Progress with the In-Medium No-Core Shell Model

Peter Gysbers
The Facility for Rare Isotope Beams
at Michigan State University

PAINT - Feb 24, 2026

Acknowledgements

- FRIB/MSU: H. Hergert, **M. Gajdosik**
- NotreDame: M. Caprio, R. Stroberg, **S. Vittal**
- TRIUMF: P. Navrátil, **M. Gennari** (→ JGUMainz)
- LLNL: K. Kravvaris, M. Atkinson (→ Reed)
- TUD: R. Roth, E. Gebrerufael, K. Vobig, T. Mongelli, **C. Wenz**

Funding

- DOE Collaboration: Nuclear Theory for New Physics (NTNP)

U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- Limitations of the NCSM
- IMSRG-Improved Methods
  - In-Medium No-Core Shell Model (IMNCSM)
- Preliminary Results
  - Applications to intruder states ($^{10}\mathrm{Be}$)
- Open questions and speculations

No-Core Shell Model (NCSM)

(also known as NCCI)

- Solve the nuclear many-body problem via matrix diagonalization

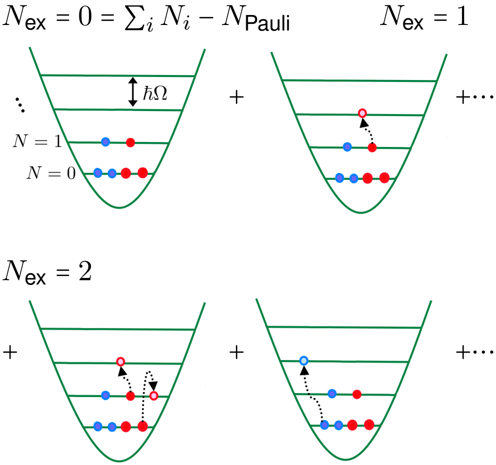
$$H|\Psi_k\rangle = E_k|\Psi_k\rangle$$

- Expand over a basis of configurations (filling single-particle harmonic oscillator orbitals)

$$|\Psi_k\rangle = \sum_{N_{\rm ex}=0}^{N_{\max}} \sum_j c^k_{N_{\rm ex}j}|\Phi_{N_{\rm ex}j}\rangle$$

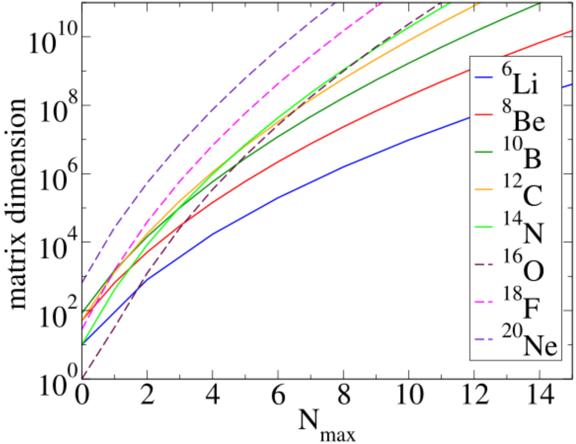
- Converge to an exact solution as $N_{\max} \to \infty$
- Evaluate matrix elements of operators:

$$\langle\Psi_f|O|\Psi_i\rangle = \sum_{\alpha\beta}^{A}\langle\alpha|O|\beta\rangle\langle\Psi_f|a^\dagger_\alpha a_\beta|\Psi_i\rangle$$



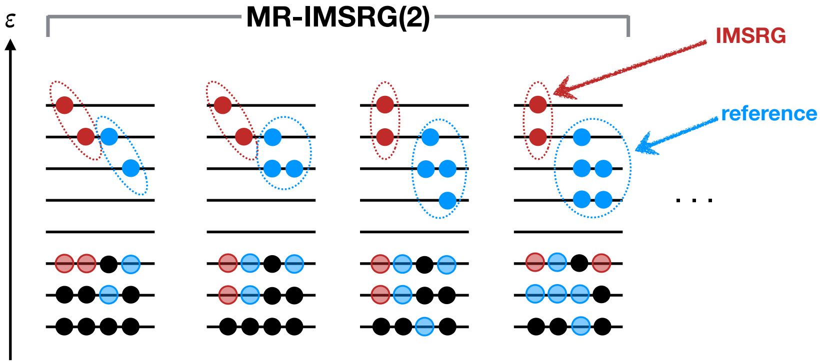
Motivation

- Heavier nuclei allow more possible configurations
  → the cost of storing the Hamiltonian matrix explodes
- Can we tune the basis (with IMSRG) to reduce the size required?



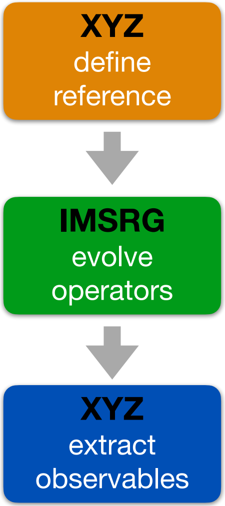
Yang et al (2013)

Correlated Reference States



MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)

IMSRG-Improved Methods



* mean field or **explicitly correlated**

IMSRG-Improved Methods

- Choose/find a reference state
- Normal-Order the Hamiltonian with respect to that reference
- Evolve Hamiltonian with IMSRG (and any operators)
- De-Normal-Order back to the vacuum representation (if necessary)
- Use effective Hamiltonian in many-body method to extract observables

Vacuum Normal-Ordering

= Standard Second Quantization

- Normal-ordered operators: $A^i_j = a^\dagger_i a_j$, $A^{ij}_{kl} = a^\dagger_j a^\dagger_i a_k a_l$, etc,
  - with respect to the vacuum, i.e. $\langle 0| A |0\rangle = 0$

$$
\begin{aligned}
H &= T_{\text{int}} + V \\
&= \left(1 - \frac{1}{A}\right) T^{(1)} + \frac{1}{A} T^{(2)} + V^{(2)} + V^{(3)} \\
&= \sum t^{\circ}_{\circ} A^{\circ}_{\circ} + \frac{1}{4} \sum \left(t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ}\right) A^{\circ\circ}_{\circ\circ} + \frac{1}{36} \sum v^{\circ\circ\circ}_{\circ\circ\circ} A^{\circ\circ\circ}_{\circ\circ\circ}
\end{aligned}
$$

Reference Normal-Ordering

Given a reference state $|\Psi\rangle$:

- Compute the density matrices: $\rho^i_j = \langle\Psi| A^i_j |\Psi\rangle$ and $\rho^{ij}_{kl} = \langle\Psi| A^{ij}_{kl} |\Psi\rangle$, etc
  - Define operators $\tilde{A}$ such that $\langle\Psi| \tilde{A} |\Psi\rangle = 0$

$$
\begin{aligned}
H =& E + \sum f^{\circ}_{\circ} \tilde{A}^{\circ}_{\circ} + \frac{1}{4} \sum \Gamma^{\circ\circ}_{\circ\circ} \tilde{A}^{\circ\circ}_{\circ\circ} + \frac{1}{36} \sum W^{\circ\circ\circ}_{\circ\circ\circ} \tilde{A}^{\circ\circ\circ}_{\circ\circ\circ} \\
E =& \sum {\color{red} t^{\circ}_{\circ}} \rho^{\circ}_{\circ} + \frac{1}{4} \sum {\color{green} (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ})} \rho^{\circ\circ}_{\circ\circ} + \frac{1}{36} \sum {\color{blue} v^{\circ\circ\circ}_{\circ\circ\circ}} \rho^{\circ\circ\circ}_{\circ\circ\circ} \\
f^{\circ}_{\circ} =& {\color{red} t^{\circ}_{\circ}} + \sum {\color{green} (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ})} \rho^{\circ}_{\circ} + \frac{1}{4} \sum {\color{blue} v^{\circ\circ\circ}_{\circ\circ\circ}} \rho^{\circ\circ}_{\circ\circ} \\
\Gamma^{\circ\circ}_{\circ\circ} =& {\color{green} (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ})} + \sum {\color{blue} v^{\circ\circ\circ}_{\circ\circ\circ}} \rho^{\circ}_{\circ} \\
W^{\circ\circ\circ}_{\circ\circ\circ} =& {\color{blue} v^{\circ\circ\circ}_{\circ\circ\circ}}
\end{aligned}
$$

Reference Normal-Ordering

Given a reference state $|\Psi\rangle$:

- Compute the density matrices: $\rho^i_j = \langle\Psi| A^i_j |\Psi\rangle$ and $\rho^{ij}_{kl} = \langle\Psi| A^{ij}_{kl} |\Psi\rangle$, etc
  - Define operators $\tilde{A}$ such that $\langle\Psi| \tilde{A} |\Psi\rangle = 0$

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

$$E = \sum t^{\circ}_{\circ} \rho^{\circ}_{\circ} + \frac{1}{4} \sum (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ}) \rho^{\circ\circ}_{\circ\circ} + \frac{1}{36} \sum v^{\circ\circ\circ}_{\circ\circ\circ} \rho^{\circ\circ\circ}_{\circ\circ\circ}$$

$$f^{\circ}_{\circ} = t^{\circ}_{\circ} + \sum (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ}) \rho^{\circ}_{\circ} + \frac{1}{4} \sum v^{\circ\circ\circ}_{\circ\circ\circ} \rho^{\circ\circ}_{\circ\circ}$$

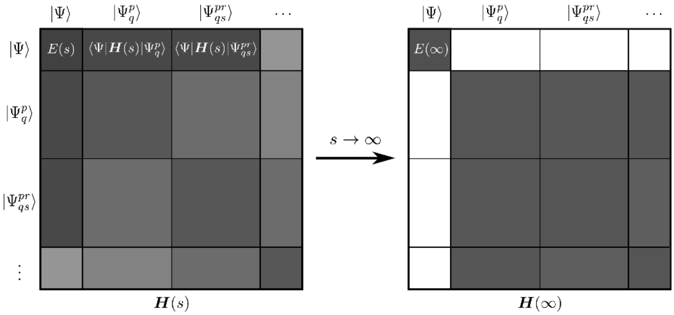
$$\Gamma^{\circ\circ}_{\circ\circ} = (t^{\circ\circ}_{\circ\circ} + v^{\circ\circ}_{\circ\circ}) + \sum v^{\circ\circ\circ}_{\circ\circ\circ} \rho^{\circ}_{\circ}$$

$$\cancel{W^{\circ\circ\circ}_{\circ\circ\circ} = v^{\circ\circ\circ}_{\circ\circ\circ}}$$ NO2B approx.

IMSRG-Improved Methods

- Choose/find a reference state
- Normal-Order the Hamiltonian with respect to that reference
- Evolve Hamiltonian with IMSRG (and any operators)
- De-Normal-Order back to the vacuum representation (if necessary)
- Use effective Hamiltonian in many-body method to extract observables

IMSRG: In-Medium Similarity Renormalization Group

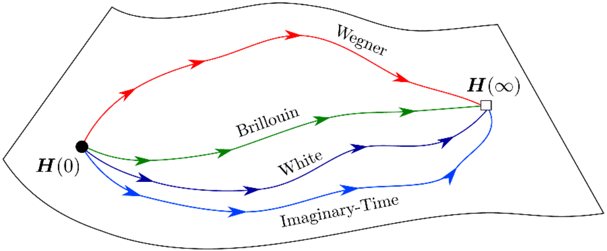


- continuous unitary transformation
- solve flow equation: $\frac{d}{ds}H(s) = [\eta(s), H(s)]$

E. Gebrerufael (2017)

IMSRG (cont.)

- Choose $\eta(s)$ to decouple reference state from excitations
- $E(s) = \langle\Psi| H(s) |\Psi\rangle$ converges to an eigenstate



E. Gebrerufael (2017)

IMSRG (cont.)

Advantages

- soft scaling with A (never construct $H(s)$ explicitly)
- 3N interaction included via the normal-ordered two-body approximation (NO2B)

Disadvantages

- ground state only
- formulated for 0^+ states (only even nuclei)

Compromises

- $\eta(s)$ not computed exactly
  - IM-SRG(2): include only up to 2-body flow equations
  - include only up to 2-body irreducible densities ($\lambda^{(2)}$) in contractions

IMSRG-Improved Methods

- Choose/find a reference state
- Normal-Order the Hamiltonian with respect to that reference
- Evolve Hamiltonian with IMSRG (and any operators)
- De-Normal-Order back to the vacuum representation (if necessary)
- Use effective Hamiltonian in many-body method to extract observables

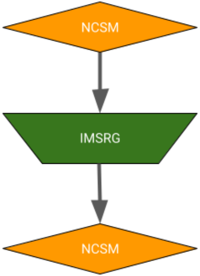
De-Normal-Ordering

Reconstruct a Vacuum Normal-Ordered Hamiltonian

$$
\begin{aligned}
H(s) &= h + \sum h^{\circ}_{\circ} A^{\circ}_{\circ} + \sum h^{\circ\circ}_{\circ\circ} A^{\circ\circ}_{\circ\circ} \\
h &= E(s) - \sum f^{\circ}_{\circ}(s) \rho^{\circ}_{\circ} - \frac{1}{4} \sum \Gamma^{\circ\circ}_{\circ\circ}(s) \left(\rho^{\circ\circ}_{\circ\circ} - 4 \rho^{\circ}_{\circ} \rho^{\circ}_{\circ} \right) \\
h^{\circ}_{\circ} &= f^{\circ}_{\circ}(s) - \sum \Gamma^{\circ\circ}_{\circ\circ}(s) \rho^{\circ}_{\circ} \\
h^{\circ\circ}_{\circ\circ} &= \Gamma^{\circ\circ}_{\circ\circ}(s)
\end{aligned}
$$

IM-NCSM

- Calculate a reference state with NCSM in the $N_{\text{max}}^{\text{ref}}$ space
- Normal-Order the Hamiltonian with respect to that reference
- Evolve Hamiltonian with IMSRG (and any operators)
- De-Normal-Order back to the vacuum representation
- Use effective Hamiltonian in NCSM to extract observables



IM-NCSM: The best of both worlds

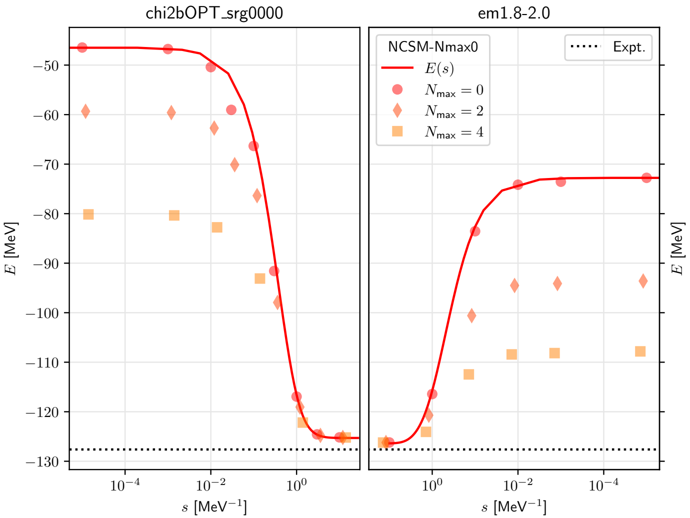
IMSRG

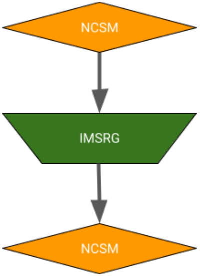
- polynomial-scaling with A (never construct H explicitly)
- include 3N via NO2B approximation

NCSM

- easy access to excited states and observables
- no restrictions to even nuclei

^{16}O: Ground State ($N_{\text{max}}^{\text{ref}} = 0$)

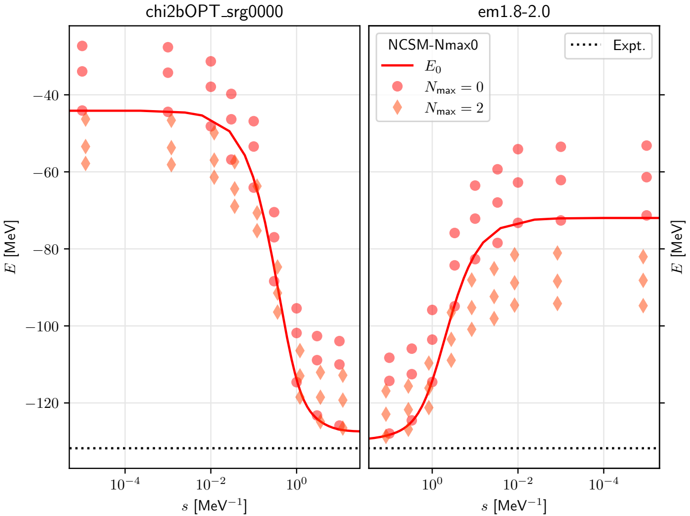




Eta: White
$e_{\text{max}} = 8$
$\hbar\Omega = 20$MeV

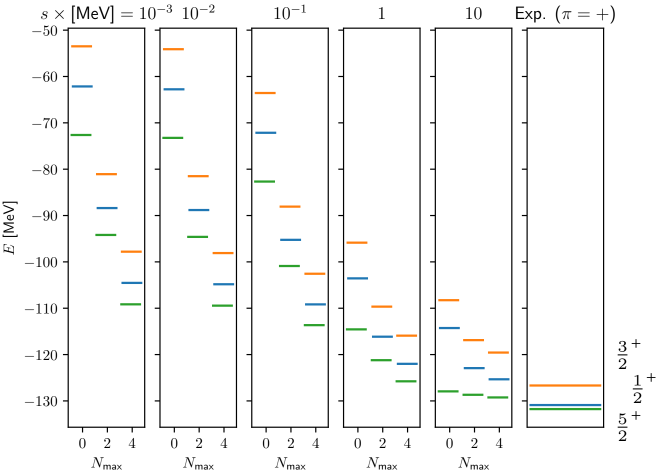
Odd-A: ^{17}O ($N_{\mathrm{max}}^{\mathrm{ref}} = 0$)

- use the scalar part of the ground state $\frac{5}{2}^{+}$ density as the reference (0^{+} "pseudo-state")



Eta: White
$e_{\mathrm{max}} = 8$
$\hbar\Omega$ = 20MeV

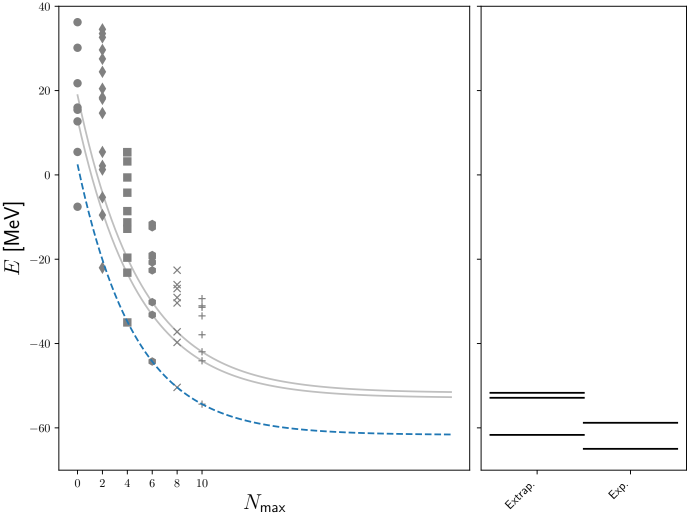
Odd-A: ^{17}O ($N_{\text{max}}^{\text{ref}} = 0$)



Eta: White
$e_{\text{max}} = 8$
$\hbar\Omega$ = 20MeV
Int: em1.8-2.0

^{10}Be: A Case Study

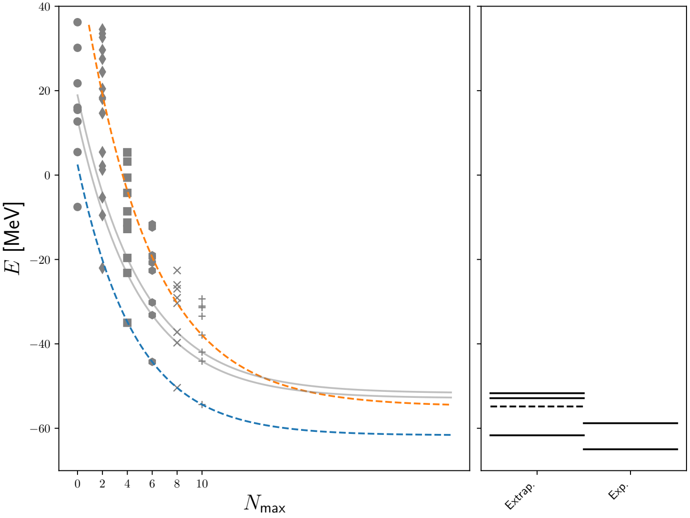
(only 0^+ states)
Int: chi2bOPT



N_{max}	Dim.
0	51
2	10111
4	430137
6	9213794
8	129146347
10	1342798788

^{10}Be: A Case Study

(only 0^+ states)
Int: chi2bOPT



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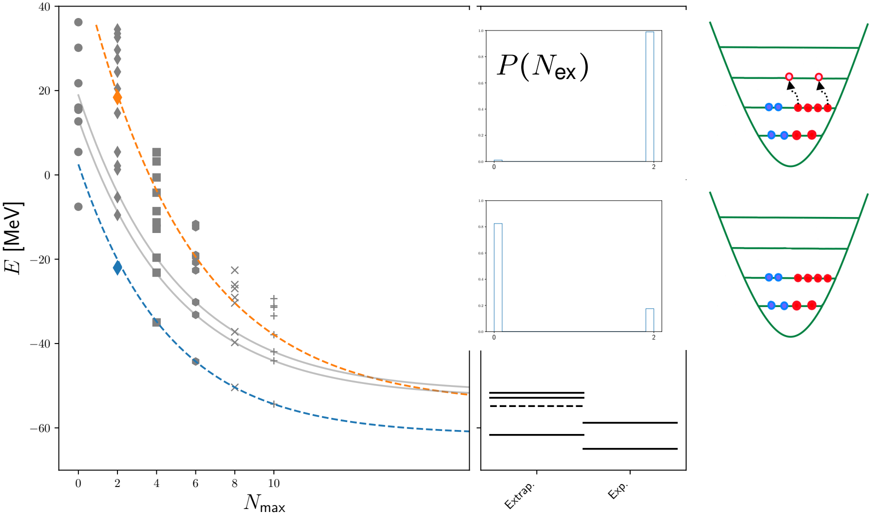
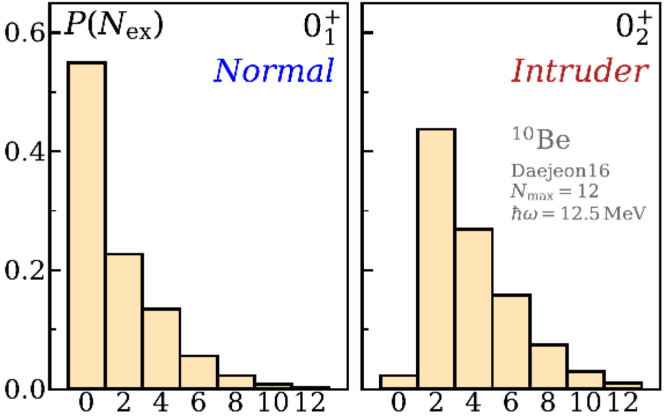


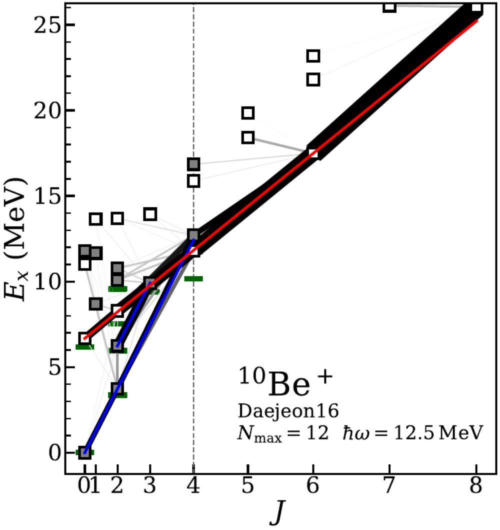
N_{max}	Dim.
0	51
2	10111
4	430137
6	9213794
8	129146347
10	1342798788

^{10}Be: $P(N_{\mathrm{ex}})$ $N_{\mathrm{max}} = 12$



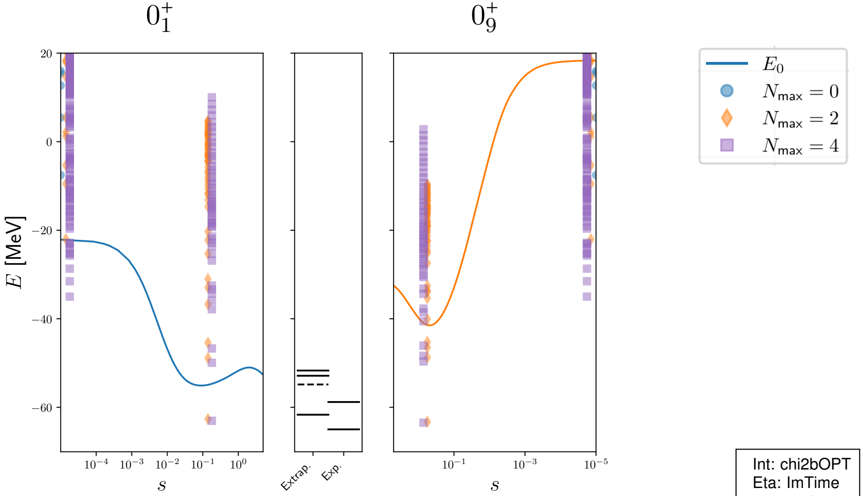
Caprio (PAINT2024)

$^{10}\mathrm{Be}$ Rotational Bands: $E_x \propto \frac{J(J+1)}{2I}$



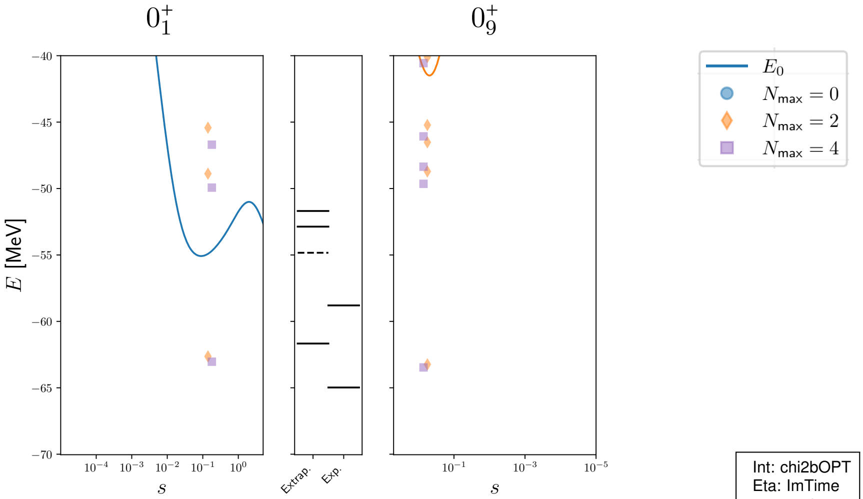
Caprio (PAINT2024)

^{10}Be: IMSRG with $N_{\max}^{\text{ref}} = 2\ 0^+$ References



Int: chi2bOPT
Eta: ImTime
$e_{\max}$ = 8
$\hbar\Omega$ = 20MeV

^{10}Be: IMSRG with $N_{\text{max}}^{\text{ref}} = 2$ 0^+ References

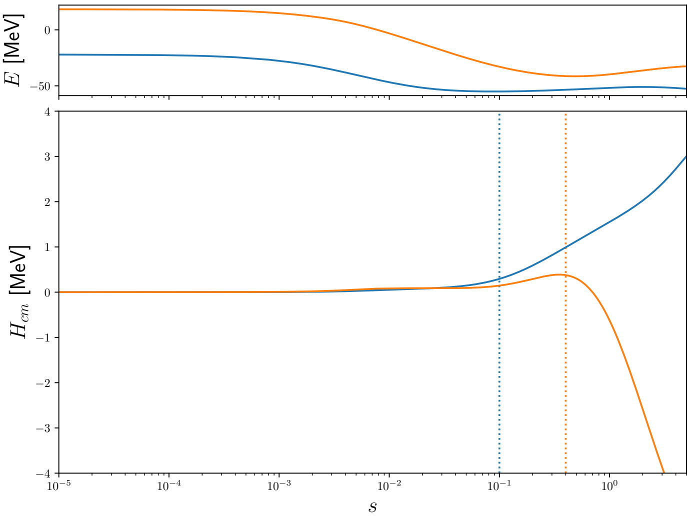


Int: chi2bOPT
Eta: ImTime
$e_{\text{max}} = 8$
$\hbar\Omega = 20$MeV

Co-evolving Operators

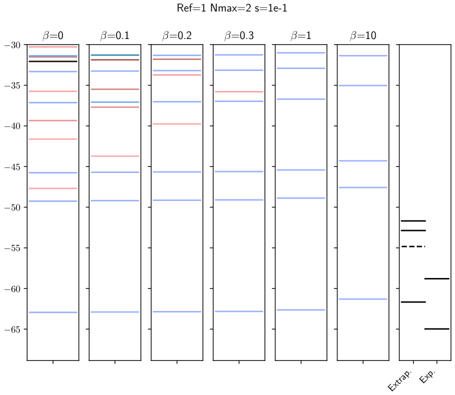
- Center of mass Hamiltonian
- N_{ex}
- Isospin

H_{cm} Flow

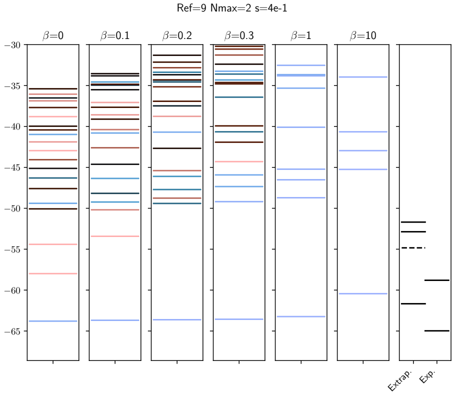


$H(s) + \beta H_{\mathrm{cm}}(s)$

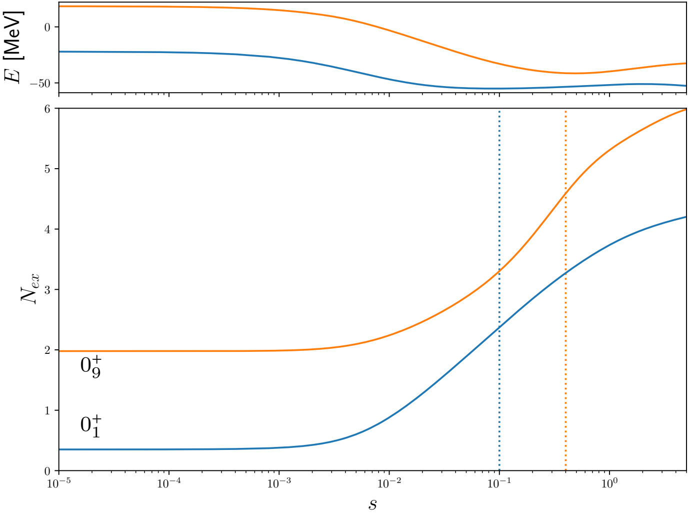
0_1^+



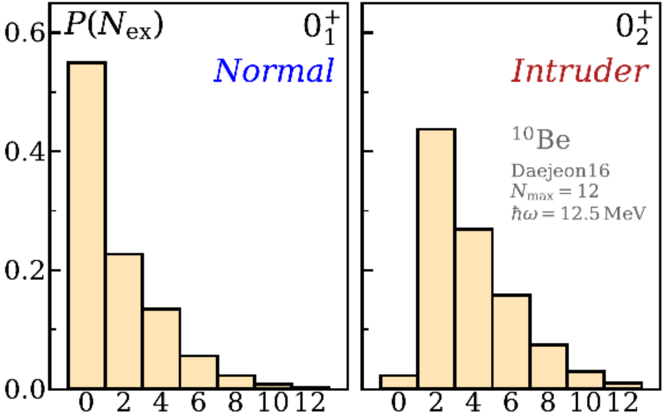
0_9^+



N_{ex} Flow



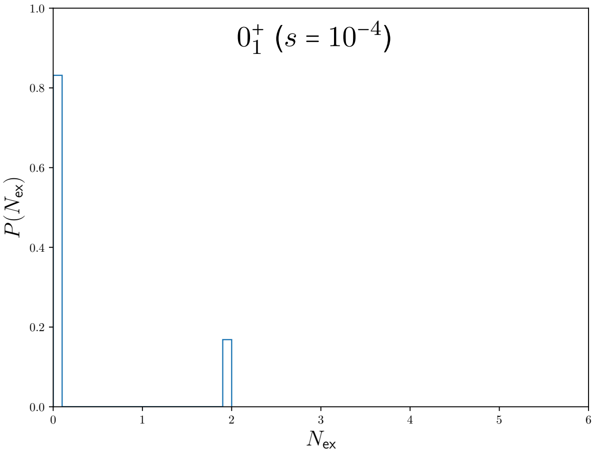
N_{ex} Flow



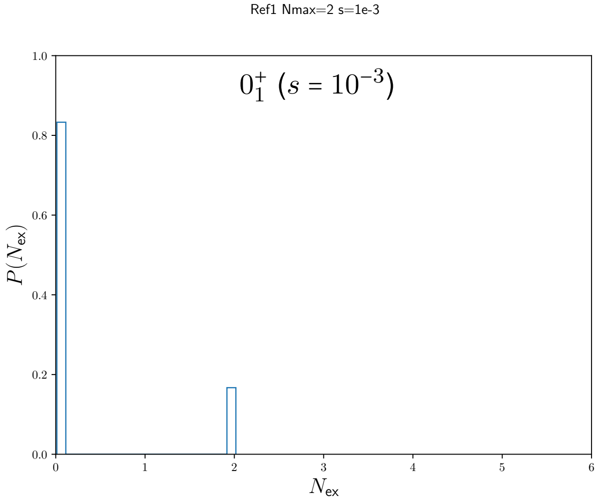
$< N_{\text{ex}} >\sim 5$ $\quad$ $< N_{\text{ex}} >\sim 10$

N_{ex} Flow

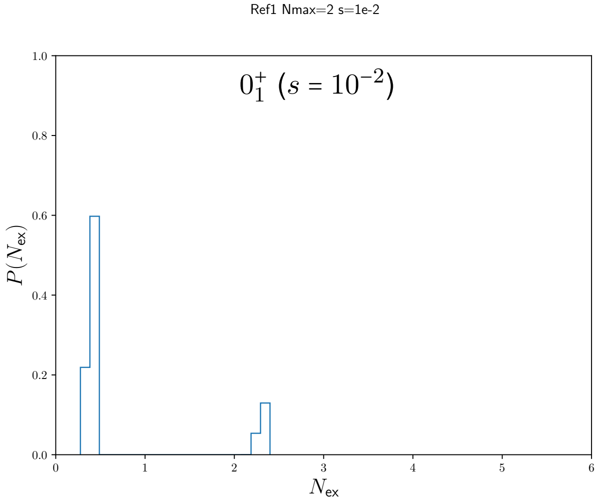
Ref1 Nmax=2 s=1e-4



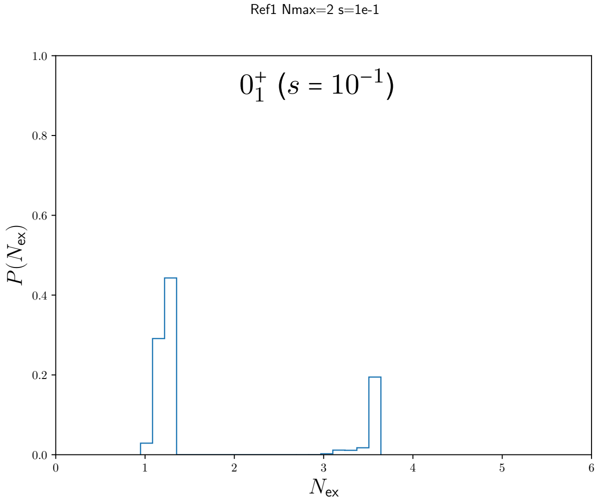
N_{ex} Flow



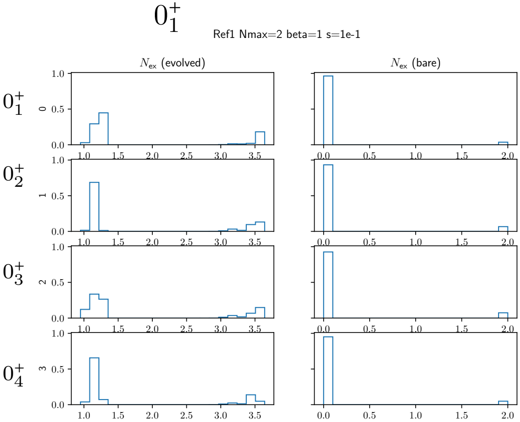
N_{ex} Flow

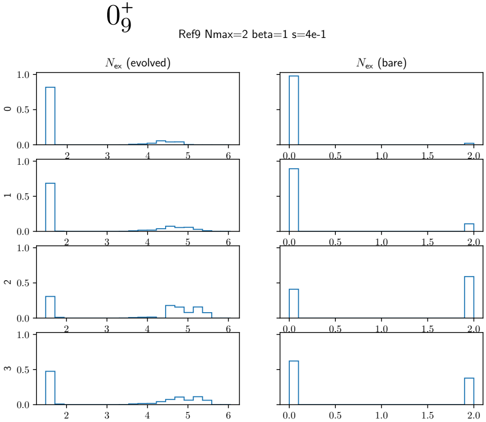


N_{ex} Flow

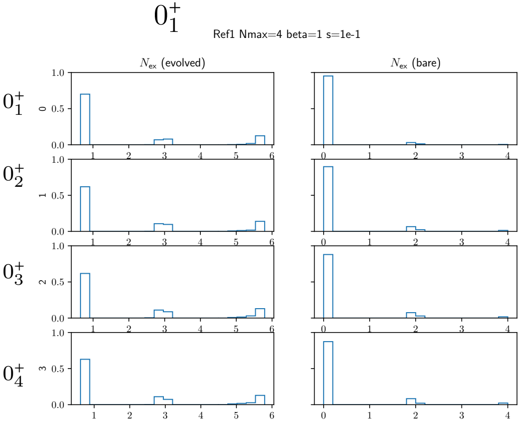


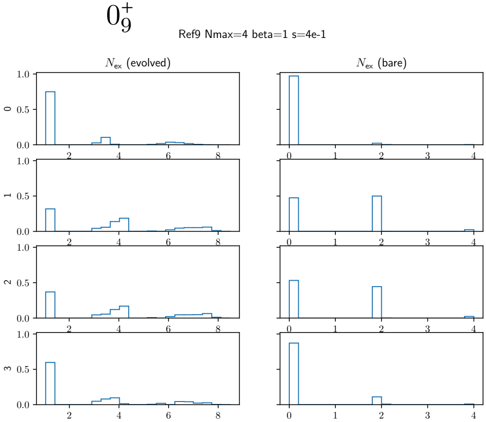
$P(N_{ex})$ for $N_{max} = 2$ ($N_{max}^{ref} = 2$)



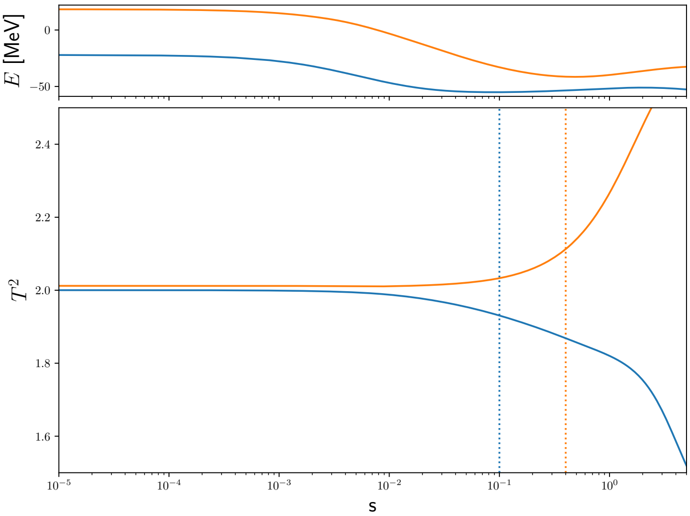


$P(N_{\mathrm{ex}})$ for $N_{\mathrm{max}} = 4$ ($N_{\mathrm{max}}^{\mathrm{ref}} = 2$)





Induced Isospin Breaking



Open Questions

- How do we account for induced isospin breaking in β decay corrections (δ_C)?
- How do we interpret evolved N_{ex}?
- Can we target other experimentally known states by choosing the right reference states?
  - $N_{\text{max}} = 4$ precursor for α excitations? ($^{12}\mathrm{C}$ Hoyle state, 0_2^+ in even oxygens)
  - or invent a density with a particular symmetry

Conclusion: A lot more to explore...

- IMSRG is a convergence accelerator!
- Development in progress to improve NCSM calculations
  - apply to open-shell nuclei, excited states, transition operators
  - e.g. push the mass range for super-allowed decays
- Try different IM-improved combinations
  - target intruder states or particular symmetries
  - IM-NCSMC
  - IM-GCM-SA-NCSM
- Uncertainty quantification
  - increase eMax, optimize $\hbar\Omega$
  - reference state dependence
  - interaction dependence
  - vary IMSRG generators