Ab Initio Electromagnetic Transitions with the IMSRG

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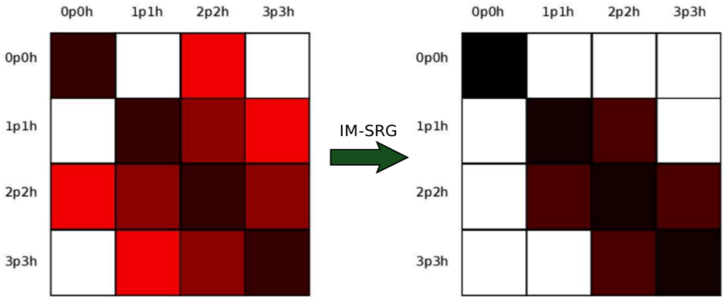
IMSRG

IMSRG rotates the Hamiltonian into a coordinate system where simple methods (e.g. Hartree-Fock) are approximately exact:

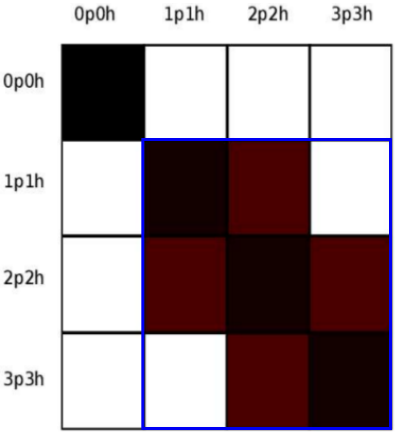
$$\bar{H}(s) = U(s) H U^{\dagger}(s)$$

$\bar{H}(0)$ "Bare" Hamiltonian $\qquad$ $\bar{H}(\infty)$ "Dressed" Hamiltonian



Approaches for Excited States

- Additional processing needed for excited states.
- GS-decoupling has softened couplings between excitation rank.
- Equations-of-motion: Approximately diagonalize excitation block.



Equations-of-Motion IMSRG

- EOM-IMSRG equation, in terms of evolved operators:

$$[\bar{H}(s), \bar{X}_\nu^\dagger(s)]|\Phi_0\rangle = \omega_\nu \bar{X}_\nu^\dagger(s)|\Phi_0\rangle$$

- IMSRG: No correlations between ground and excited states.

$$\bar{X}_\nu^\dagger = \sum_{ph} \bar{x}_h^p a_p^\dagger a_h + \frac{1}{4} \sum_{pp'hh'} \bar{x}_{hh'}^{pp'} a_p^\dagger a_{p'}^\dagger a_{h'} a_h$$

Truncation to two-body ladder operators: EOM-IMSRG(2,2).

Effective Operators in the IMSRG

IMSRG unitary transformation can be explicitly constructed:

$$U(s) = e^{\Omega(s)}$$

IMSRG via Magnus expansion:

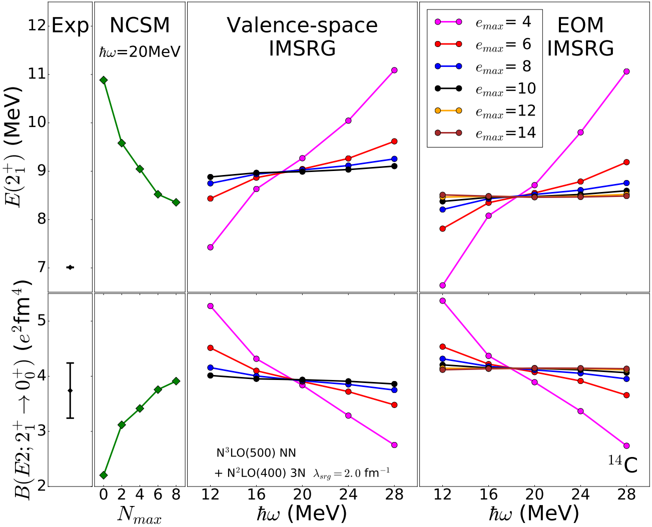
$$\frac{d\Omega}{ds} = \eta + [\Omega, \eta] - \frac{1}{2}[\Omega, [\Omega, \eta]] + \cdots$$

Effective operators from Baker-Campbell-Hausdorff:

$$\bar{O}(s) = O + [\Omega, O] + \frac{1}{2}[\Omega, [\Omega, O]] + \cdots$$

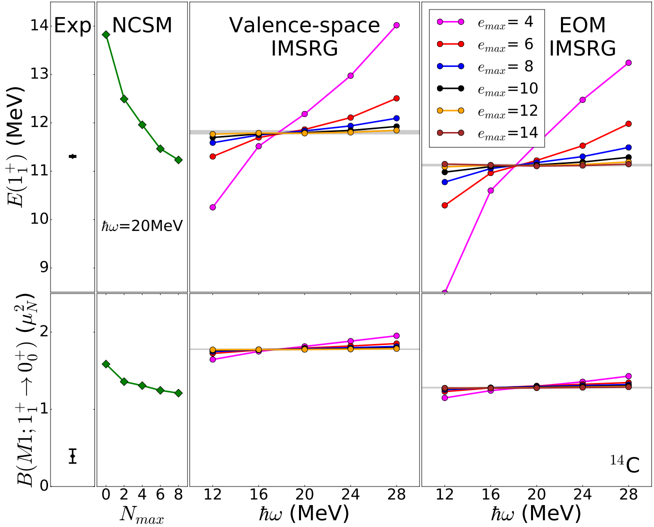
T. Morris, N. Parzuchowski, S. Bogner, Phys. Rev. C **92**, 034331 (2015).

Electromagnetic Observables: ^{14}C



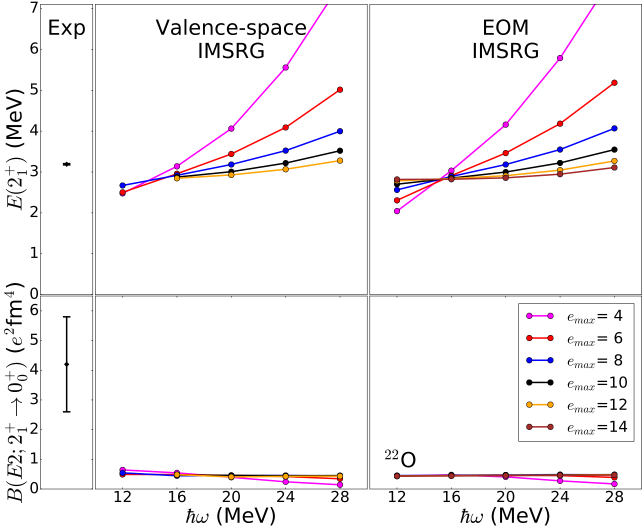
PRELIMINARY Exp: Pritychenko et. al., Nucl. Data Tables **107**, 1 (2016).

Electromagnetic Observables: ^{14}C



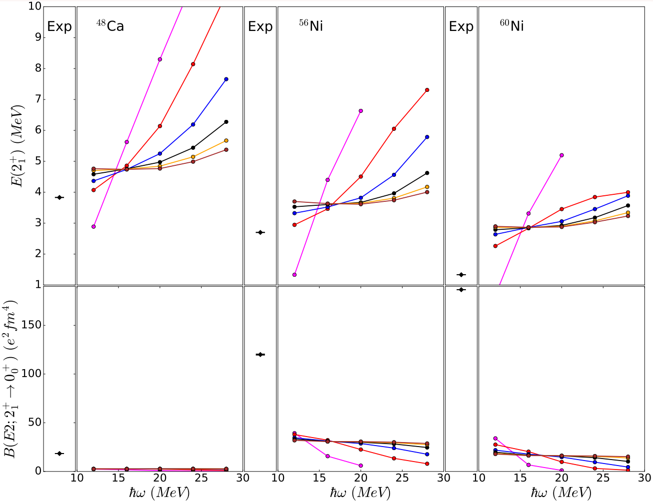
PRELIMINARY Exp: Ajzenberg-Selove, Nuc. Phys. A **1523**, 1 (1991).

Electromagnetic Observables: ^{22}O



PRELIMINARY Exp: Pritychenko et. al., Nucl. Data Tables **107**, 1 (2016).

Electromagnetic Observables: ^{48}Ca, ^{56,60}Ni



PRELIMINARY Exp: Pritychenko et. al., Nucl. Data Tables **107**, 1 (2016).

Perturbative Triples Correction: EOM-IMSRG({3},2)

EOM-IMSRG({3},2): $\mathcal{O}(N^7)$:

$$\bar{X}_\nu^\dagger = X_{1p1h} + X_{2p2h}$$

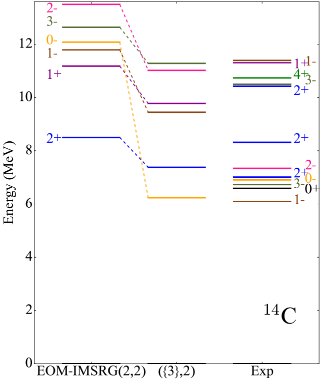
$$\delta E_\nu = \sum_{\substack{ijk\\abc}} \frac{|\langle \Phi_{ijk}^{abc} | \bar{H} \bar{X}_\nu^\dagger | \Phi_0 \rangle|^2}{\omega_\nu^{(0)} - \langle \Phi_{ijk}^{abc} | \bar{H} | \Phi_{ijk}^{abc} \rangle}$$

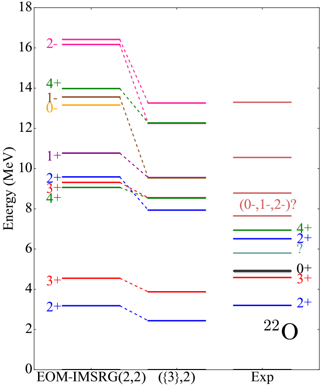
N. Parzuchowski, T. Morris, S. Bogner, arXiv:1611.00661

EOM-IMSRG({3},2) for ^{14}C, ^{22}O

E.M. N^{3}LO(500) + Navratil N^{2}LO 3N(400) λ=2.0 fm^{-1}

$e_{max} = 8$ $\hbar\omega = 20$ MeV





PRELIMINARY Exp: NNDC ENDSF

Summary/Outlook

- Spectra and observables are now available with EOM- and VS-IMSRG
  - Results are consistent with NCSM.
  - E2 strengths consistently under-predicted (except ^{14}C).
- Moving Forward...
  - EOM-IMSRG is systematically improvable, perturbative corrections are possible.
  - Next: multi-reference-EOM-IMSRG (Heiko's talk) for static correlations and open shells.

Thank you!

IMSRG at MSU:
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Jason Holt

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Gaute Hagen

NSCL

MICHIGAN STATE UNIVERSITY

Equations-of-Motion (EOM) Methods for Excited States

Define a ladder operator $X_\nu^\dagger$ such that:

$$|\Psi_\nu\rangle = X_\nu^\dagger|\Psi_0\rangle$$

Eigenvalue problem re-written in terms of $X^\dagger$:

$$\hat{H}|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle \rightarrow [H, X_\nu^\dagger]|\Psi_0\rangle = (E_\nu - E_0)X_\nu^\dagger|\Psi_0\rangle$$

Approximations are made for $X_\nu^\dagger$, $|\Psi_0\rangle$.

$$RPA: \quad |\Psi_0\rangle \approx |\Phi_{HF}\rangle \qquad X_\nu^\dagger = \sum_{ph}[x_h^p a_p^\dagger a_h + y_h^p a_h^\dagger a_p]$$

Method Comparison in 2D Quantum Dots

Method	RMS Error
(2,2)	0.095
({3},2)-MP	0.066
({3},2)-EN	0.031

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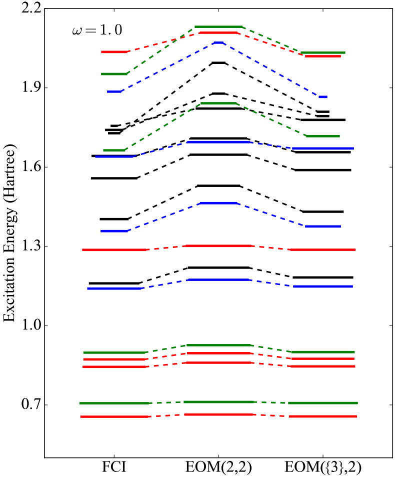


Solving the IM-SRG equations

$$\frac{d\bar{H}}{ds} = [\eta(s), \bar{H}(s)] \qquad \eta(s) \propto \bar{H}^{OD}(s)$$

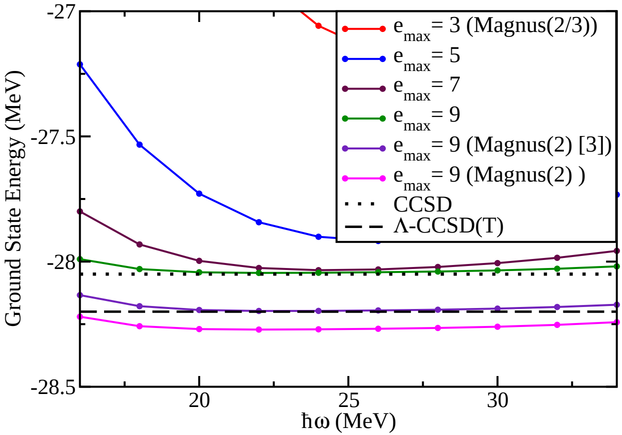
- Transform operators via flow equation.
  - requires very precise ODE solver
  - small step sizes in s needed for convergence
- Construct the unitary transformation explicitly.
  - Magnus expansion

$$U(s) = e^{-\Omega(s)}$$

$$\frac{d\Omega}{ds} = \eta(s) - \frac{1}{2}[\Omega(s), \eta(s)] + \frac{1}{12}[\Omega(s), [\Omega(s), \eta(s)]] + \ldots$$

  - less precision needed, larger step sizes

Corrections to IM-SRG(2) with ^{4}He



CC results: G. Hagen et. al., PRC **82** 034330 (2010).

Center of Mass Treatment

$$H_{cm} = T_{cm} + \frac{1}{2} m A \Omega^2 R_{cm}^2 - \frac{3}{2}\hbar\Omega$$

H_{cm} is evolved as an effective operator in IM-SRG:

$$\frac{dH_{cm}(s)}{ds} = [\eta(s), H_{cm}(s)]$$

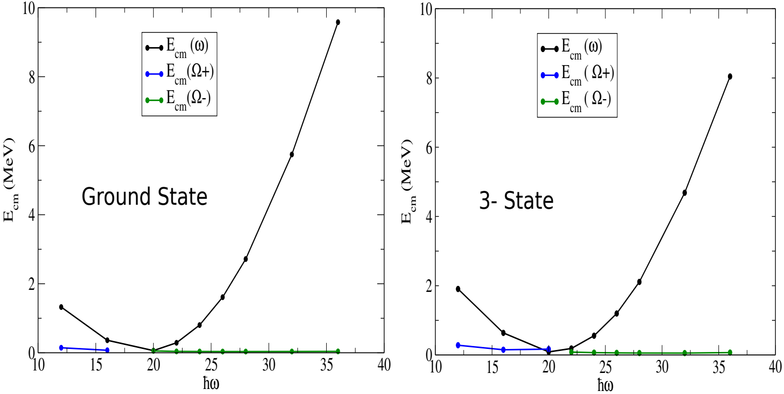
CoM frequency Ω calculated in the manner of Hagen et. al.

$$\hbar\Omega = \hbar\omega + \frac{2}{3}E_{cm}(\omega, s) \pm \sqrt{\frac{4}{9}(E_{cm}(\omega, s))^2 + \frac{4}{3}\hbar\omega E_{cm}(\omega, s)}$$

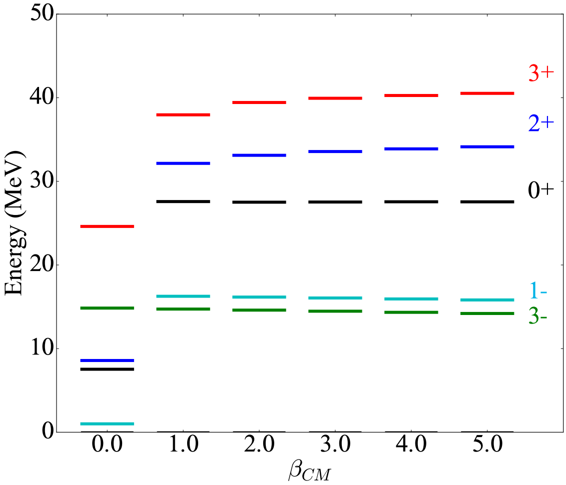
G. Hagen, T. Papenbrock, and D. J. Dean,
Phys. Rev. Lett. 103, 062503 (2009).

CoM diagnostic for ^{16}O 3- state

E.M. N3LO Λ=500 NN at λ_{SRG}=2.0 fm^{-1}



Lawson CoM Treatment: $H = H_{int} + \beta_{CM} H_{CM}(\Omega)$



Lawson for ^{14}C