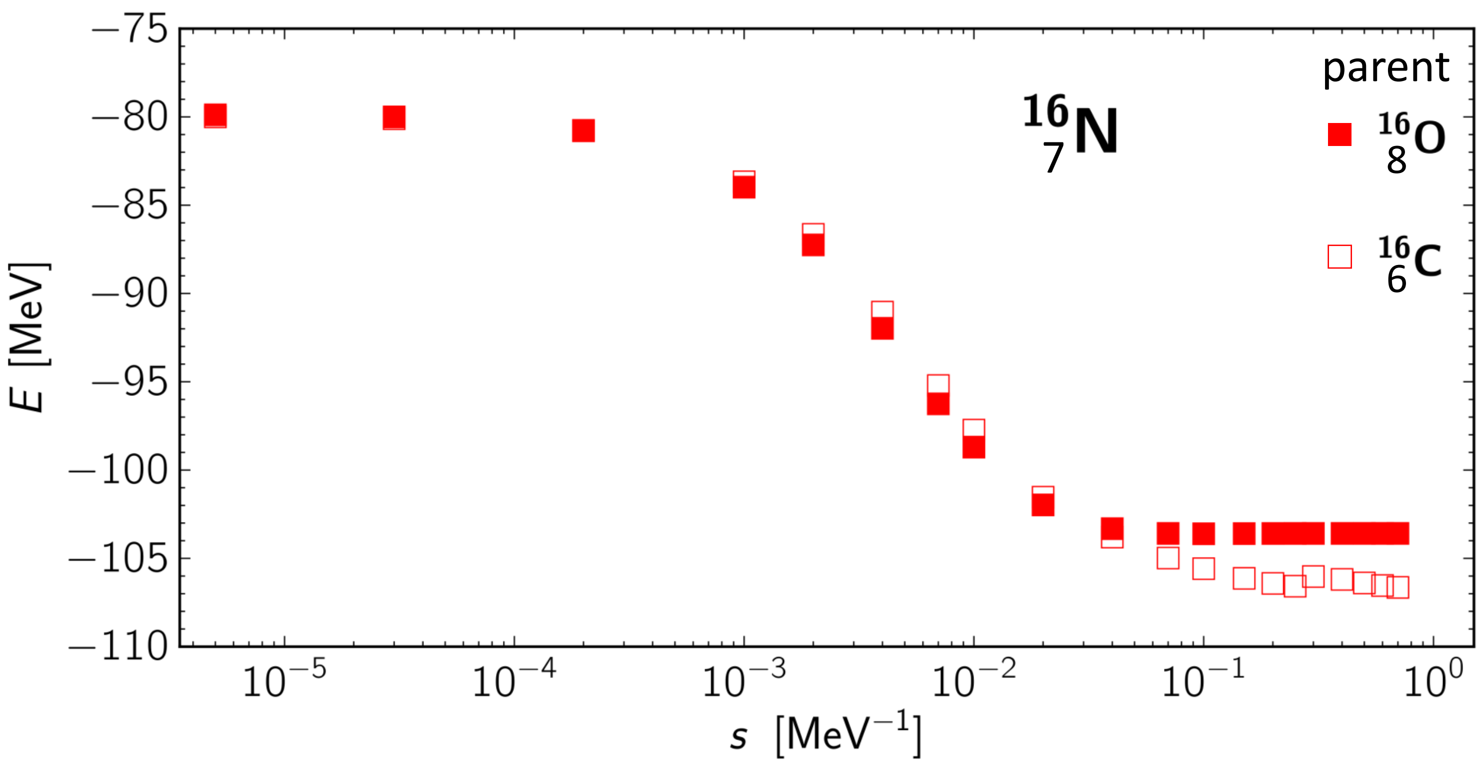
^{16}C

$e_{max} = 12$

- 4^+ simply not calculated in NCSM
- first excited 0^+ shows same behaviour as in ^{12}C

Results

IM-NCSM: Particle-Attached Particle-Removed Form.



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Imag. Time

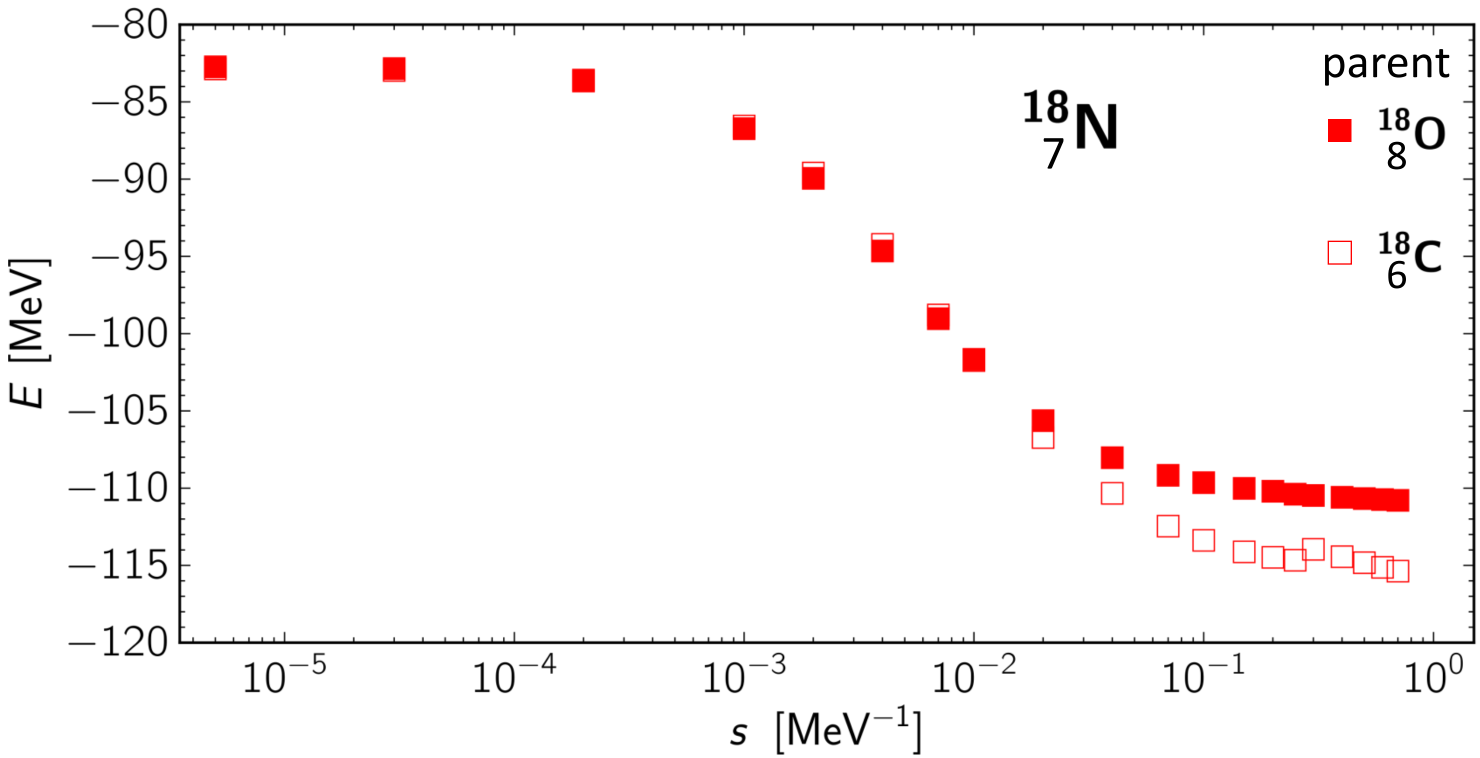
$N^{ref}_{max} = 0$

$e_{max} = 12$

$N_{max} = 2$

- eigenvalues for small flow parameter independent on parent nucleus
- eigenvalues for large flow paremter show dependence on parent nucleus
- deviation at the level of 4 MeV (< 4%)

Results
IM-NCSM: Particle-Attached Particle-Removed Form.



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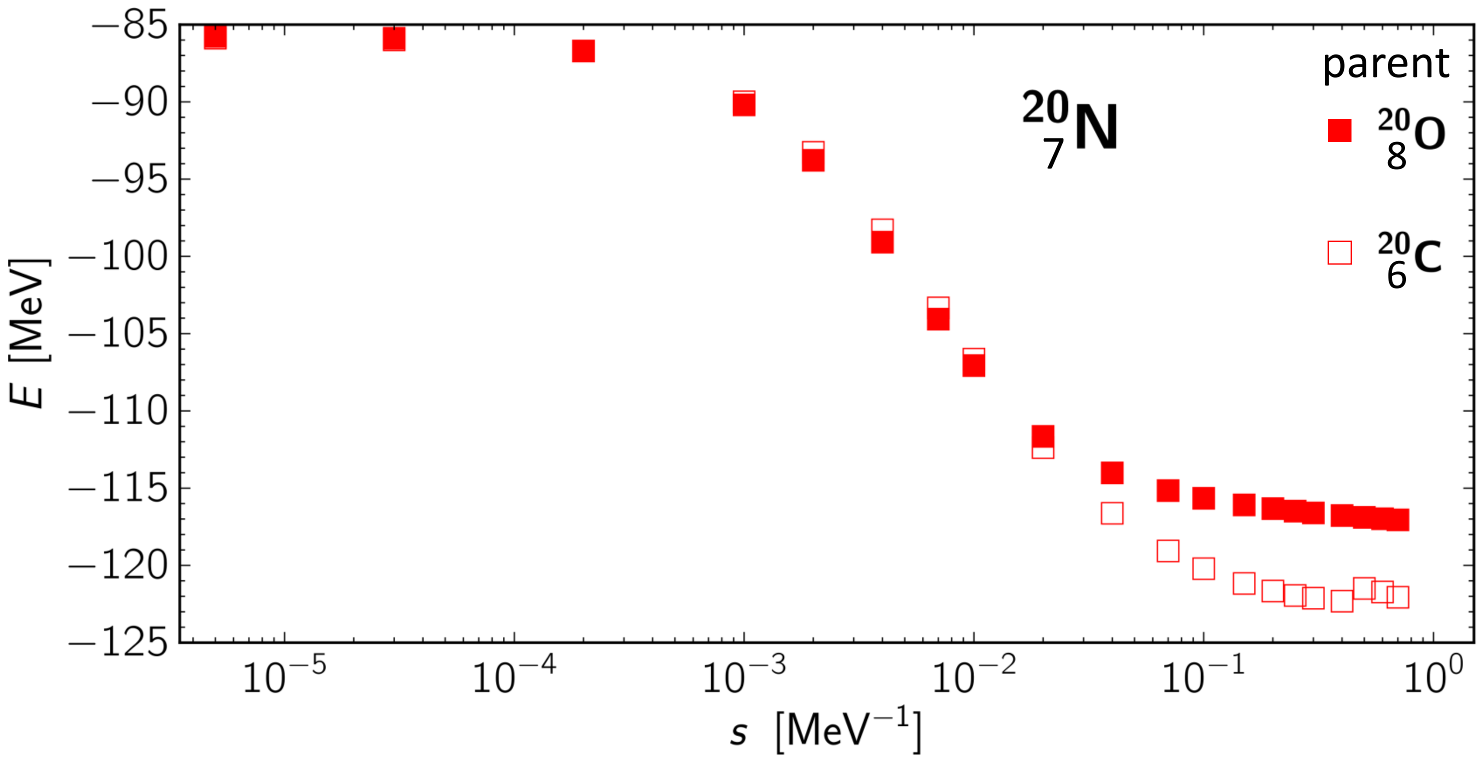
$N_{max}^{ref} = 0$

$e_{max} = 12$
$N_{max} = 2$

- deviation at the level of 5 MeV (< 5%)

IM-NCSM: Particle-Attached Particle-Removed Form.



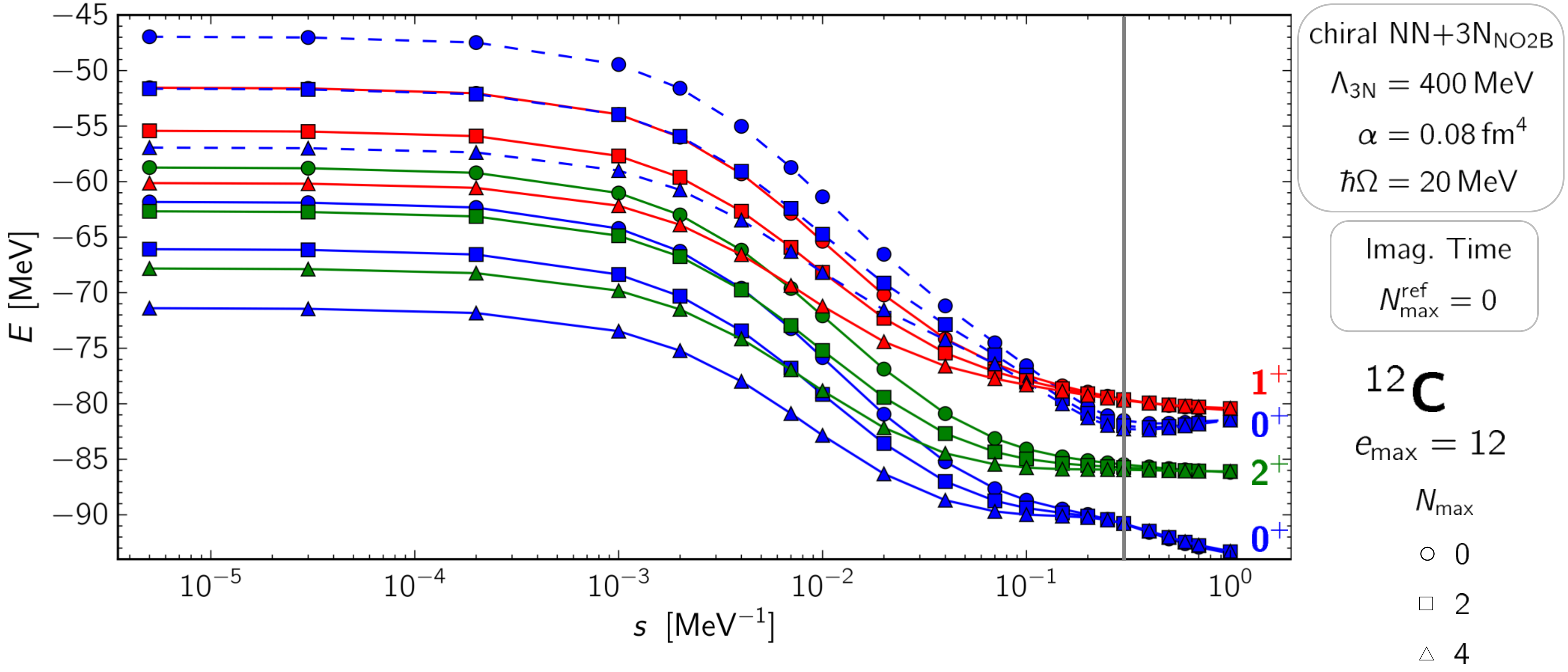
chiral NN+$3N_{NO2B}$
$\Lambda_{3N} = 400$ MeV
$\alpha = 0.08\ \mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

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

$e_{max} = 12$
$N_{max} = 2$

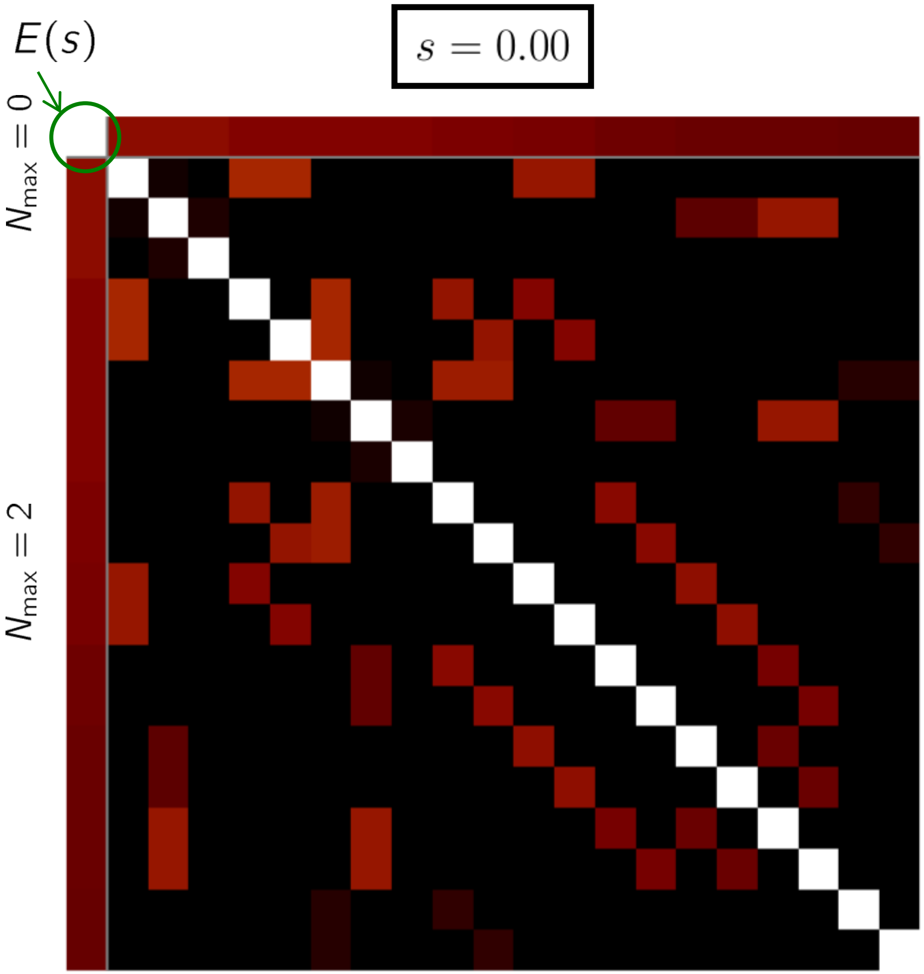
- deviation at the level of 5 MeV (< 5%)

Evolution of Excitation Energies – On Absolute Scale



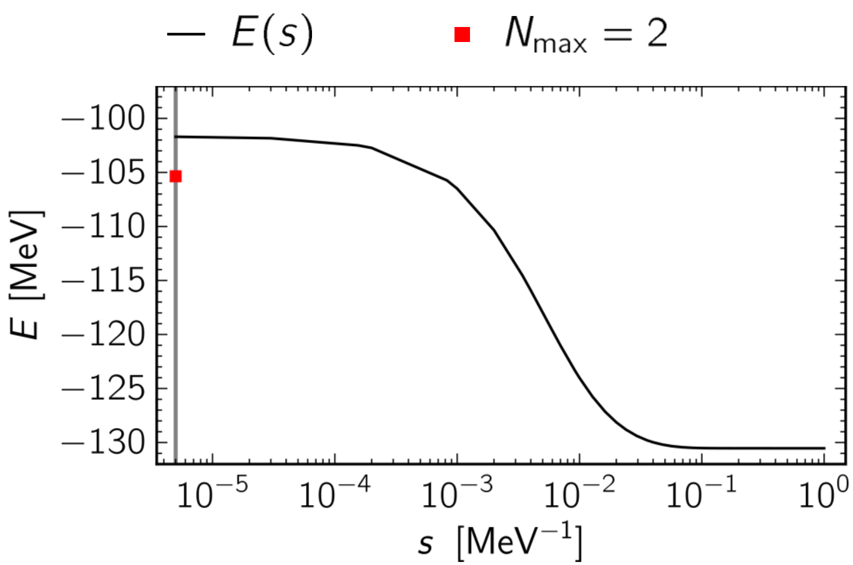
- 2^+ perfectly converged on absolute scale
- induced many-body contribution different for each state

Novel Approach: IM-NCSM
Hamilton Matrix in *A*-Body Basis: ^{16}O



N_{max}=0
Slater det.

N_{max}=2
Slater determinants

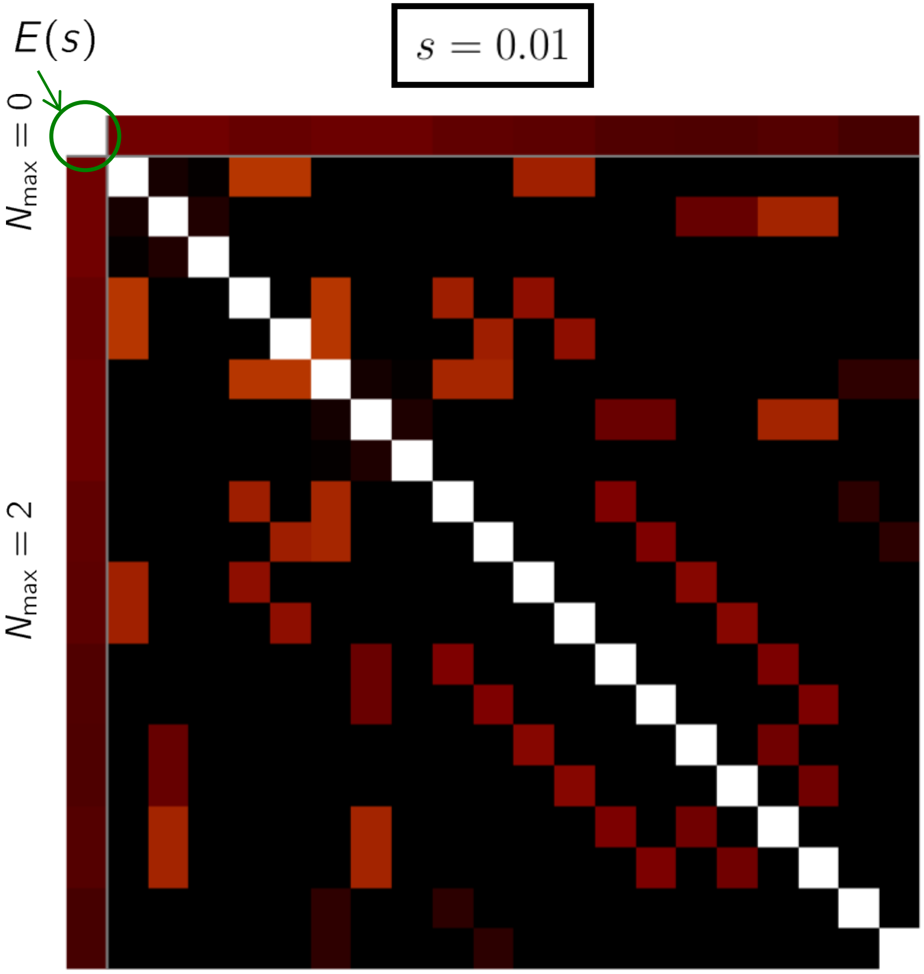


$E(s)$ converges monotonically against N_{max}=2 eigenvalue

IM-SRG decouples reference state from N_{max} =2 space

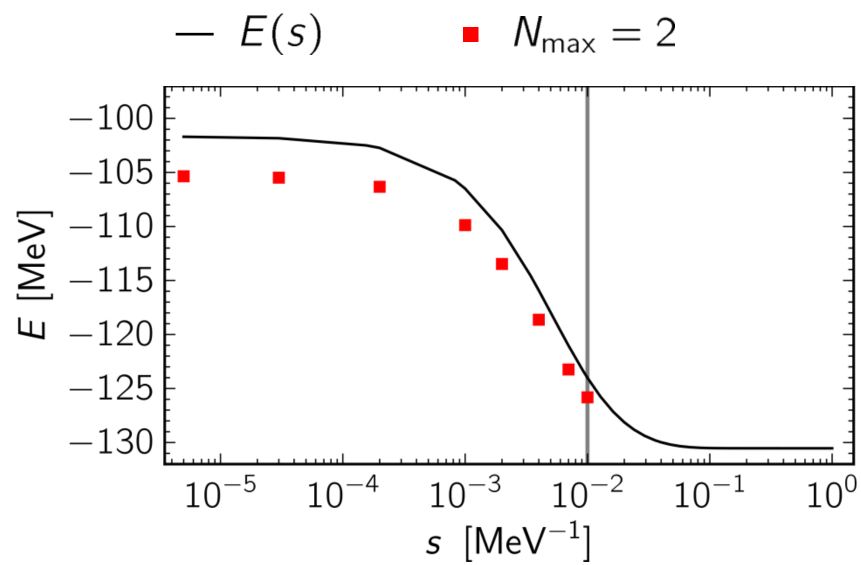
Novel Approach: IM-NCSM

Hamilton Matrix in *A*-Body Basis: ^{16}O



N_{max}=0
Slater det.

N_{max}=2
Slater determinants



$E(s)$ converges monotonically against N_{max}=2 eigenvalue

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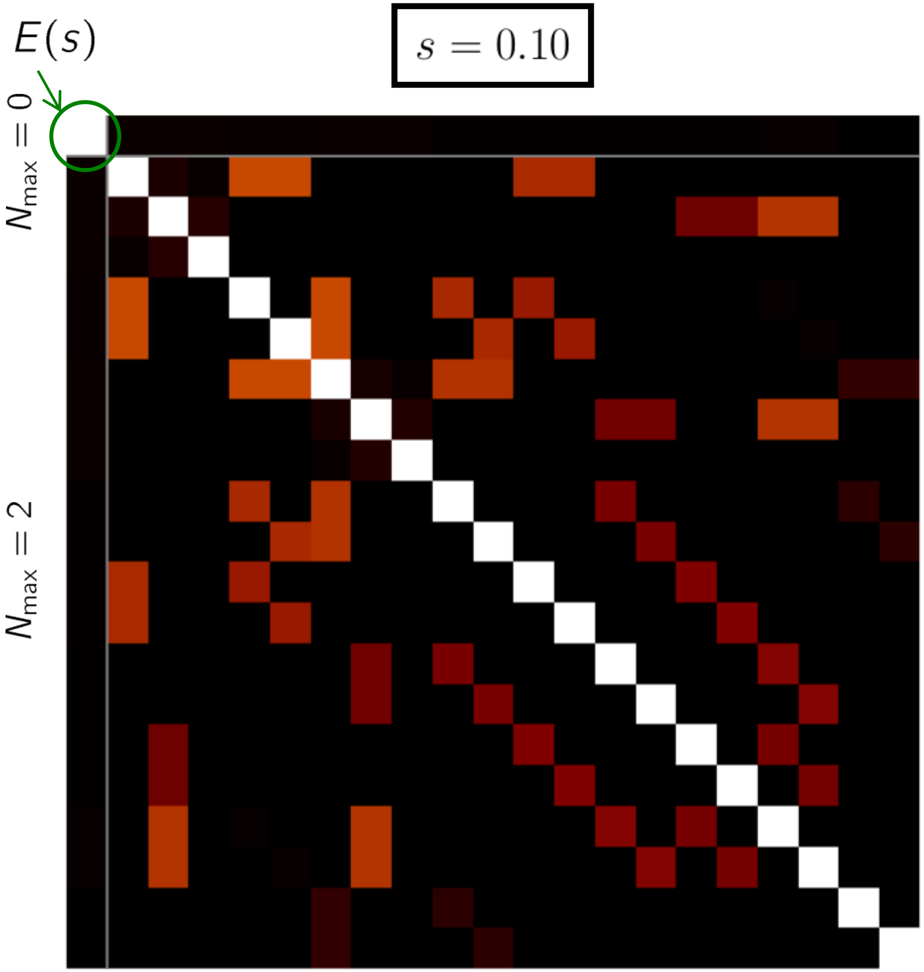
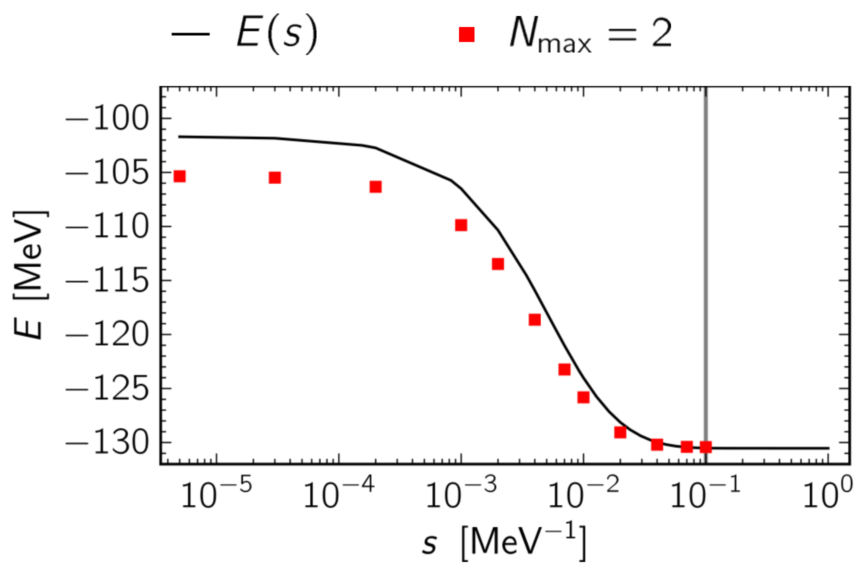
Hamilton Matrix in *A*-Body Basis: ^{16}O



N_{max}=0 Slater det.

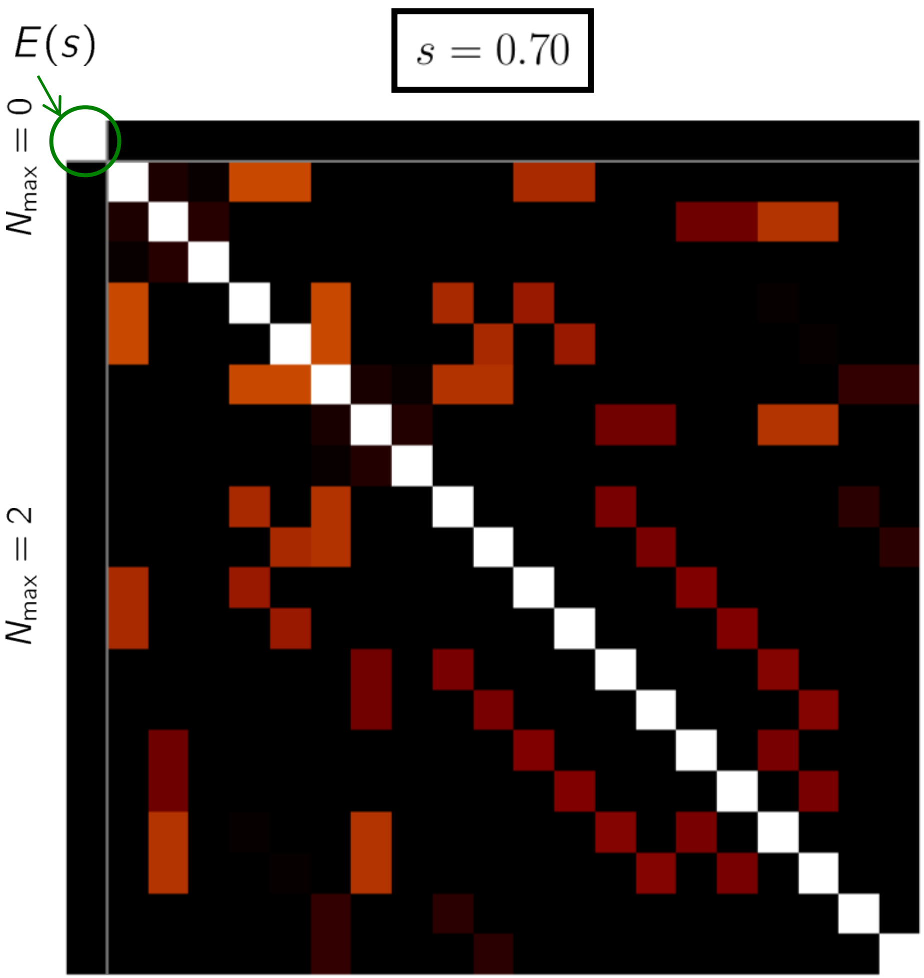
N_{max}=2 Slater determinants



E(*s*) converges monotonically against N_{max}=2 eigenvalue

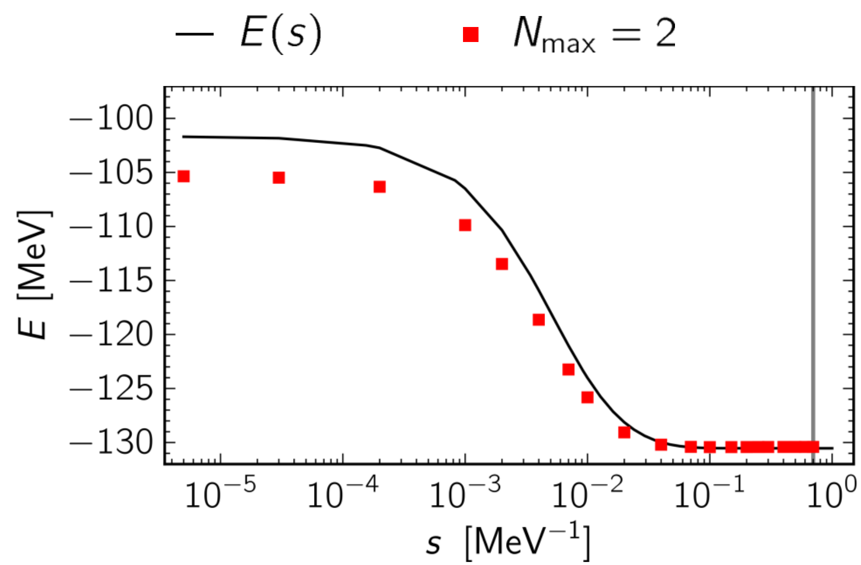
IM-SRG decouples reference state from N_{max} =2 space

Hamilton Matrix in *A*-Body Basis: ^{16}O



N_{max}=0
Slater det.

N_{max}=2
Slater determinants

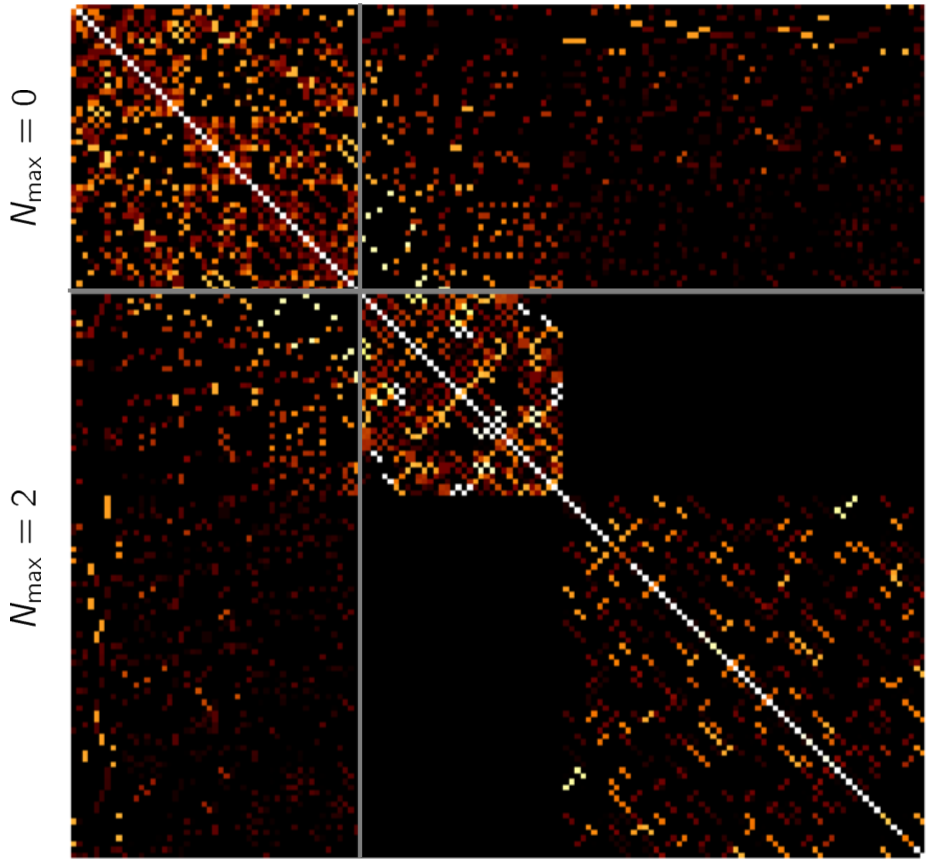


$E(s)$ converges monotonically against N_{max}=2 eigenvalue

IM-SRG decouples reference state from N_{max} =2 space

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

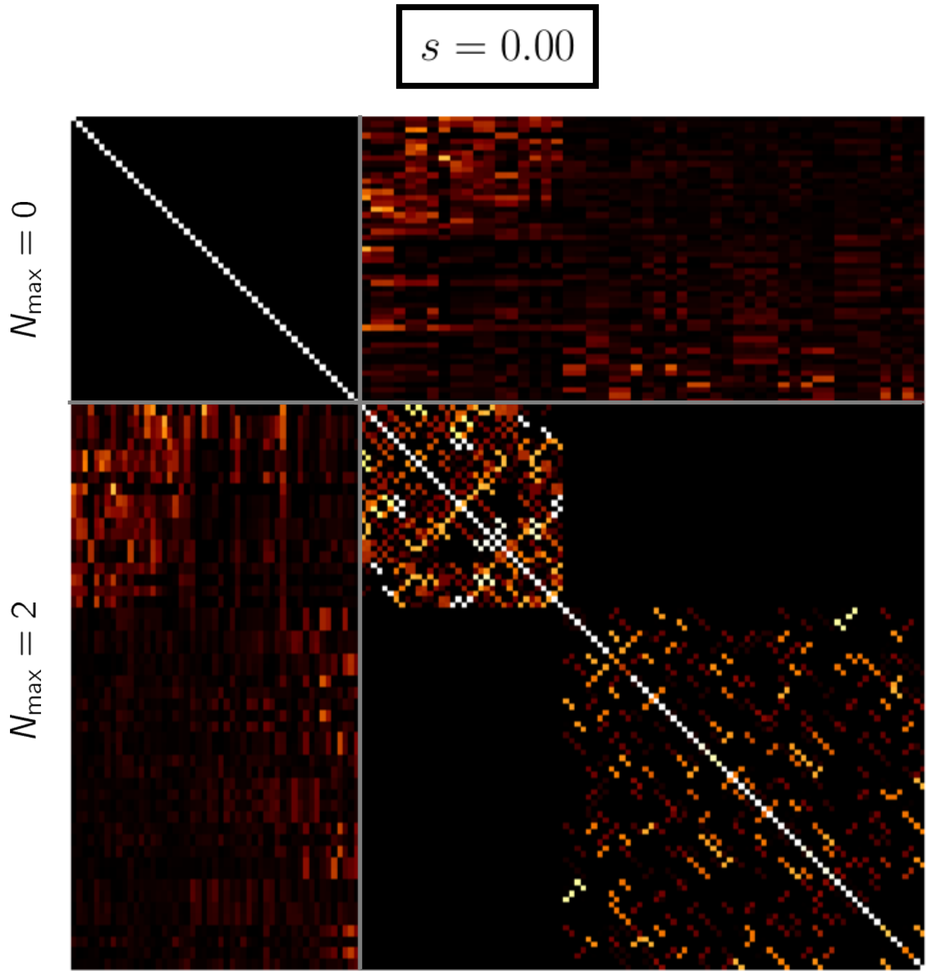
$s = 0.00$



N_{max}=0 Slater determinants

N_{max}=2 Slater determinants

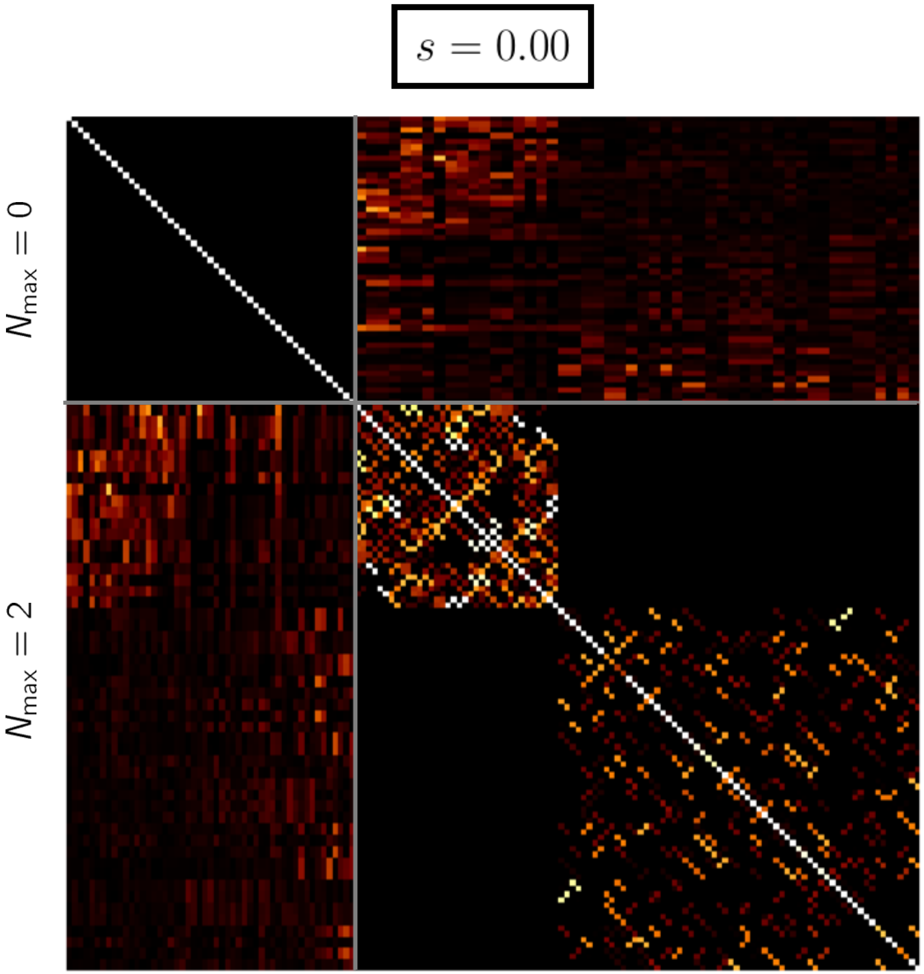
Novel Approach: IM-NCSM
Hamilton Matrix in A-Body Basis: ^{12}C



N_{max}=0
eigenstates

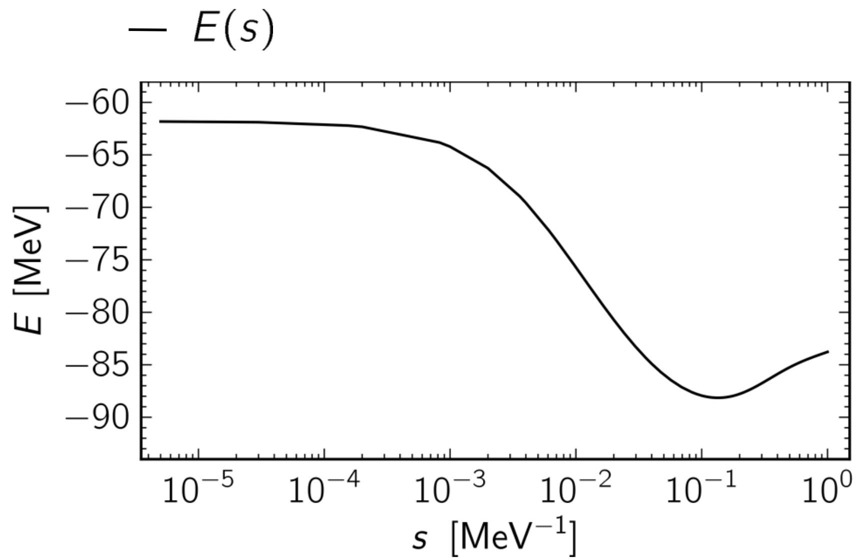
N_{max}=2
Slater determinants

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

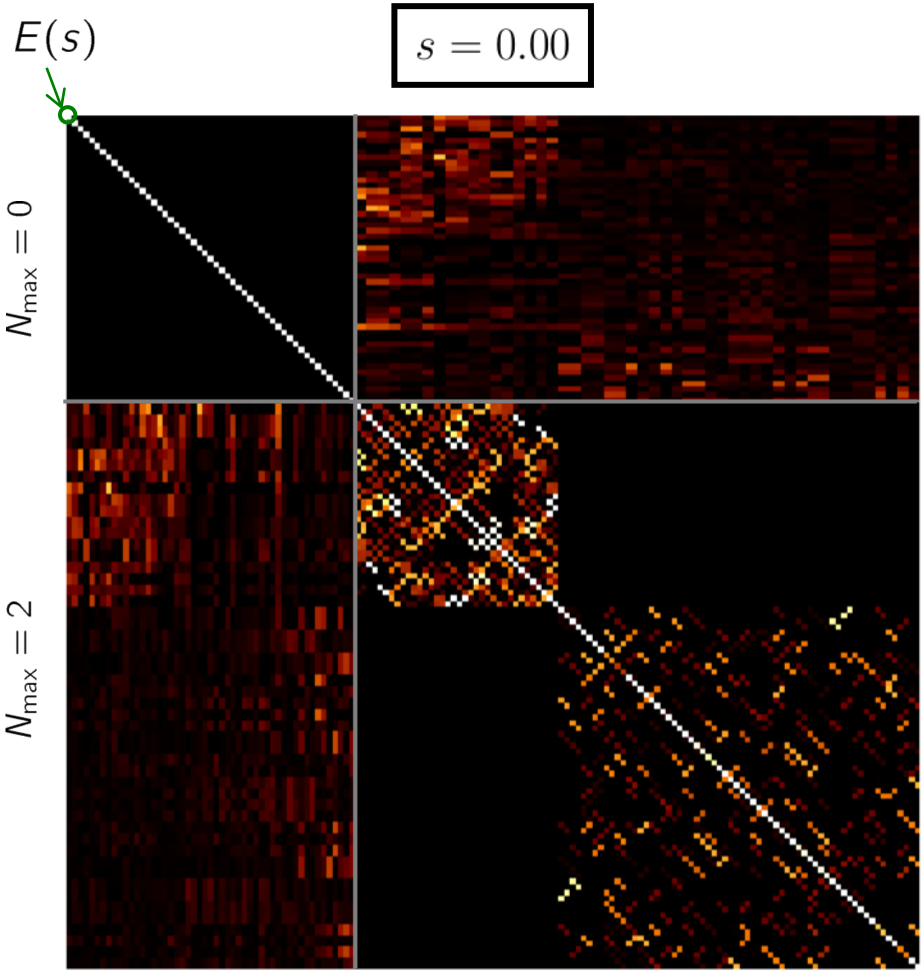


N_{max}=0
eigenstates

N_{max}=2
Slater determinants

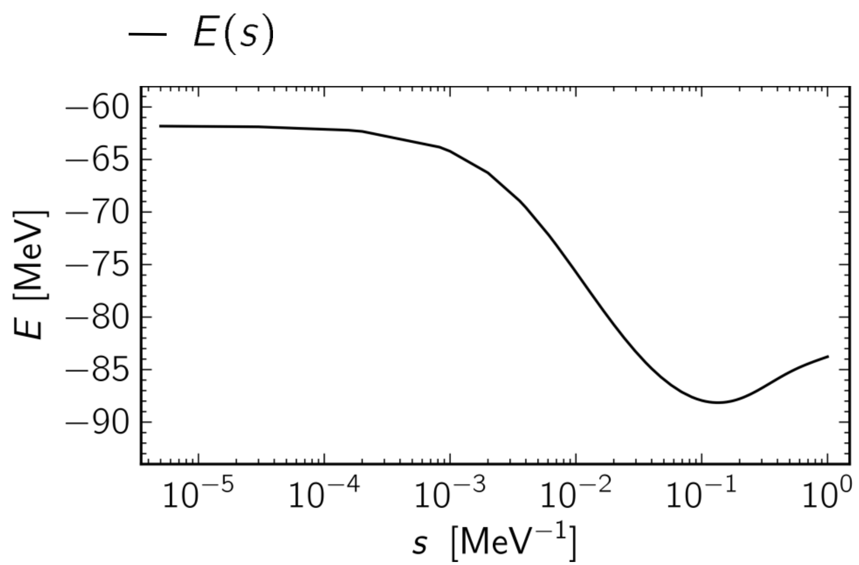


Novel Approach: IM-NCSM
Hamilton Matrix in *A*-Body Basis: ^{12}C

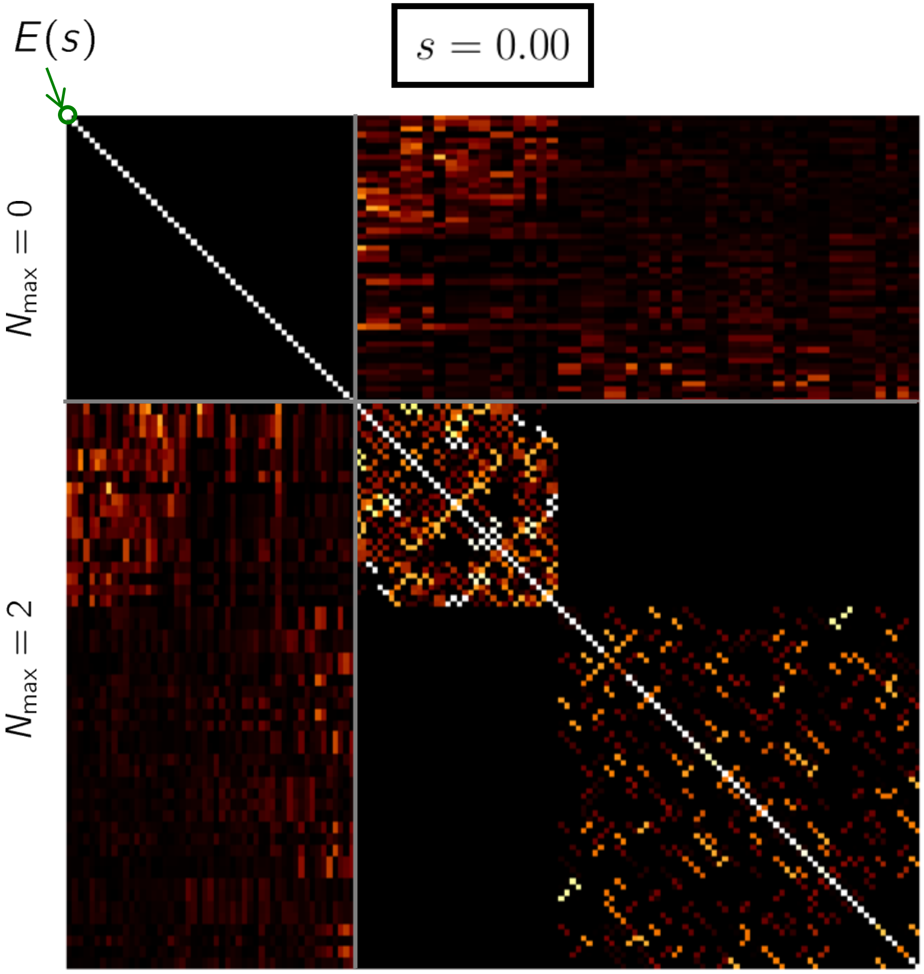


N_{max}=0
eigenstates

N_{max}=2
Slater determinants

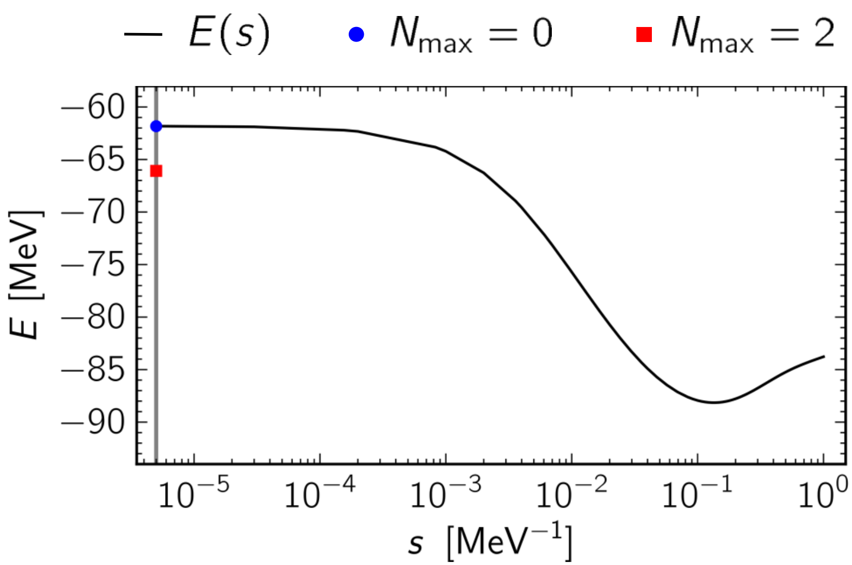


Novel Approach: IM-NCSM
Hamilton Matrix in *A*-Body Basis: ^{12}C



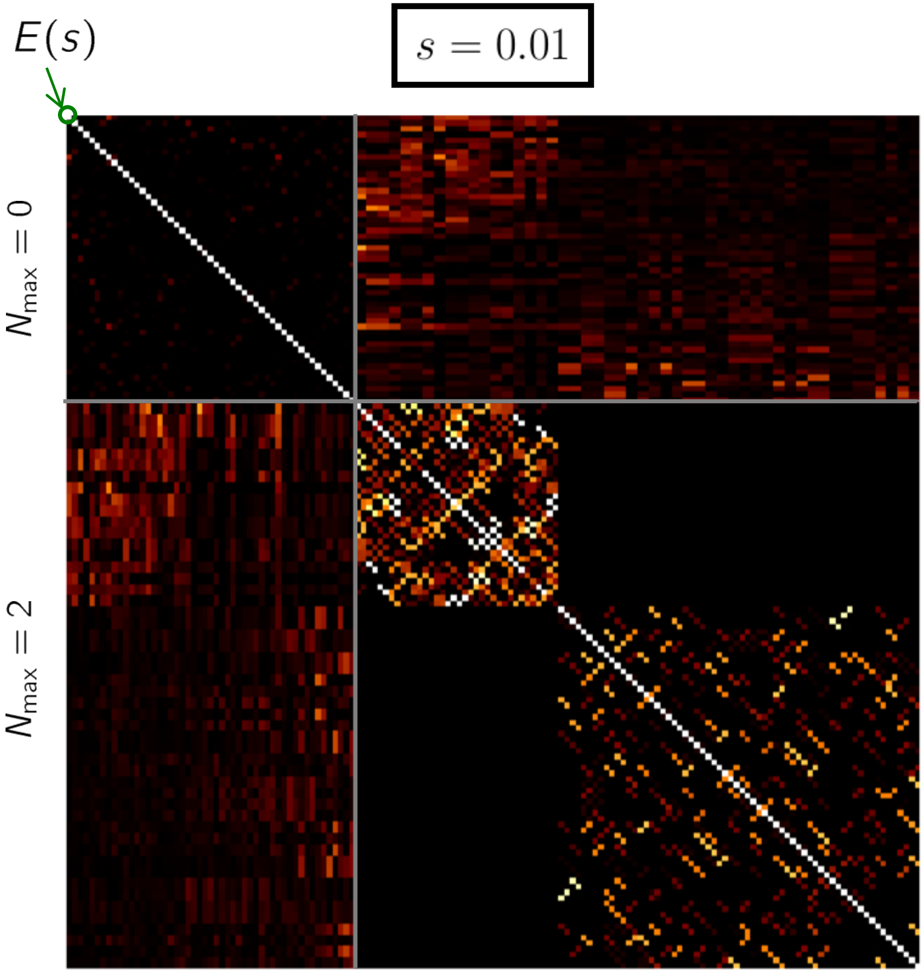
N_{max}=0
eigenstates

N_{max}=2
Slater determinants



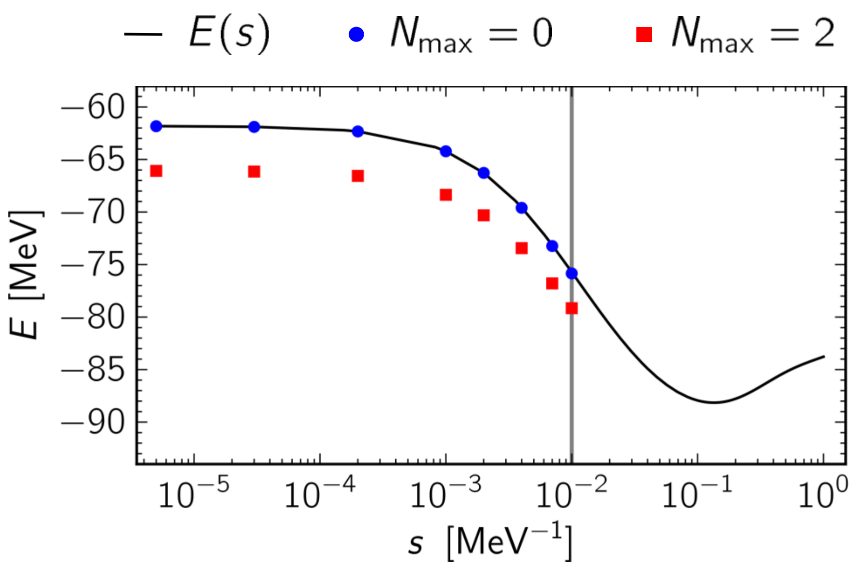
Novel Approach: IM-NCSM

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

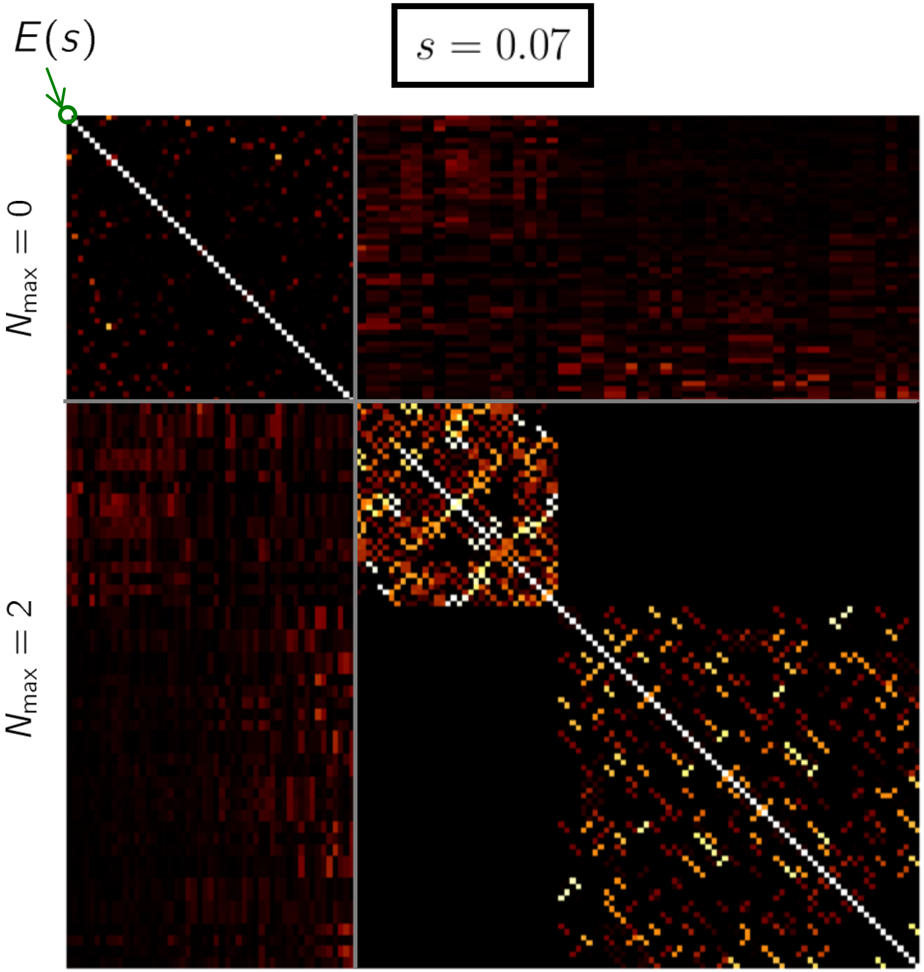


N_{max}=0
eigenstates

N_{max}=2
Slater determinants

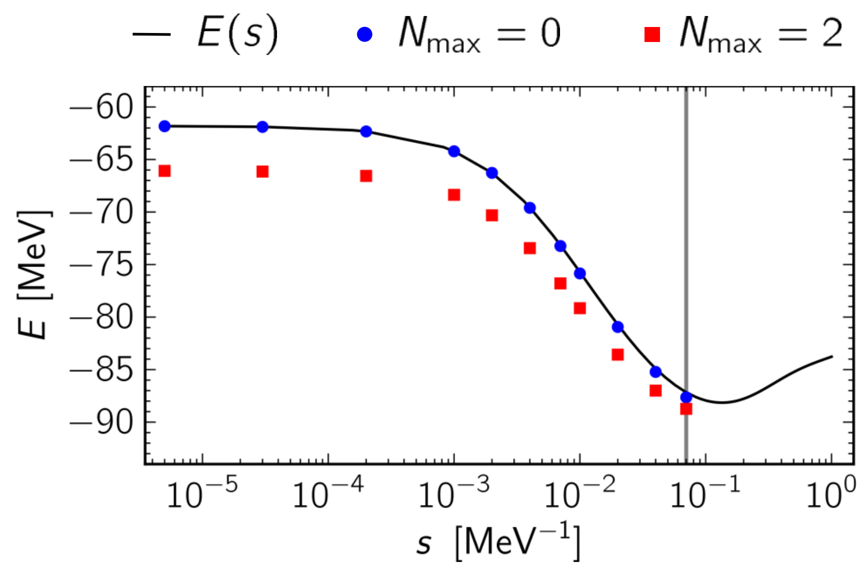


Hamilton Matrix in *A*-Body Basis: ^{12}C

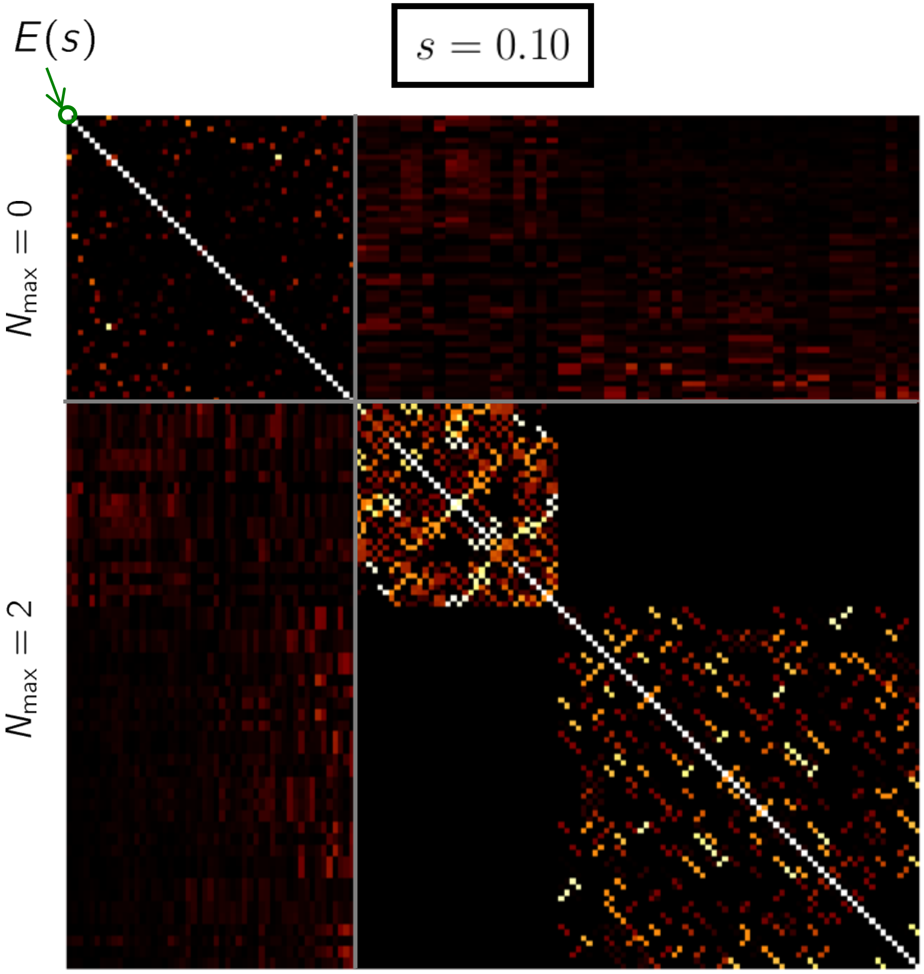


N_{max}=0
eigenstates

N_{max}=2
Slater determinants

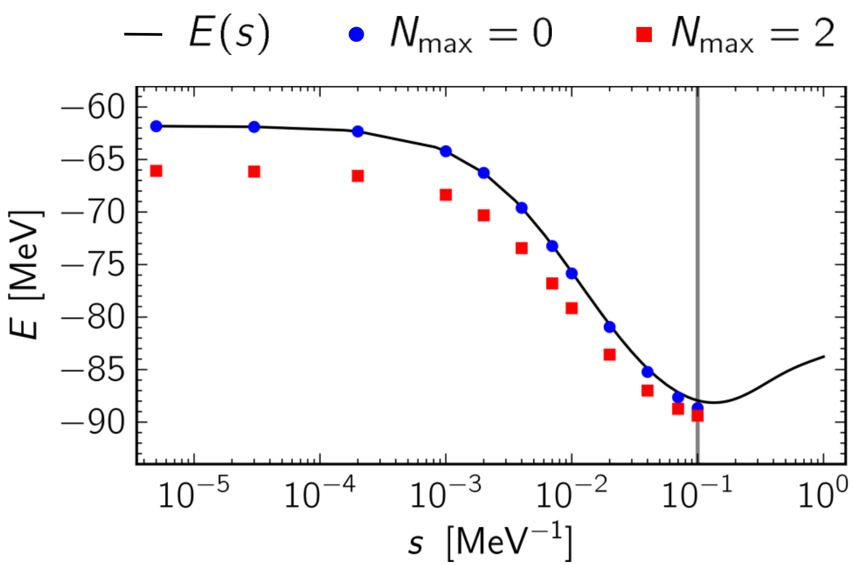


Novel Approach: IM-NCSM
Hamilton Matrix in *A*-Body Basis: ^{12}C

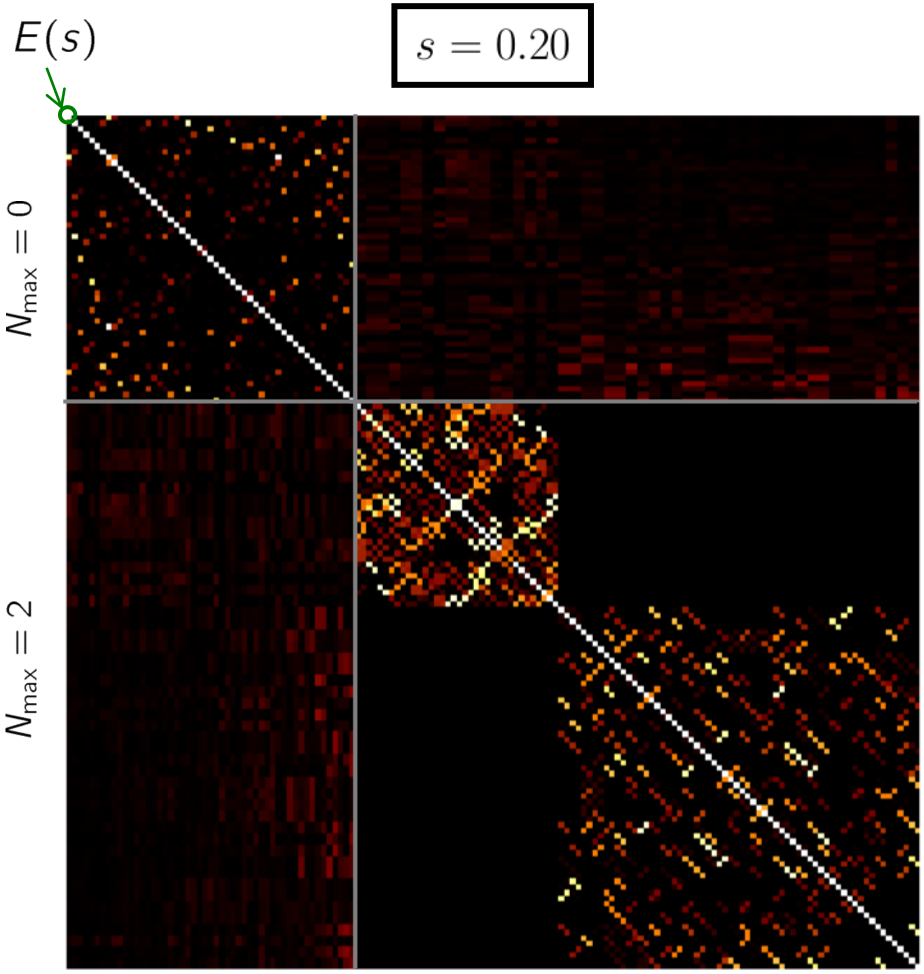


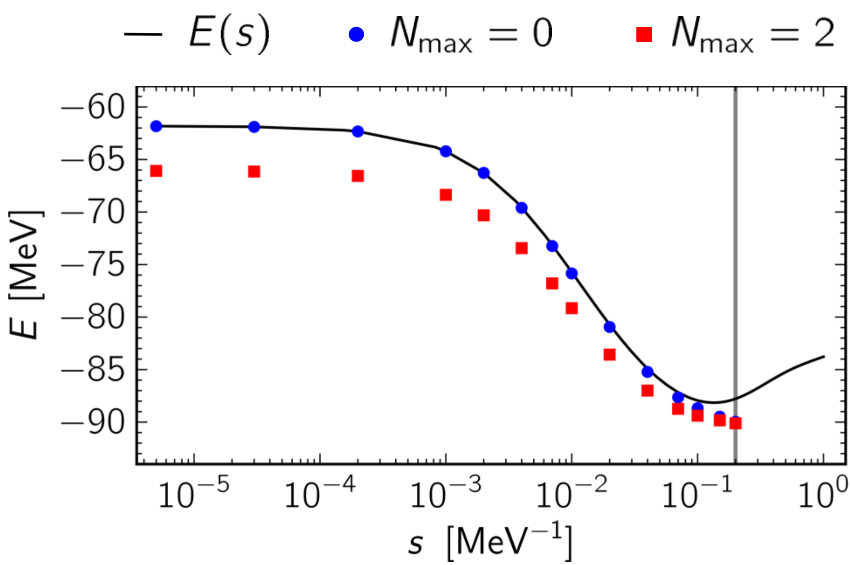
N_{max}=0 **eigenstates**

N_{max}=2 Slater determinants



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

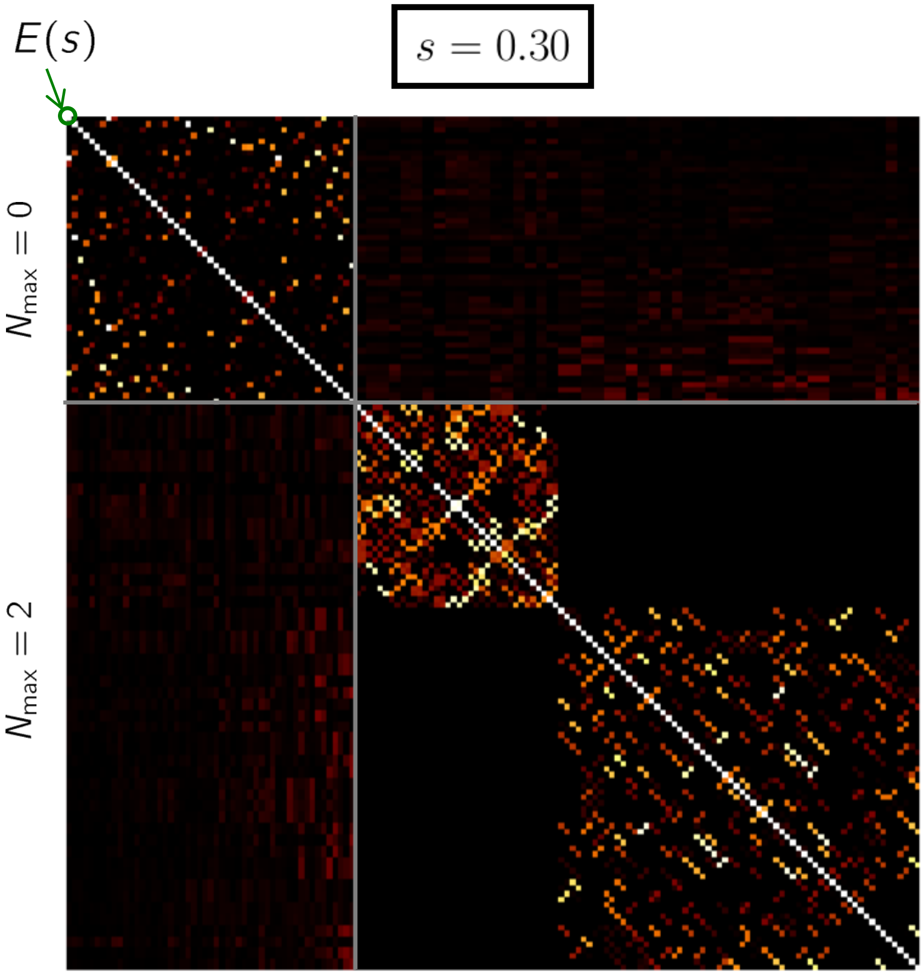




N_{max}=0
eigenstates

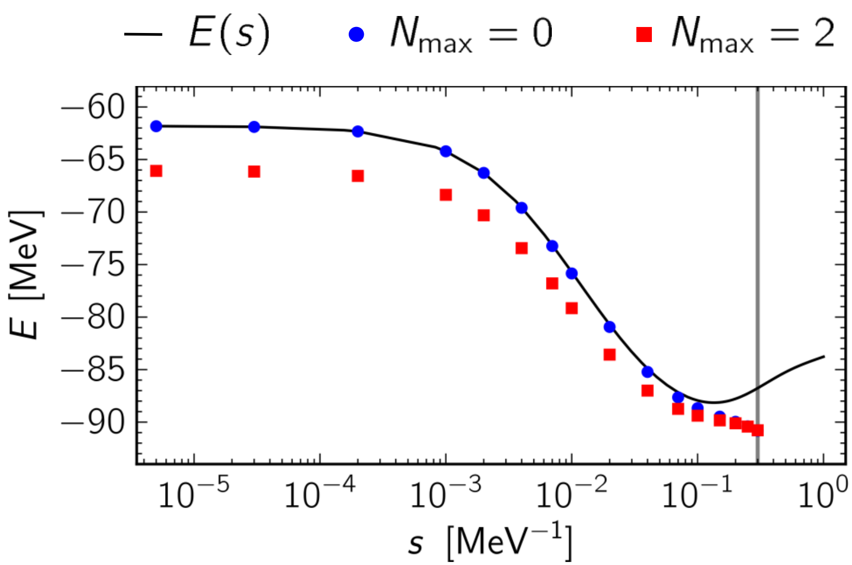
N_{max}=2
Slater determinants

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

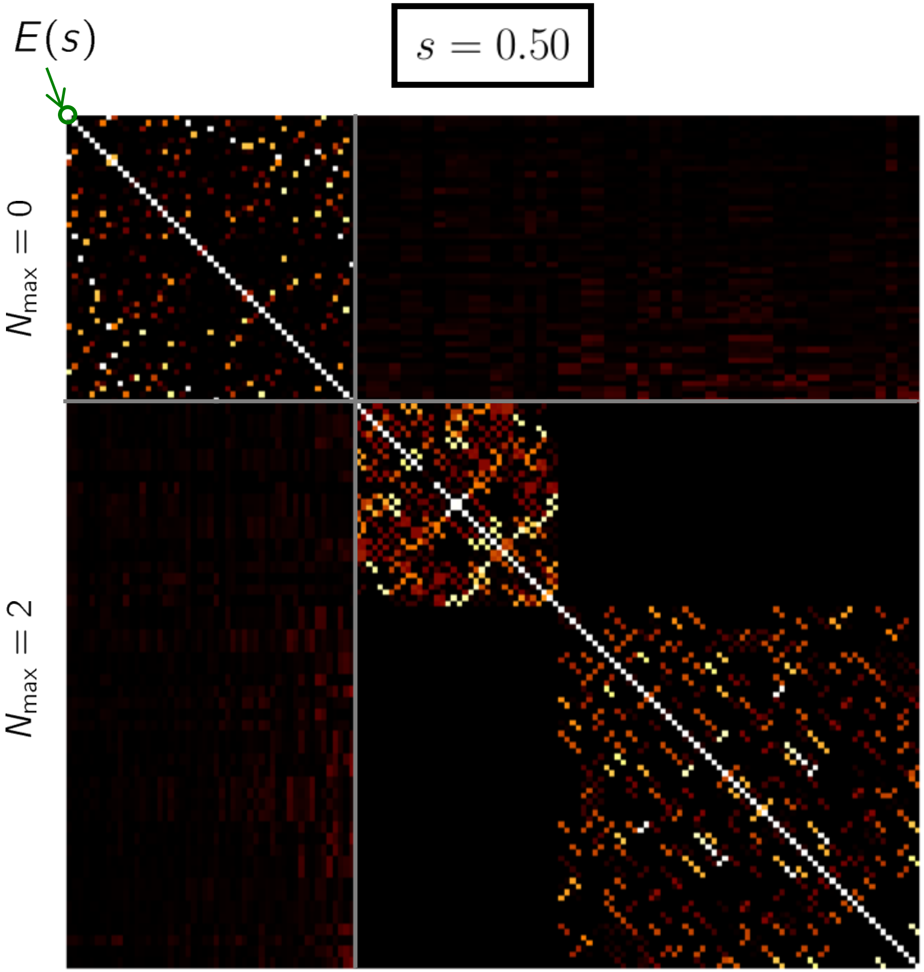


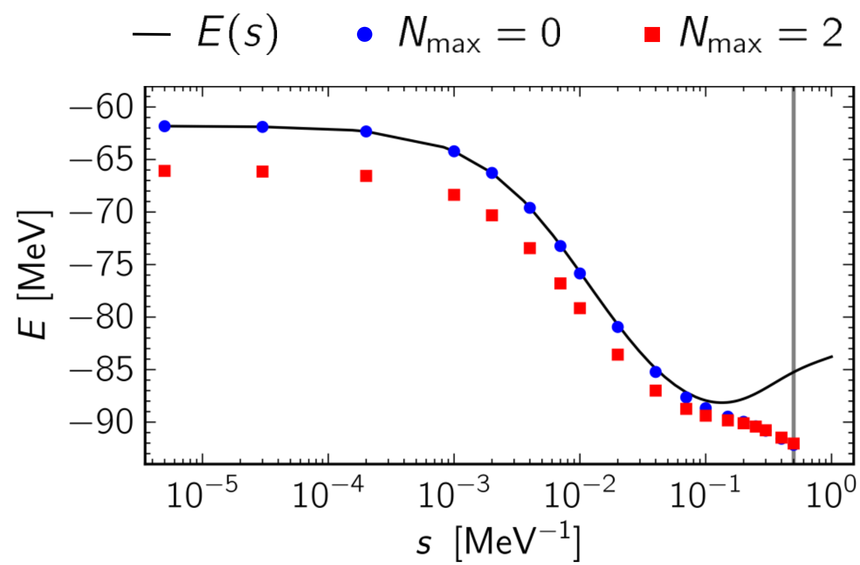
N_{max}=0
eigenstates

N_{max}=2
Slater determinants



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

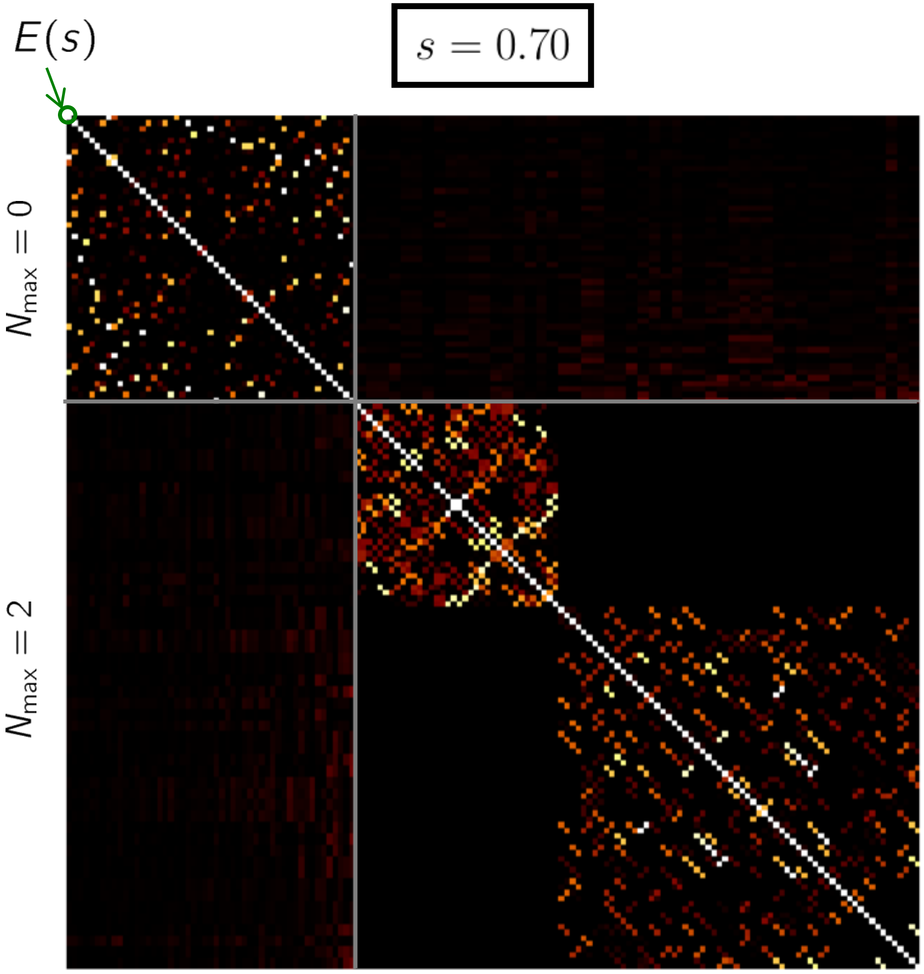




N_{max}=0 **eigenstates**

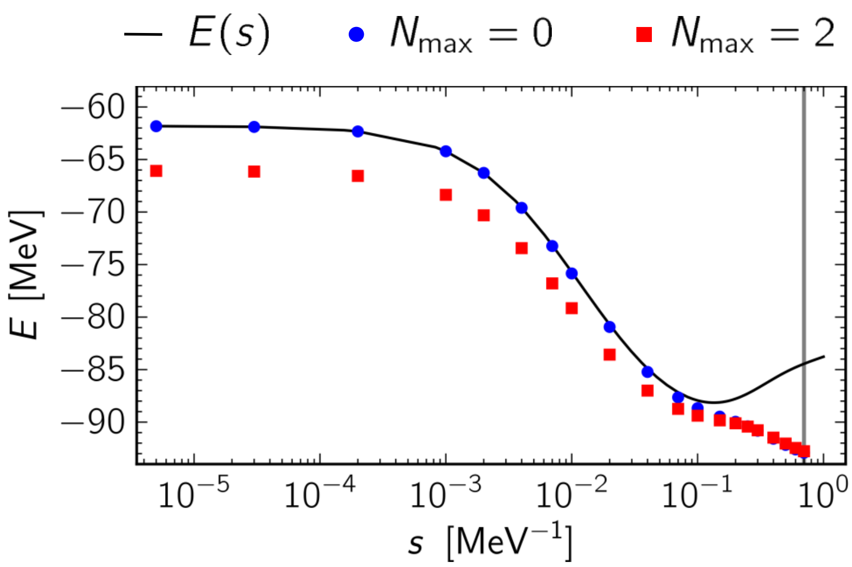
N_{max}=2 Slater determinants

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



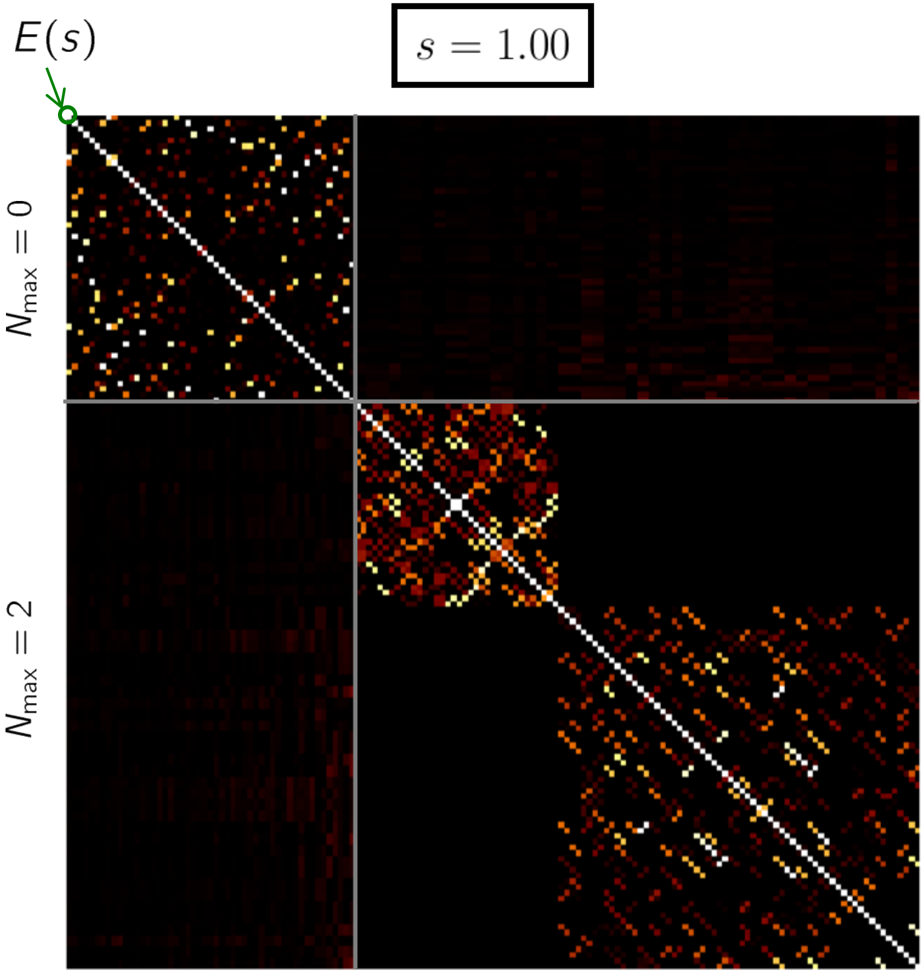
N_{max}=0
eigenstates

N_{max}=2
Slater determinants



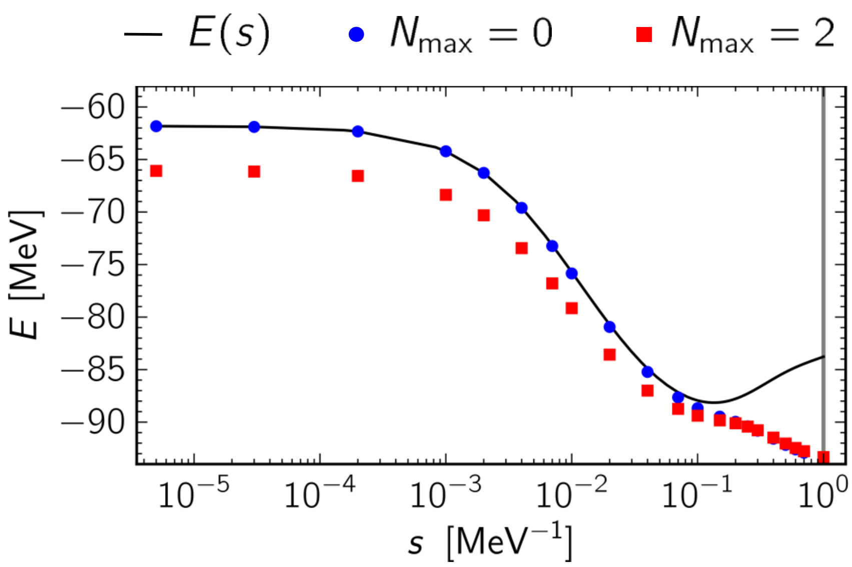
Novel Approach: IM-NCSM

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

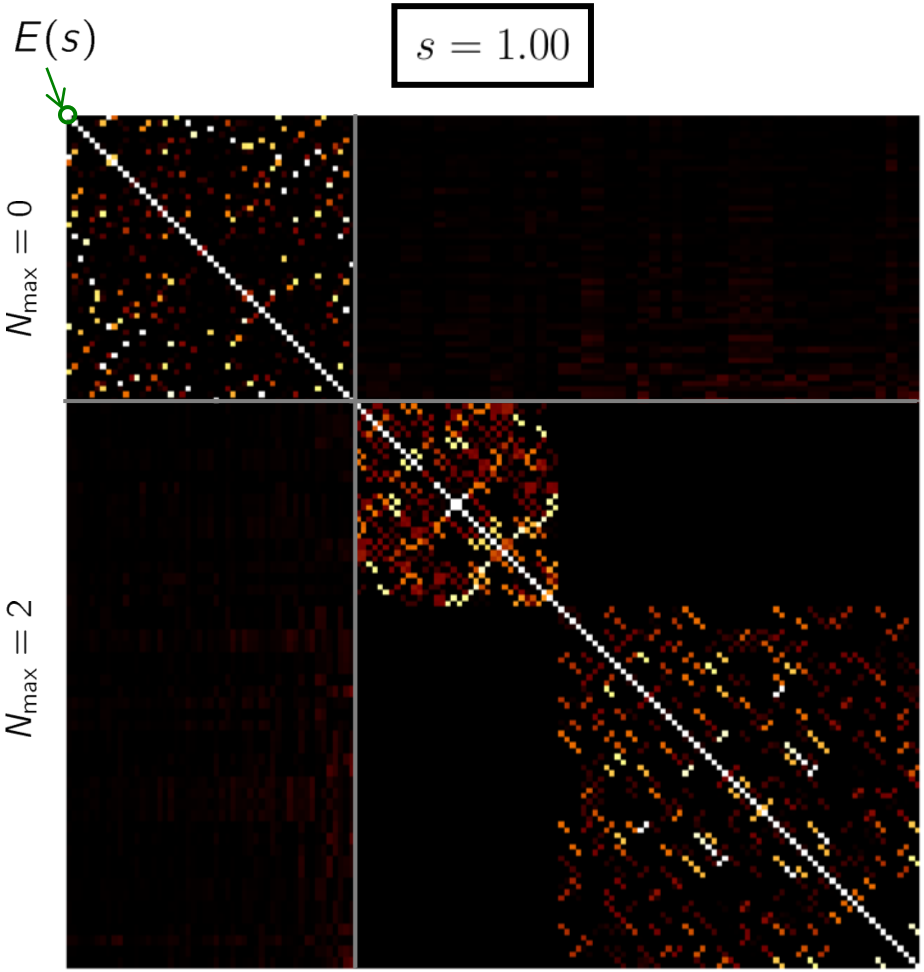


N_{max}=0
eigenstates

N_{max}=2
Slater determinants

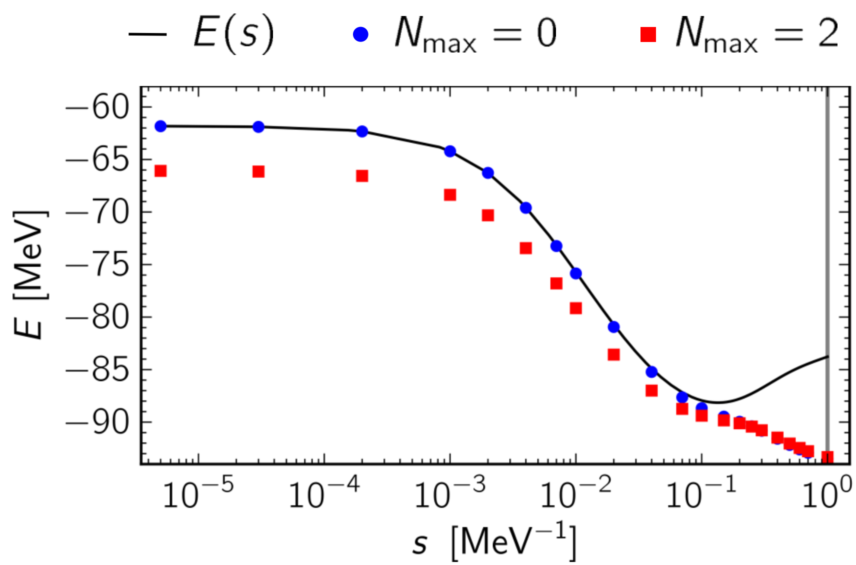


Novel Approach: IM-NCSM
Hamilton Matrix in *A*-Body Basis: ^{12}C



N_{max}=0
eigenstates

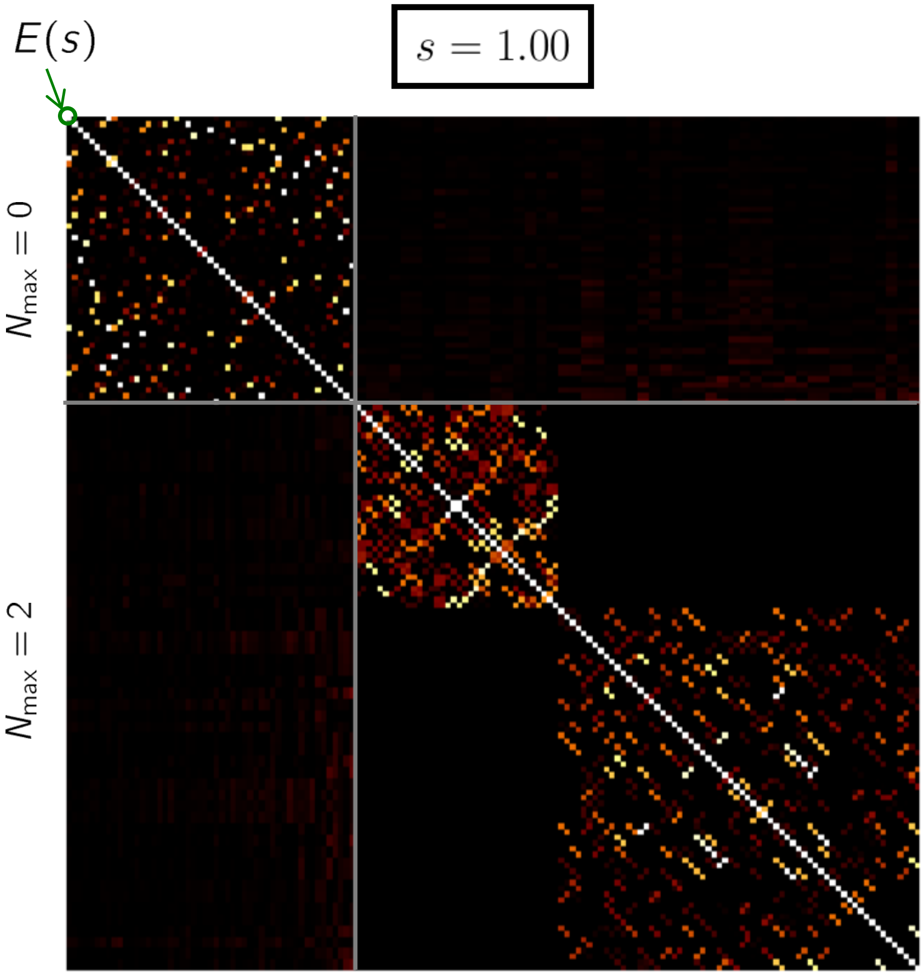
N_{max}=2
Slater determinants



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

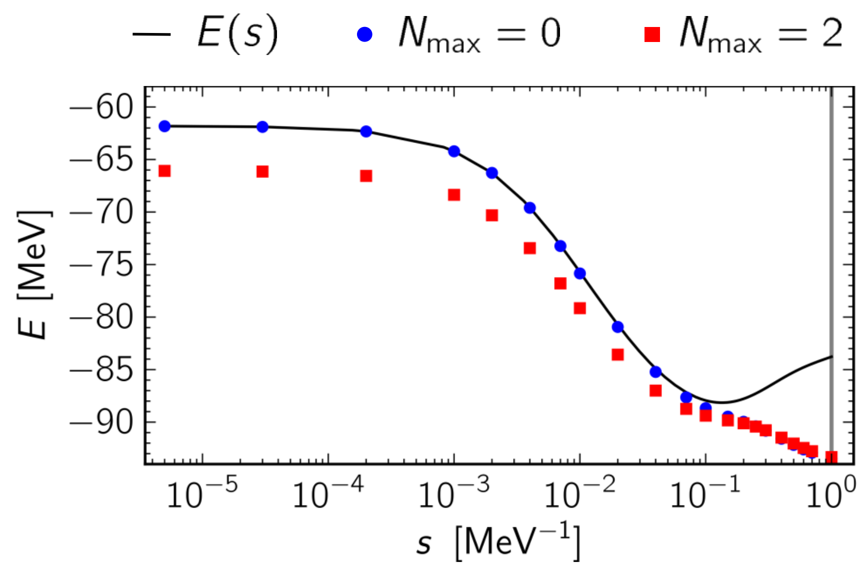
Novel Approach: IM-NCSM

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



N_{max}=0
eigenstates

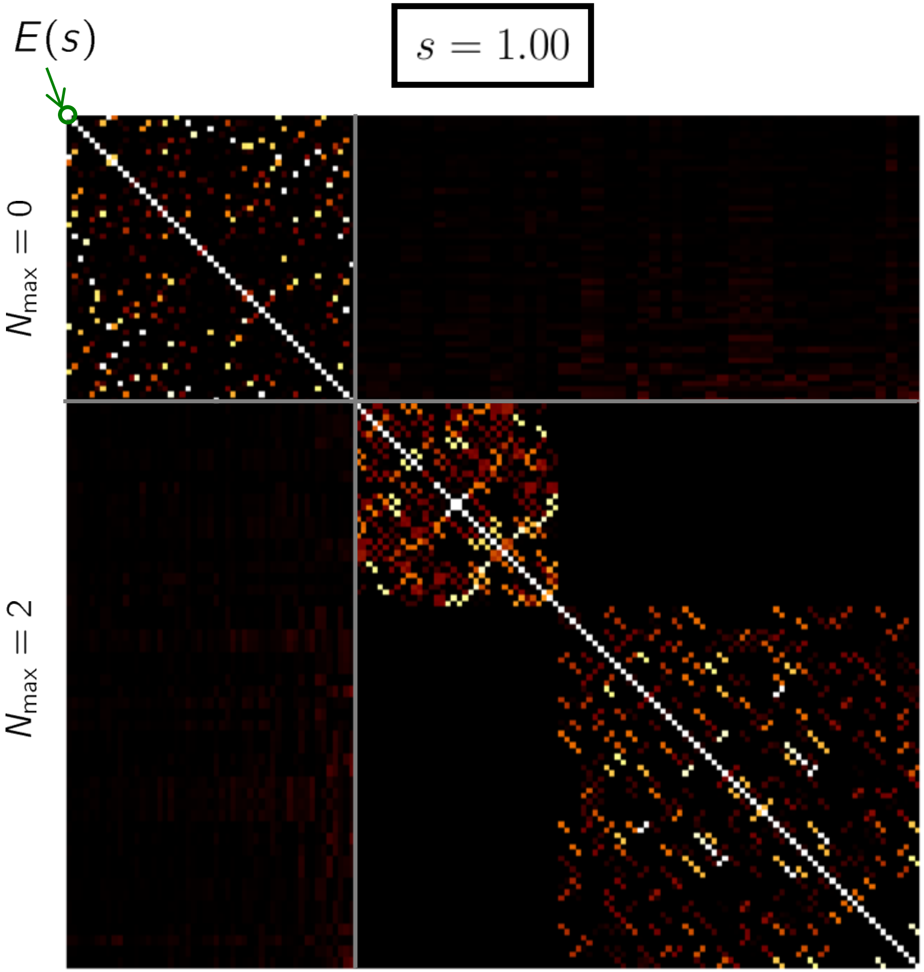
N_{max}=2
Slater determinants



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

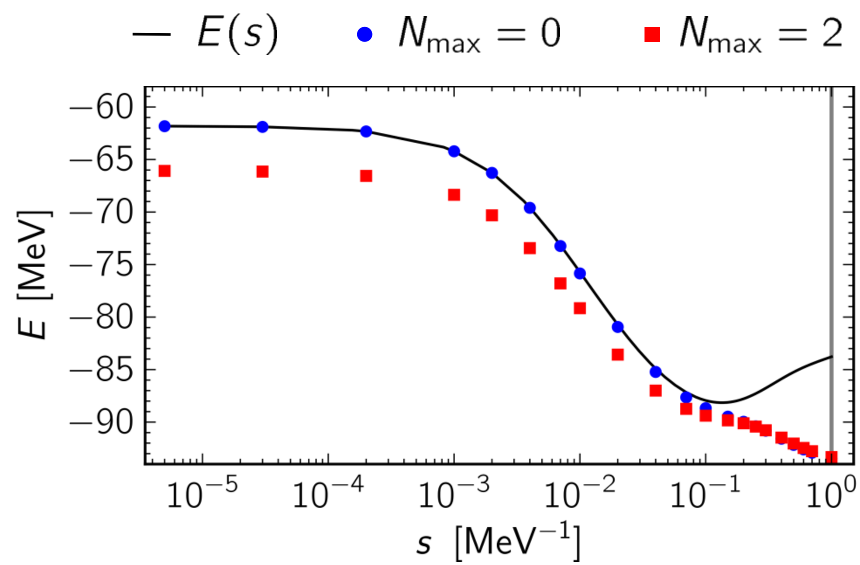
IM-SRG decouples reference state (not only) from N_{max} =2 space

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



N_{max}=0
eigenstates

N_{max}=2
Slater determinants

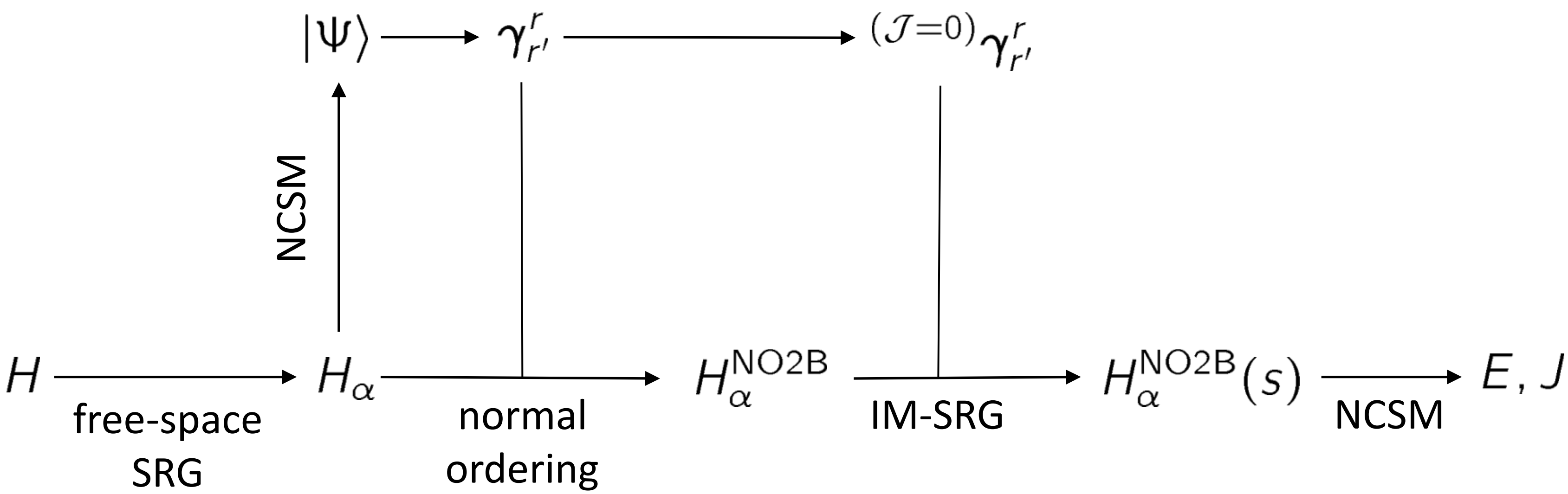


for sufficient large flow parameter eigenvalues in N_{max}=0 and N_{max}=2 equal

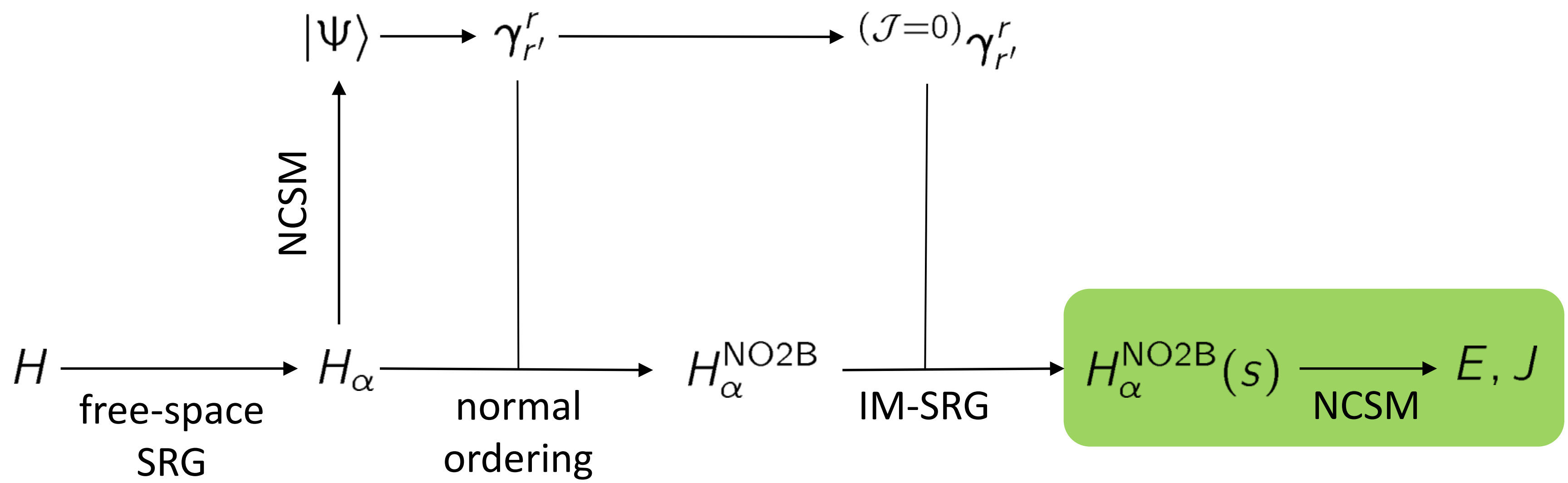
IM-SRG decouples reference state (not only) from N_{max} =2 space

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

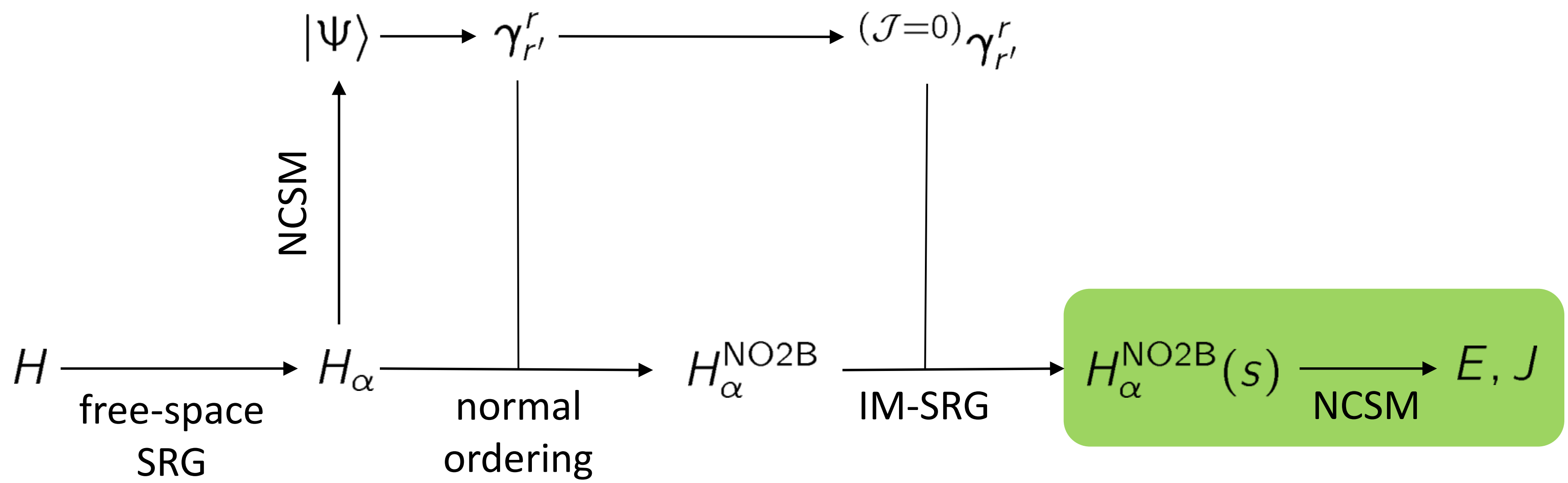
Procedure


$|\Psi\rangle$
$\gamma^{r}_{r'}$
$^{(\mathcal{J}=0)}\gamma^{r}_{r'}$
NCSM
H
free-space SRG
H_α
normal ordering
H_α^{NO2B}
IM-SRG
$H_\alpha^{\mathrm{NO2B}}(s)$
NCSM
E, J

Procedure

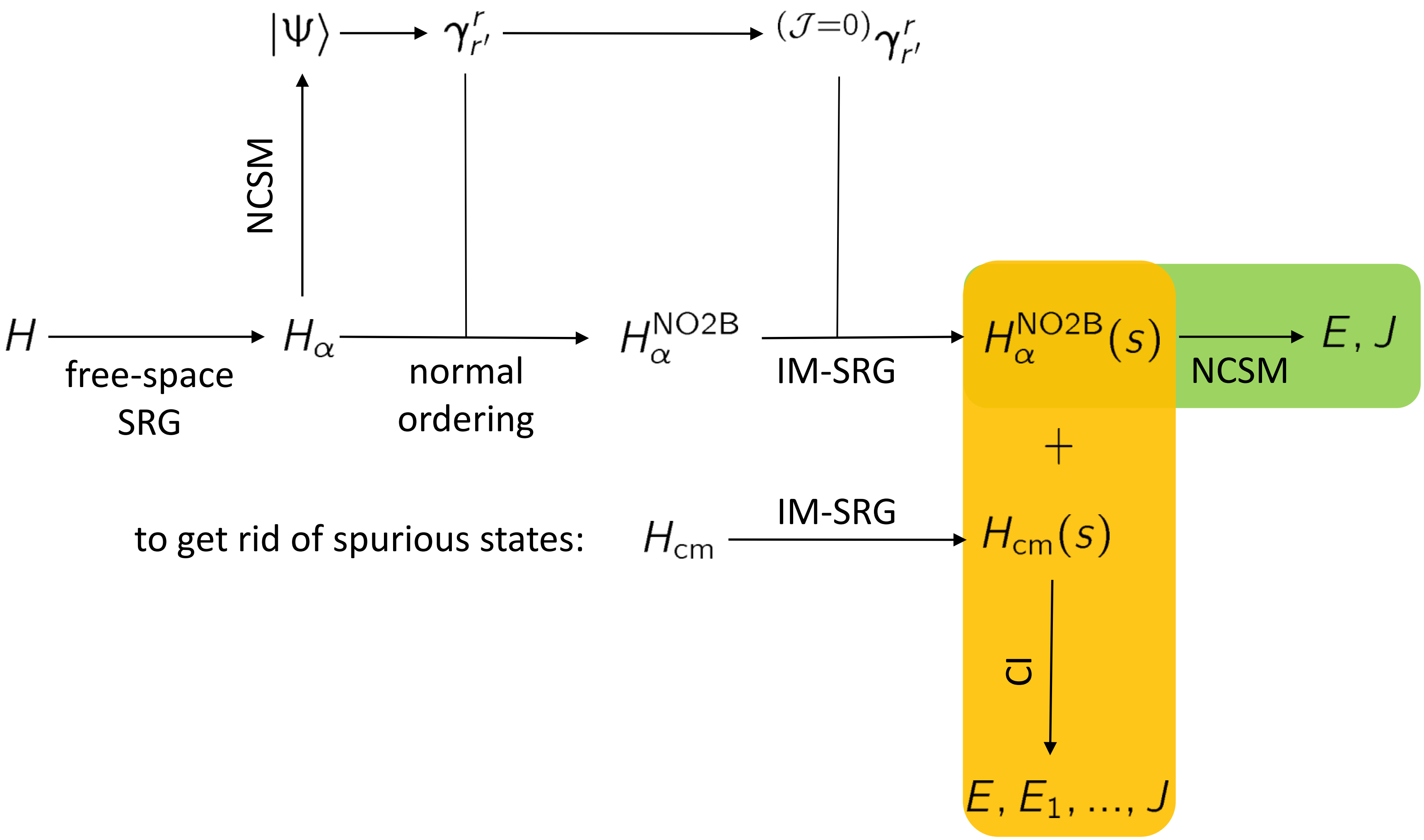

$|\Psi\rangle$
$\gamma^{r}_{r'}$
${}^{(\mathcal{J}=0)}\gamma^{r}_{r'}$
NCSM
H
free-space SRG
H_α
normal ordering
H_α^{NO2B}
IM-SRG
$H_\alpha^{\mathrm{NO2B}}(s)$
NCSM
E, J

Procedure



to get rid of spurious states: $H_{\mathrm{cm}} \xrightarrow{\text{IM-SRG}} H_{\mathrm{cm}}(s)$

Procedure


$|\Psi\rangle$
$\gamma^{r}_{r'}$
$^{(\mathcal{J}=0)}\gamma^{r}_{r'}$
NCSM
H
free-space SRG
H_α
normal ordering
H_α^{NO2B}
IM-SRG
$H_\alpha^{\text{NO2B}}(s)$
NCSM
E, J
$+$
to get rid of spurious states:
H_{cm}
IM-SRG
$H_{\text{cm}}(s)$
CI
$E, E_1, \ldots, J$

Current Implementation of Imaginary Time

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

$$\eta^{1}_{2} = \mathrm{sgn}(\Delta^{1}_{2}) \underbrace{\langle \Psi | H \tilde{a}^{1}_{2} | \Psi \rangle}_{n_1 \bar{n}_2 f^{1}_{2} + \dots} - [1 \leftrightarrow 2]$$

$$\eta^{12}_{34} = \mathrm{sgn}(\Delta^{12}_{34}) \underbrace{\langle \Psi | H \tilde{a}^{12}_{34} | \Psi \rangle}_{n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma^{12}_{34} + \dots} - [(12) \leftrightarrow (34)]$$

natural orbitals:

n_i occupation number

$\bar{n}_i = 1 - n_i$

... missing terms contain irreducible density matrix

$$\Delta^{1}_{2} = \langle \Psi | \tilde{a}^{2}_{1} H \tilde{a}^{1}_{2} | \Psi \rangle - \langle \Psi | H | \Psi \rangle = n_1 \bar{n}_2 f^{1}_{2} + \dots - E$$

$$\Delta^{12}_{34} = \langle \Psi | \tilde{a}^{34}_{12} H \tilde{a}^{12}_{34} | \Psi \rangle - \langle \Psi | H | \Psi \rangle = n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma^{12}_{34} + \dots - E$$