Explorations with the In-Medium No-Core Shell Model

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The Facility for Rare Isotope Beams
at Michigan State University

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- R. Roth, E. Gebrerufael, K. Vobig, T. Mongelli, C. Wenz

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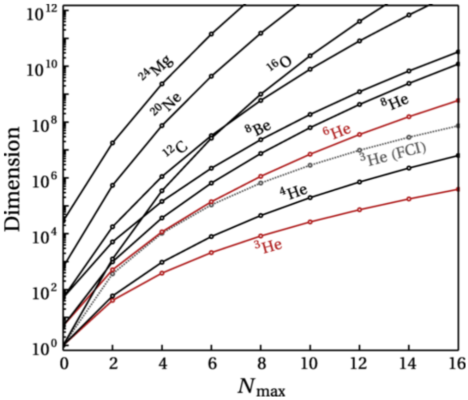
- DOE Collaboration: Nuclear Theory for New Physics (NTNP)

Outline

- IMSRG-Improved Methods
  - In-Medium No-Core Shell Model (IMNCSM)
- Preliminary Results
- Open questions and speculations

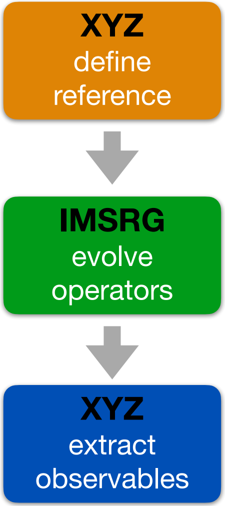
Motivation

- The NCSM requires an expansion over a huge basis
- Can we tune the basis (with IMSRG) to reduce the size required?



Fasano (2022)

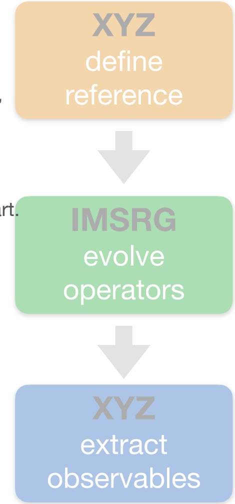
IMSRG-Improved Methods



* mean field or **explicitly correlated**

IMSRG-Improved Methods

- IMSRG for closed and open-shell nuclei: IM-HF and IM-PHFB
  - HH, Phys. Scripta, Phys. Scripta 92, 023002 (2017)
  - HH, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tuskiyama, Phys. Rept. 621, 165 (2016)
- Valence-Space IMSRG (VS-IMSRG)
  - S. R. Stroberg, HH, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci. **69**, 165
- In-Medium No Core Shell Model (IM-NCSM)
  - E. Gebrerufael, K. Vobig, HH, R. Roth, PRL **118**, 152503
- In-Medium Generator Coordinate Method (IM-GCM)
  - J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, HH PRC 98, 054311 (2018)
  - J. M. Yao et al., PRL 124, 232501 (2020)



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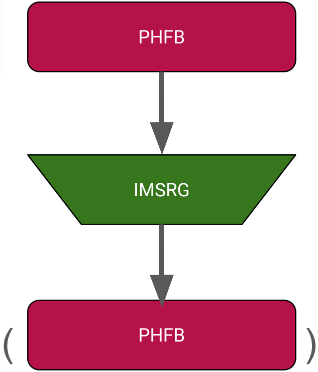

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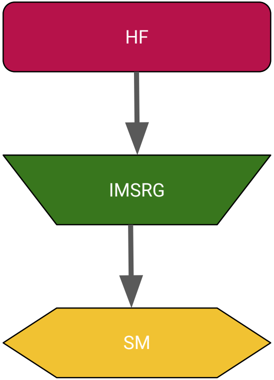

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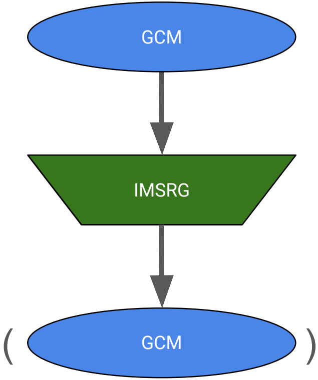

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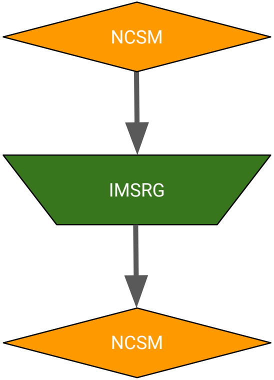

- In-Medium No Core Shell Model (IM-NCSM)
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IMSRG-Improved Methods

- 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 $\langle\Psi| \tilde{A} |\Psi\rangle = 0$

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

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

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

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

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

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

IMSRG-Improved Methods

- Choose/find a reference state
- Normal-Order the Hamiltonian with respect to that reference
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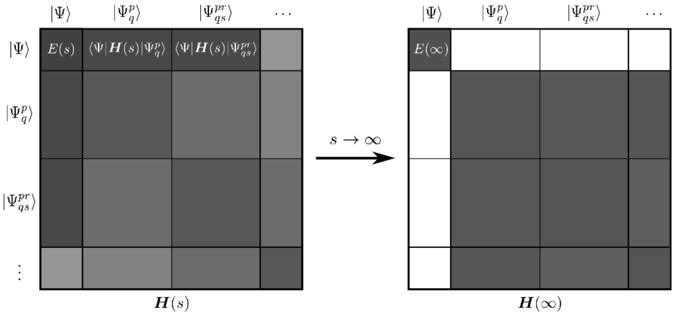
IMSRG: In-Medium Similarity Renormalization Group

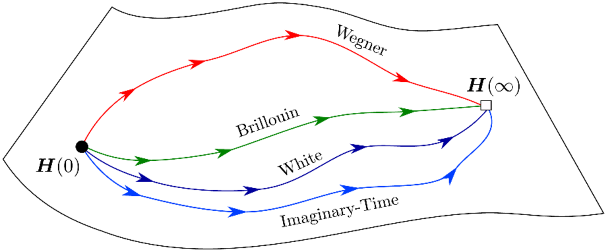


- continuous unitary transformation
- solve flow equation: $\frac{d}{ds}H(s) = [\eta(s), H(s)]$

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

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De-Normal-Ordering

Reconstruct a Vacuum Normal-Ordered Hamiltonian

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

No-Core Shell Model (NCSM)

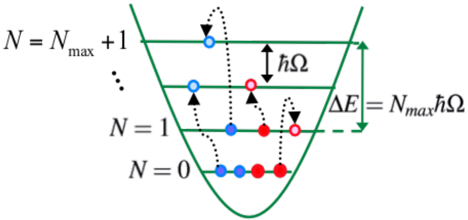
Find eigenstates of the A-body nuclear Hamiltonian:

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

Expand in anti-symmetrized products of harmonic oscillator single-particle states:

$$\left|\Psi_k\right\rangle = \sum_{N=0}^{N_{\text{max}}} \sum_j c_{Nj}^k \left|\Phi_{Nj}\right\rangle$$

Converge to an exact solution as $N_{\text{max}} \to \infty$



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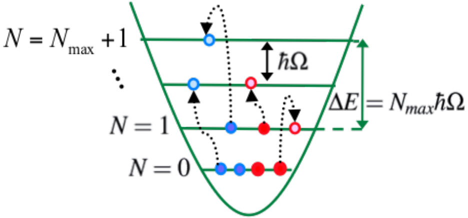


Disadvantage:

Basis size grows **factorially** with N_{max} and A!

IMNCSM: The best of both

IMSRG

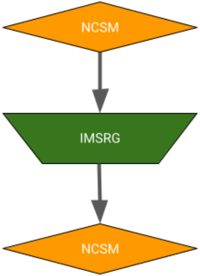
- polynomial-scaling with A
- NO2B approximation
- IM-SRG(2) approximation

NCSM

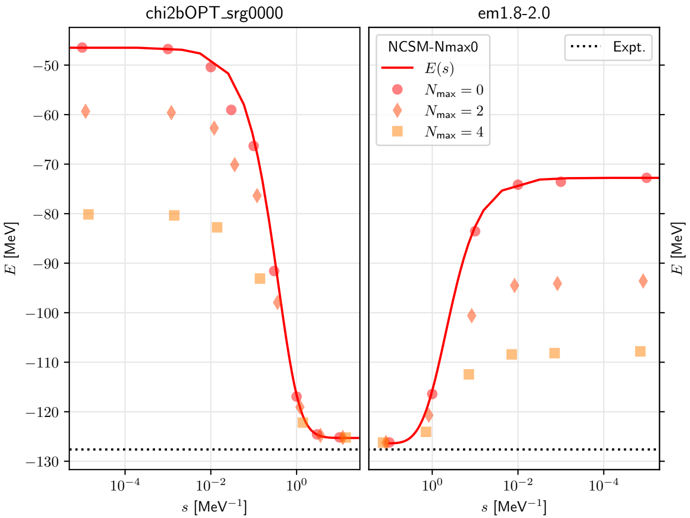
- easy access to spectroscopy
- no restrictions to even nuclei

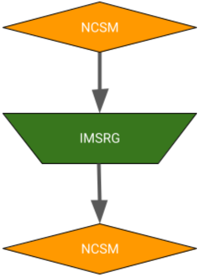
IMNCSM

- 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



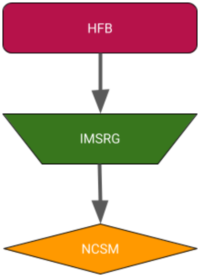
^{16}O: Ground States

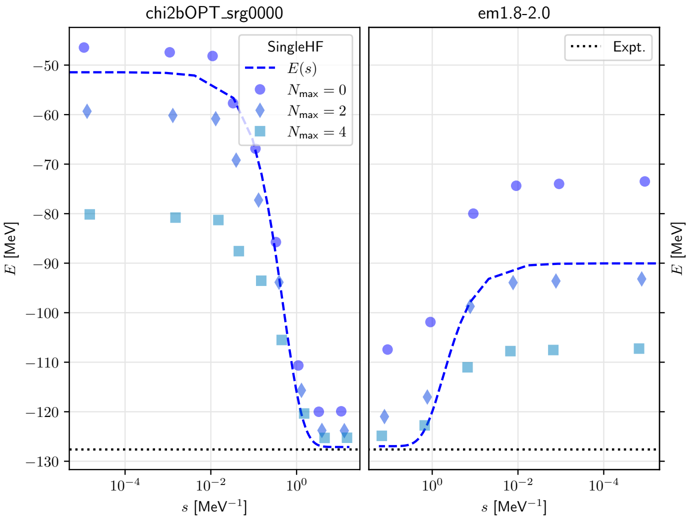




Eta: White
e_{max} = 8
$\hbar\Omega$ = 20MeV

^{16}O: Ground States





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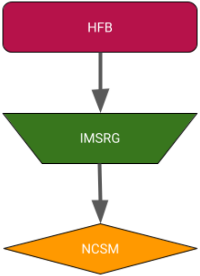
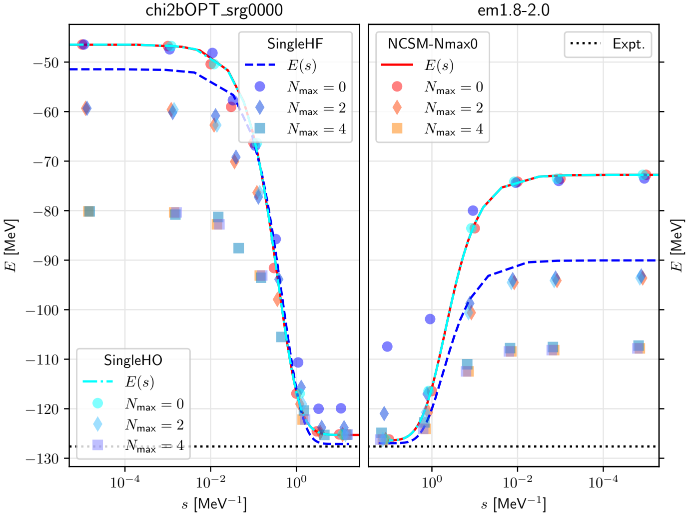
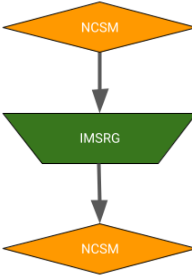
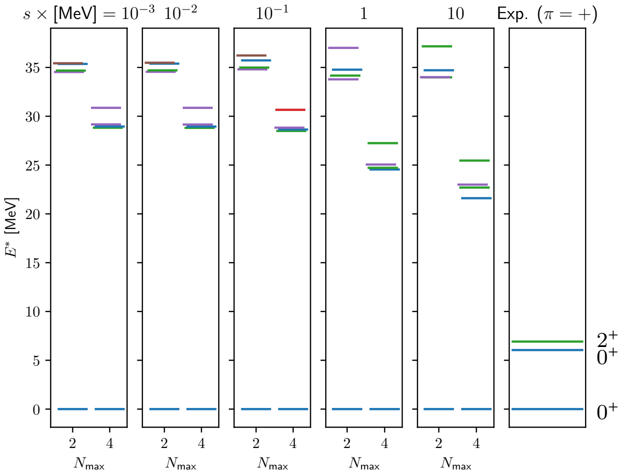






Eta: White
e_{max} = 8
$\hbar\Omega$ = 20MeV

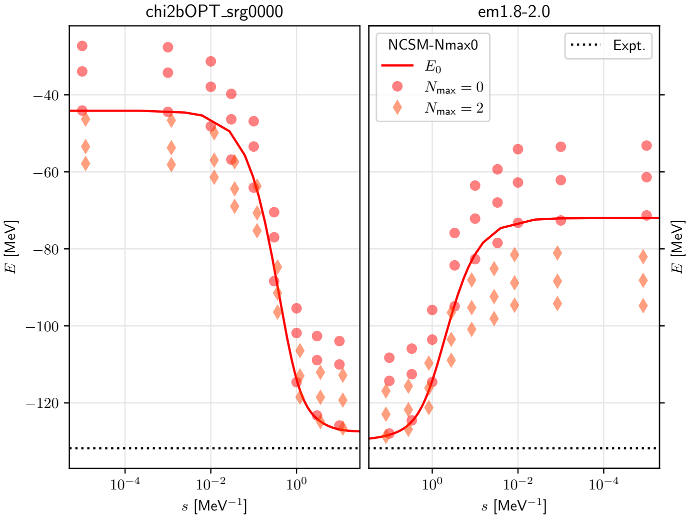
^{16}O: Excited States (NCSM $N_{\text{max}}^{\text{ref}} = 0$ Reference)



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

Odd-A: ^{17}O

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



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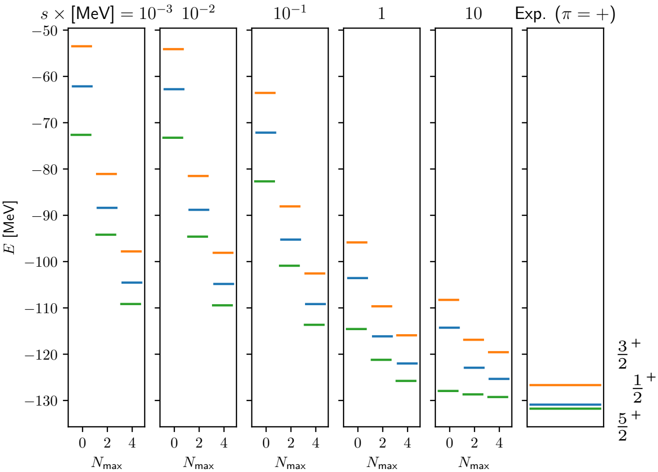

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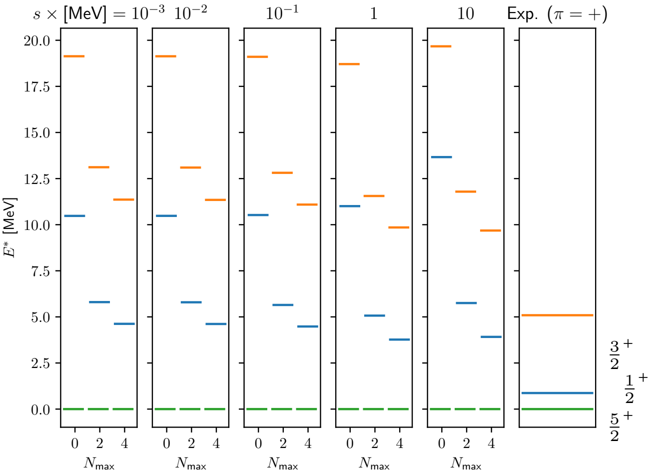

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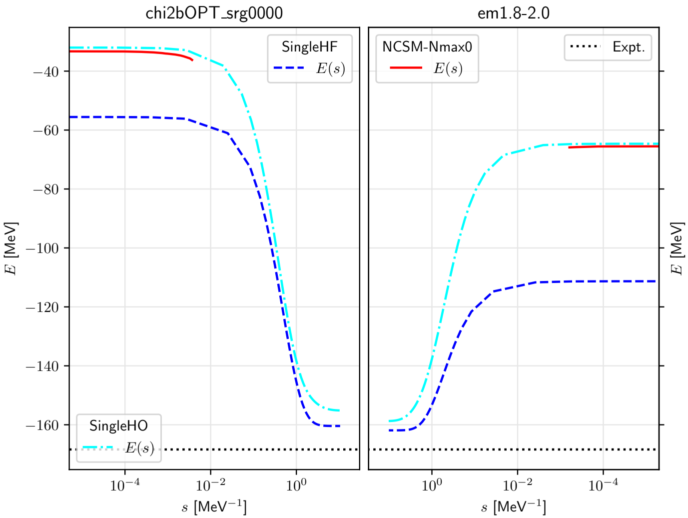
Work in Progress: ^{24}O



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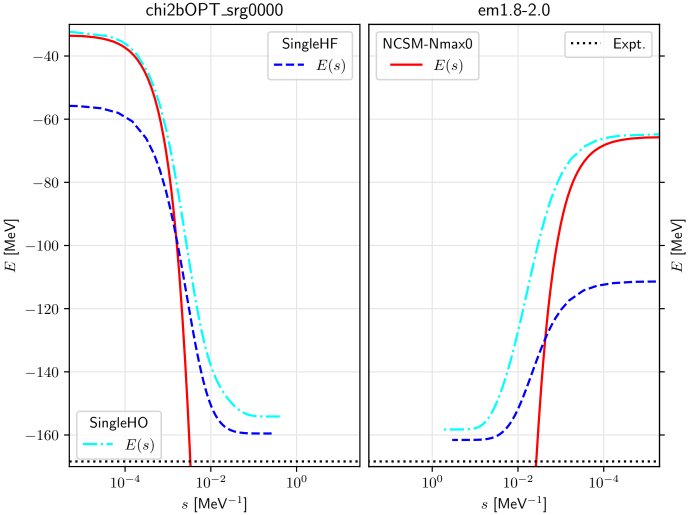
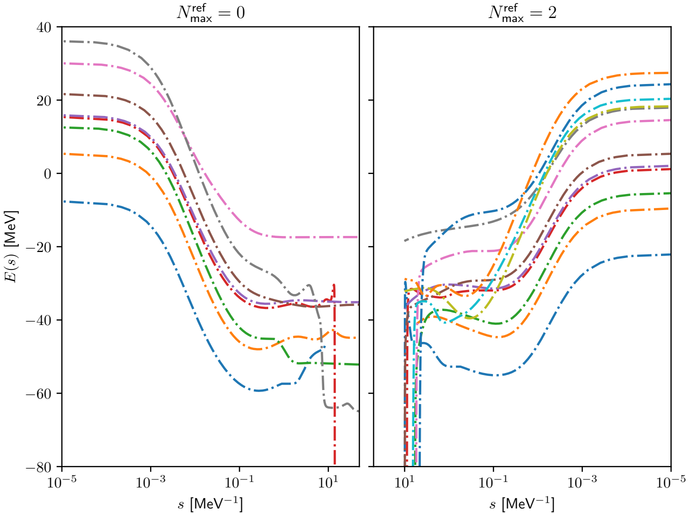


Eta: ImTime
e_{max} = 8
$\hbar\Omega$ = 20MeV

Work in Progress: ^{24}O

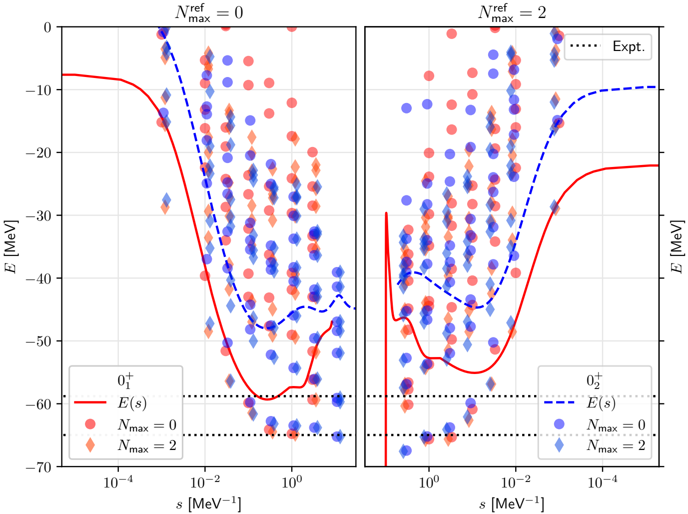
- Stalling or blow-up in the flow for some references
  - Can we catch and treat level crossings that switch the sign of η?
  - Can we optimize the ODE solver? (Adaptively relax/tighten constraints)
- Does missing $\lambda^{(3)}$ introduce instability into flow equations?
  - Can we reconstruct/approximate it from $\lambda^{(1)}$ and $\lambda^{(2)}$?

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



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

^{10}Be: 0^+ States from $N_{\text{max}}^{\text{ref}} = 0$ 0^+ References



Int: chi2bOPT
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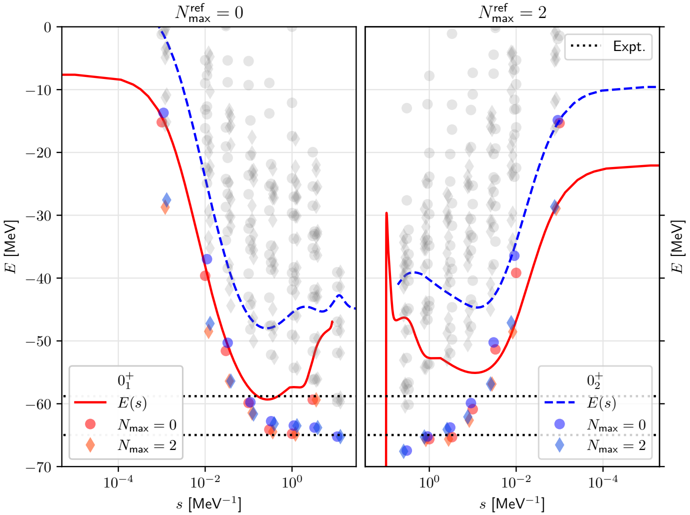

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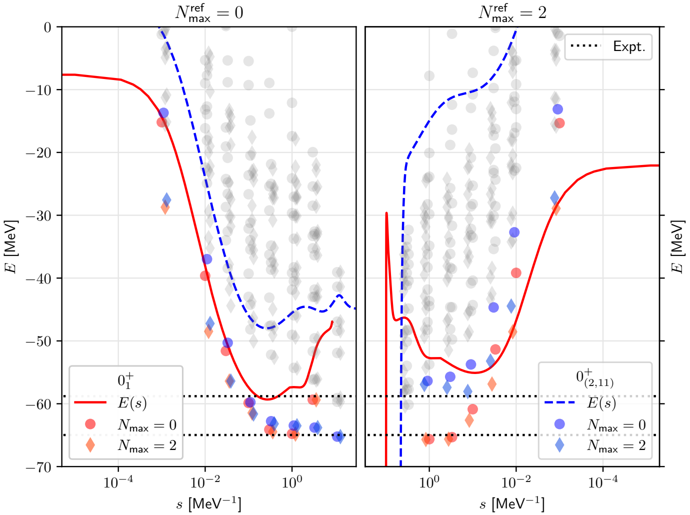


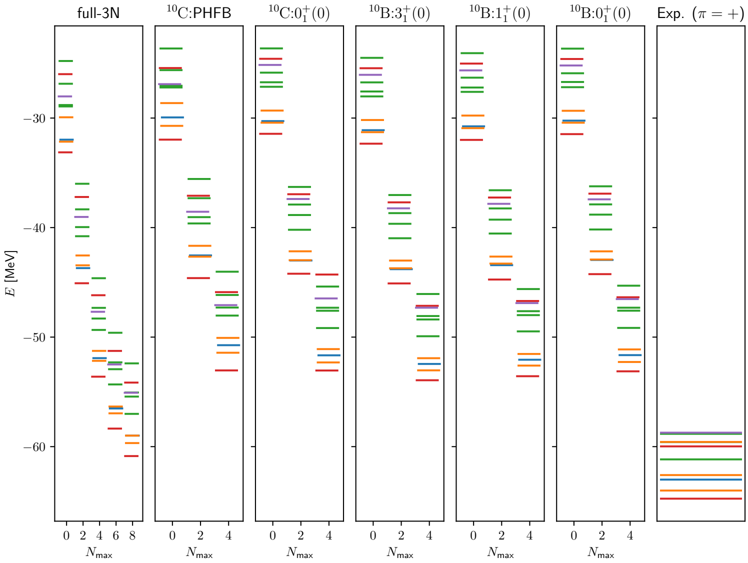
Int: chi2bOPT
Eta: ImTime
$e_{\text{max}} = 8$
$\hbar\Omega = 20\text{MeV}$

Super-Allowed Beta-Decays ($0^+ \rightarrow 0^+$)

Motivation:

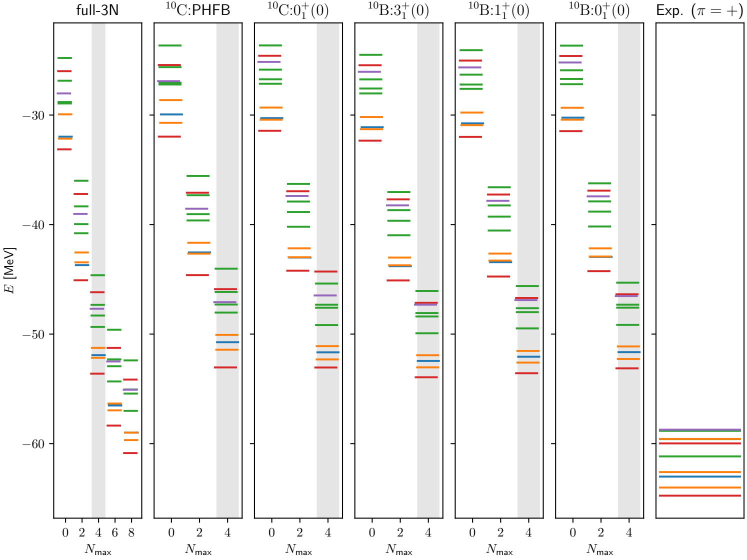
- enable extraction of V_{ud} from Fermi transition matrix elements
  - talk by M. Gennari (Tues)
- corrections depend on the full spectrum (intermediate states)
- most candidates at masses beyond the reach of NCSM (^{22}Mg, ^{26}Al, etc)

^{10}B: NCSM with NO2B interactions



Int: n4lo500-3NlnlE7
e_{max} = 6
$\hbar\Omega$ = 18MeV

^{10}B: NCSM with NO2B interactions



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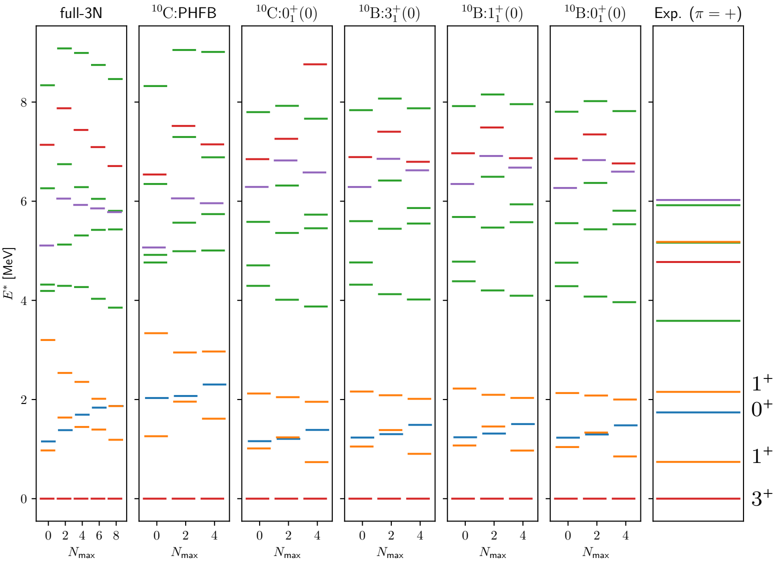
^{10}B: NCSM with NO2B interactions



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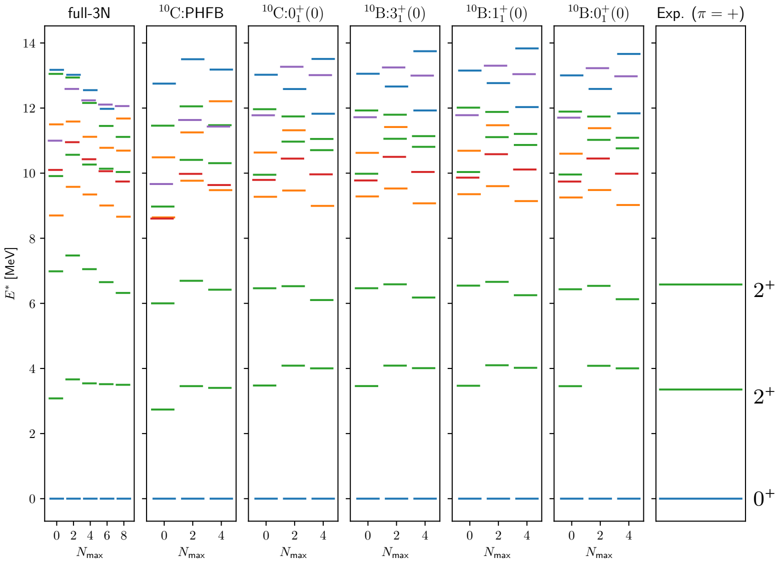
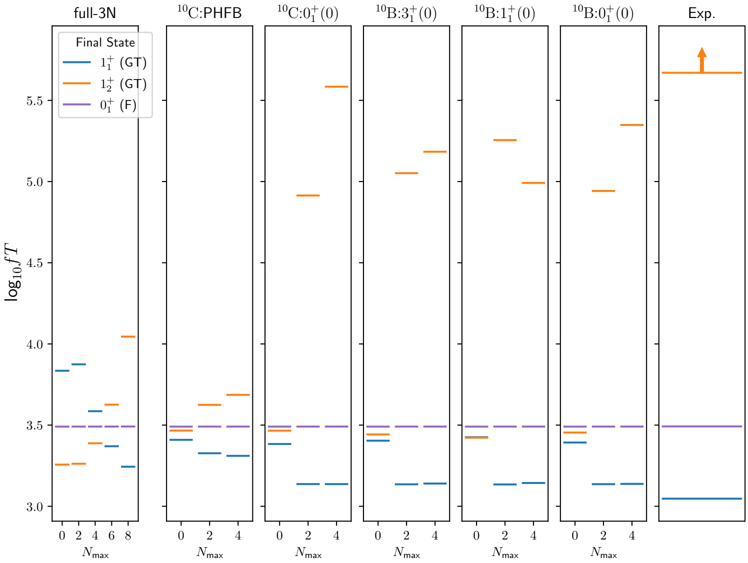
^{10}C: NCSM with NO2B interactions



Int: n4lo500-3NlnlE7
e_{max} = 6
$\hbar\Omega$ = 18MeV

$^{10}C(0^+) \to {}^{10}B$ with NO2B interactions



Int: n4lo500-3NlnlE7
$e_{\text{max}} = 6$
$\hbar\Omega = 18$MeV

$^{10}C \to {}^{10}B$

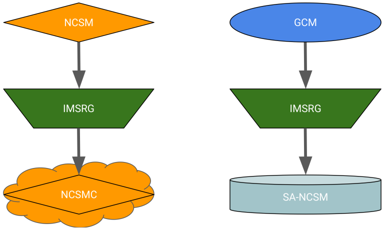
- Normal-ordering alone seems to improve mixing of 1^+ states
  - with some computational cost savings
- But IM-SRG flow stalls - requires treating of level crossings and/or $\lambda^{(3)}$ reconstruction

Open Questions

- What determines the evolution stopping criteria?
  - plateau in $E(s)$?
- Can we achieve convergence with respect to variation of reference state?
  - increase eMax? optimize $\hbar\Omega$?
- Instability and stalling during the flow
  - Can we catch and treat level crossings?
- Can we target experimentally known states by choosing the right reference states?
  - select the right low-Nmax precursor state or invent a density with a particular symmetry

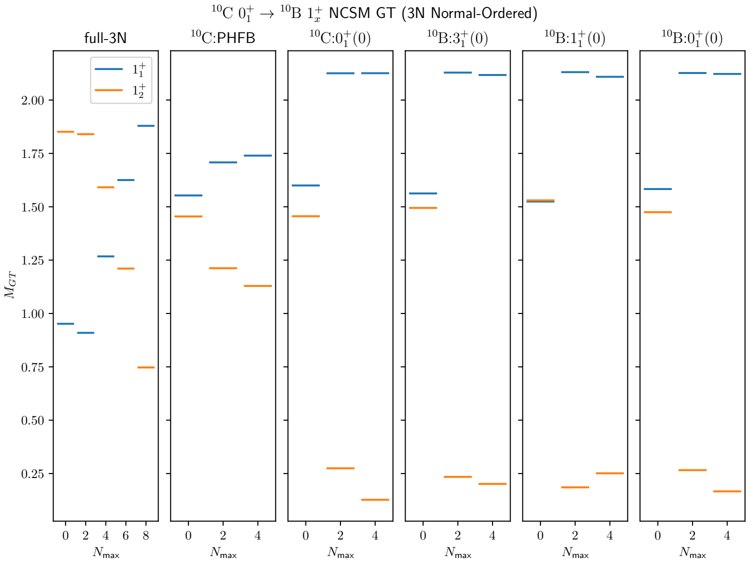
Conclusion: A lot more to explore...

- 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
  - reference state dependence
  - interaction dependence
  - IMSRG generators and evolution parameter



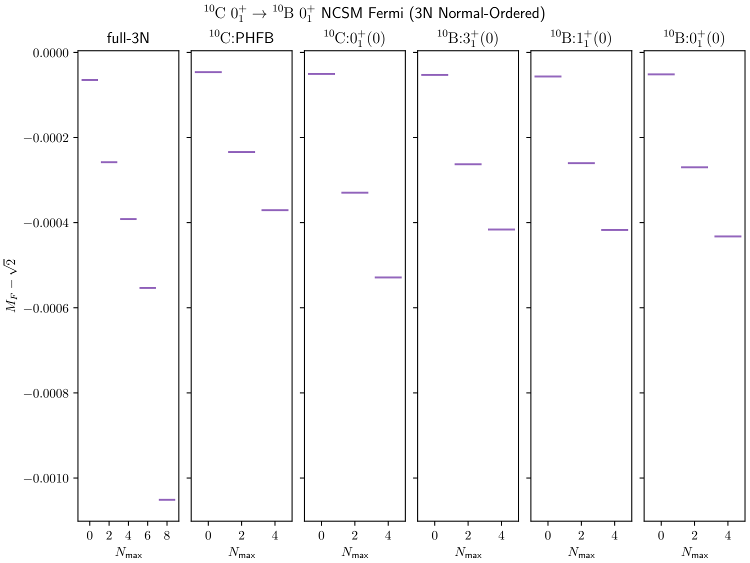
Backup Slides

$^{10}C \to {}^{10}B$ with NO2B interactions



Int: n4lo500-3NlnlE7
e_{max} = 6
$\hbar\Omega$ = 18MeV

$^{10}C \to {}^{10}B$ with NO2B interactions



Int: n4lo500-3NlnlE7
e_{max} = 6
$\hbar\Omega$ = 18MeV