Resurrecting Forgotten Many-Body Methods with Unitary Transformations

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Ab Initio Methods in Nuclear Physics

- *Ab initio*: from the beginning.
- Nucleons and pions are fundamental degrees of freedom.
- All nucleons treated as active.
- Solve many-body Schrödinger equation with realistic forces.

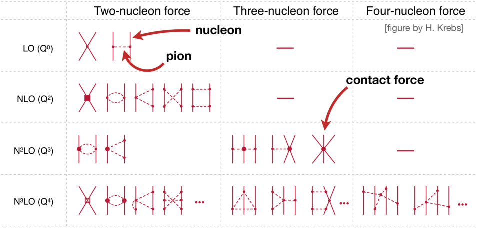
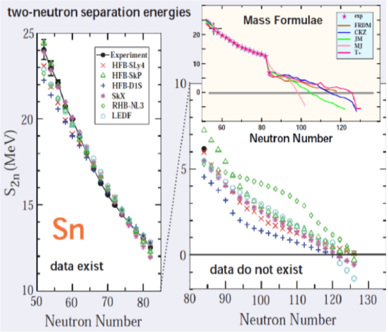
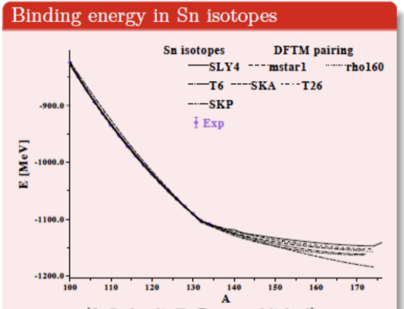


Figure: H. Hergert

Why Ab Initio? Limits of Nuclear Existence

Limited predictive power of phenomenology
(e.g. Shell Model, Skyrme...)





[J. Sadoudi, T. D., unpublished]

Why Ab Initio? Neutrinoless Double Beta Decay

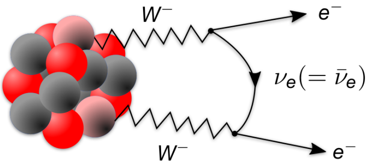


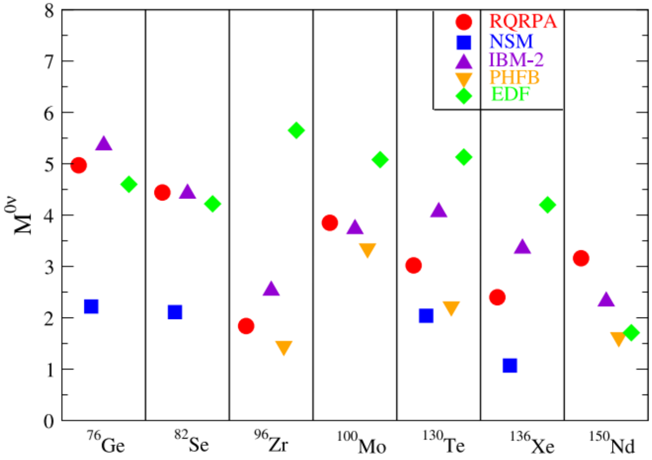
Figure: H. Hergert

- Beyond standard model physics?
- Neutrino mass scale?
- Relevant structure quantity: nuclear matrix element.

$$|m_{\beta\beta}|^2 \propto \frac{1}{|M_{0\nu\beta\beta}|^2}$$

Why Ab Initio? Neutrinoless Double Beta Decay

There is a need for a consistent effective operator formalism...



Engel, J. 2015 J. Phys. G: Nucl. Part. Phys. 42 034017

Ab Initio Progress in Nuclear Physics

Ab initio: from the beginning.

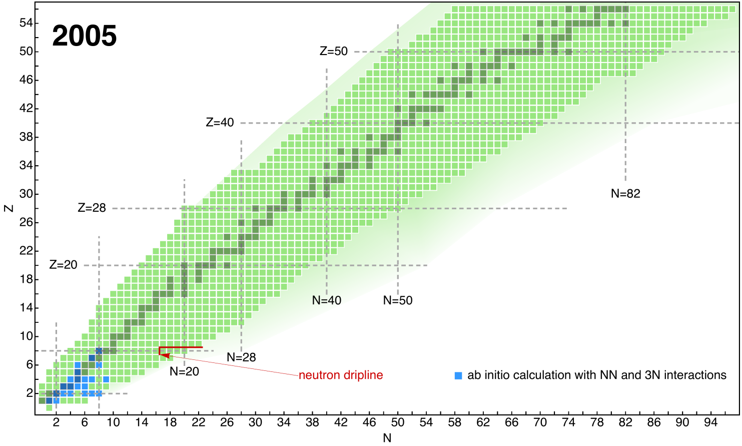


Figure: H. Hergert

Ab Initio Progress in Nuclear Physics

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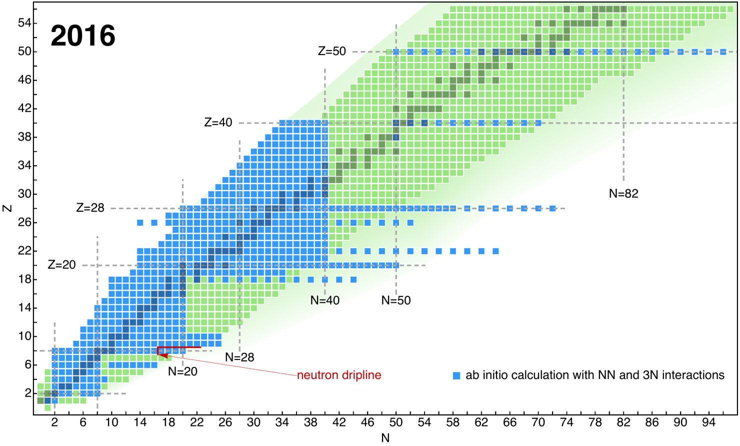

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Ab Initio Progress in Nuclear Physics

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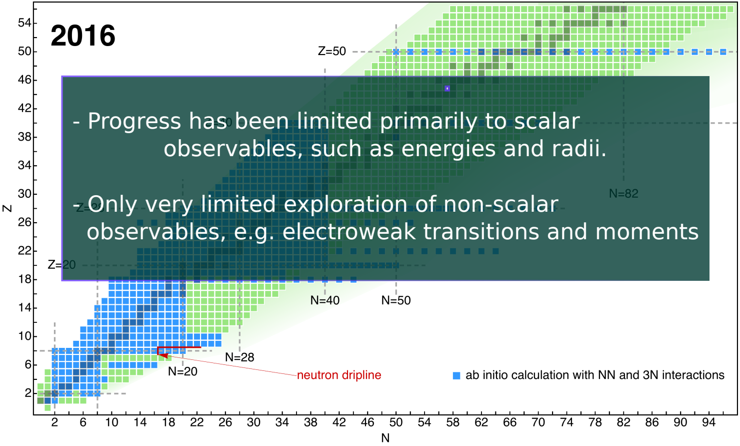
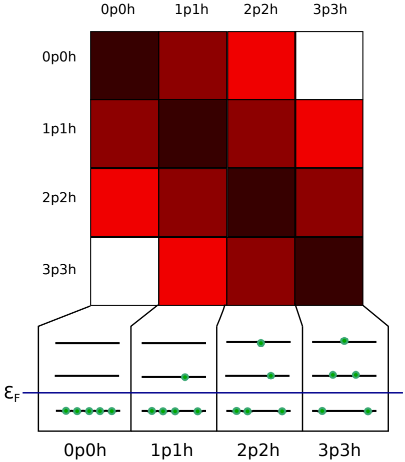


- Progress has been limited primarily to scalar observables, such as energies and radii.
- Only very limited exploration of non-scalar observables, e.g. electroweak transitions and moments

Figure: H. Hergert

Exact Calculations: Constructing the Many-Body Basis



- 0p0h – "reference state"

$$|\Phi_0\rangle \,.$$

- 1p1h – "singly-excited" state

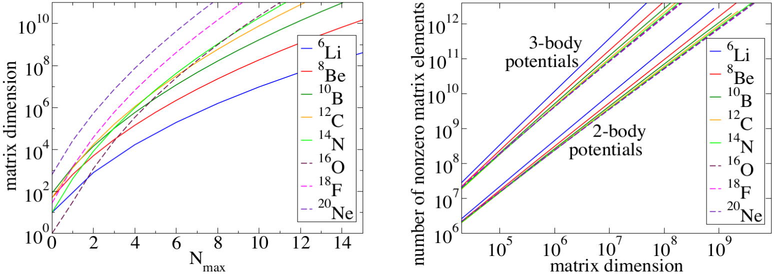
$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle \,.$$

- 2p2h – "doubly-excited"

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle \,.$$

- Completeness: up to ApAh.

Limitations of Exact Methods



from: C. Yang, H. M. Aktulga, P. Maris, E. Ng, J. Vary, Proceedings of NTSE-2013

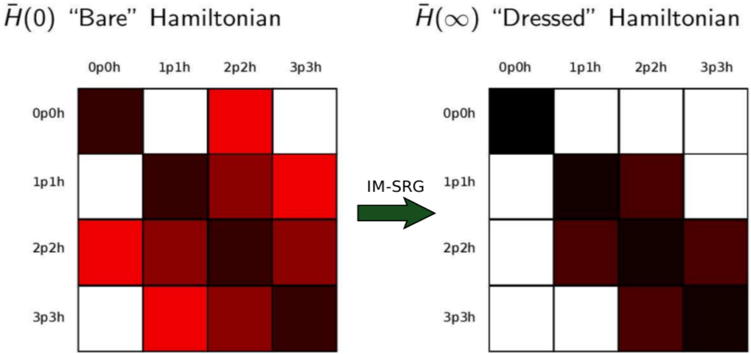
Storage of the full interaction is impossible. How to proceed?

IMSRG

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

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

K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011).



Similarity Renormalization Group (SRG)

- Apply a continuous unitary transformation.

$$\frac{d}{ds}[U^\dagger(s)HU(s)] \equiv \frac{d\bar{H}}{ds} = [\eta(s), \bar{H}(s)]$$

- η is the anti-Hermitian generator of the transformation.

$$\eta(s) \equiv \frac{dU}{ds}U^\dagger(s)$$

- Generator drives the Hamiltonian to a "diagonal" form:

$$\eta(s) = [H^d(s), H^{od}(s)]$$

- In general this is an A-body transformation.

S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001(R) (2007)

Normal Ordering to a Reference State

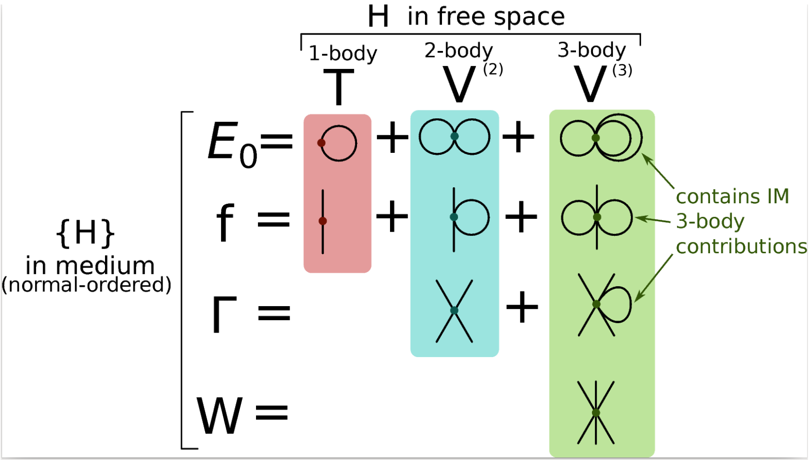


Figure: F. Yuan

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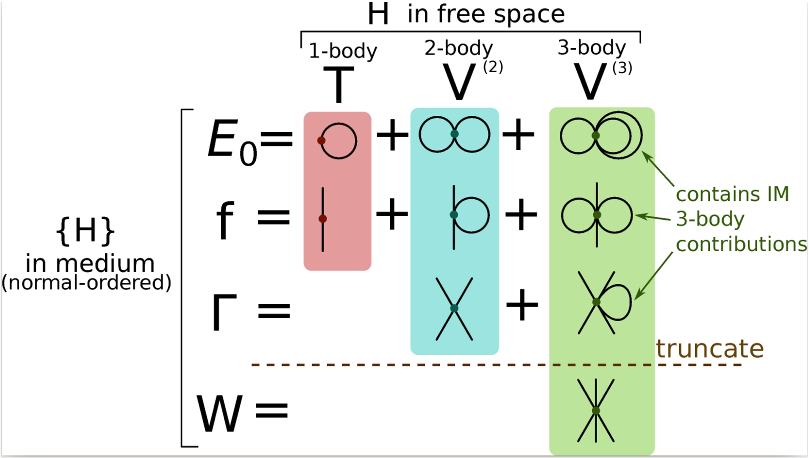
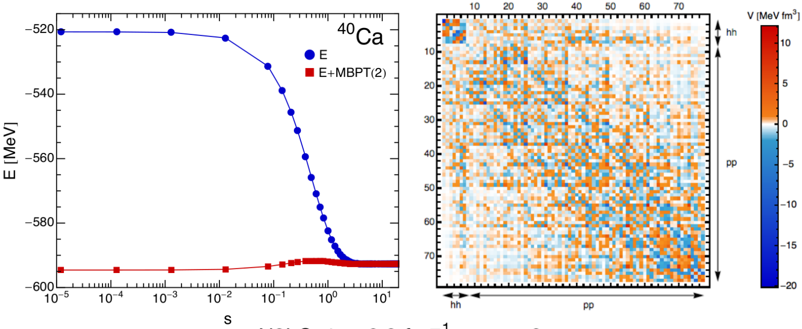


Figure: F. Yuan

IMSRG(2) Decoupling



N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

H. Hergert, *et. al.*, Phys. Rept., 621:165222, 2016.

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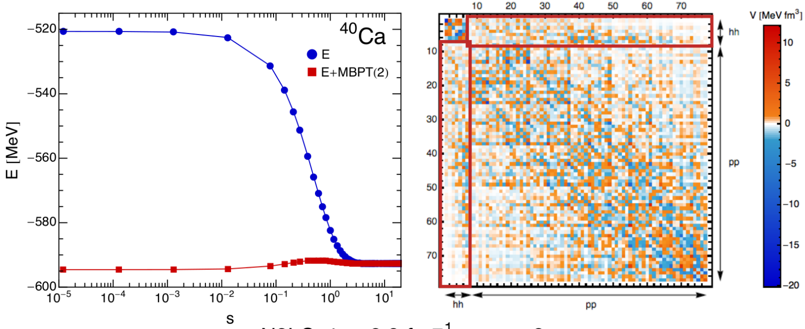

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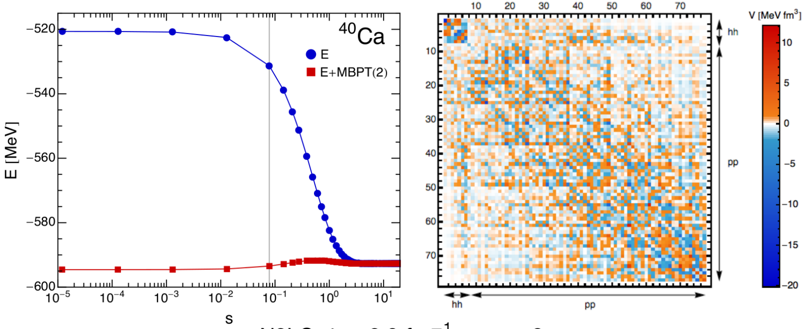

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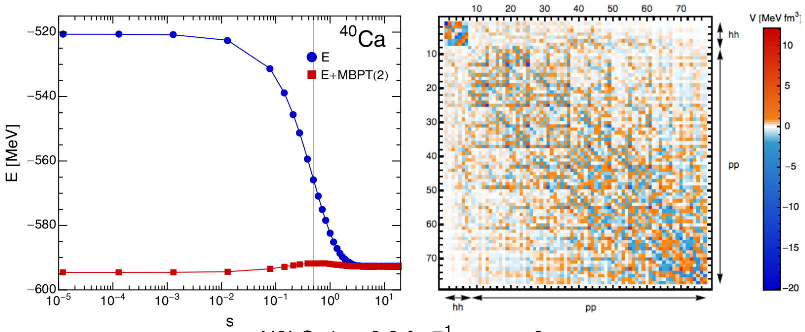

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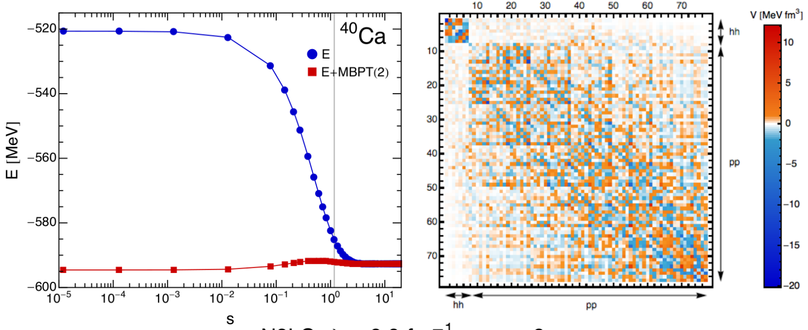

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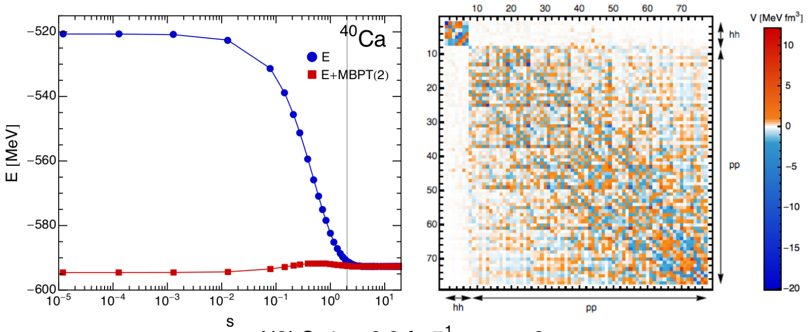

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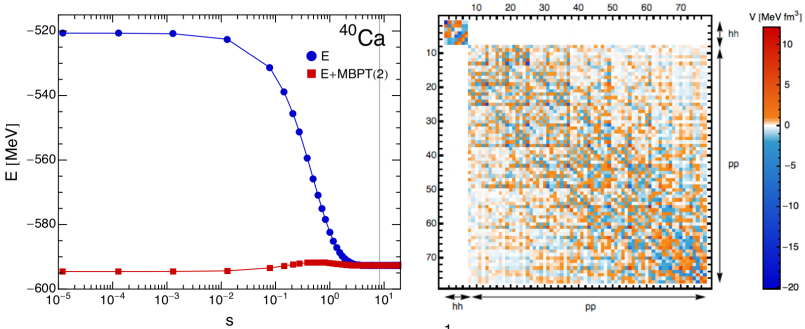
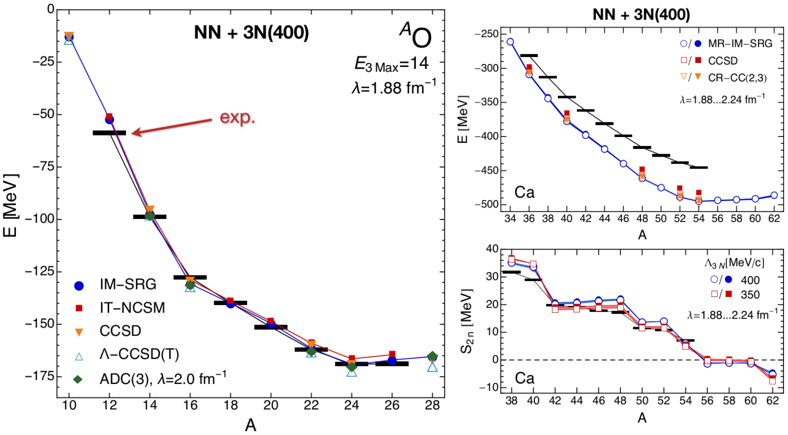


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

H. Hergert, *et. al.*, Phys. Rept., 621:165222, 2016.

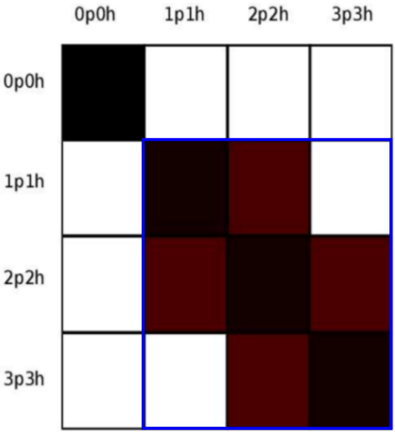
IMSRG Success with Ground States

HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)



Approaches for Excited States

- Describe excited states using ground-state-decoupled Hamiltonian?
- Couplings between excitation rank have been reduced.
- Can we approximately diagonalize the excitation block?



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 $X_\nu^\dagger$, $|\Psi_0\rangle$.

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

Equations-of-Motion IMSRG

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

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

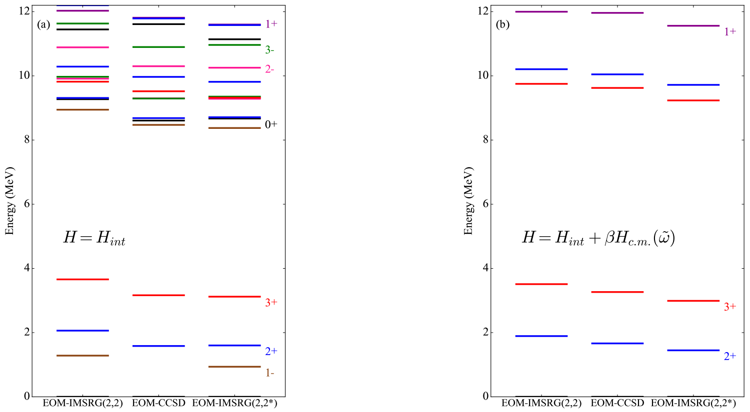
- IMSRG: No correlations between ground and excited states.

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

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

EOM-IMSRG vs. EOM-CCSD for ^{22}O

E.M. N3L0(500) λ=2.0 fm^{-1} NN only. $e_{max} = 11$ $\hbar\omega = 20$ MeV



Parzuchowski, Morris, and Bogner, Phys. Rev. C **95**, 044304 (2017)

Effective Operators in the IMSRG

IMSRG unitary transformation can be explicitly constructed:

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

The Magnus Expansion-IMSRG,

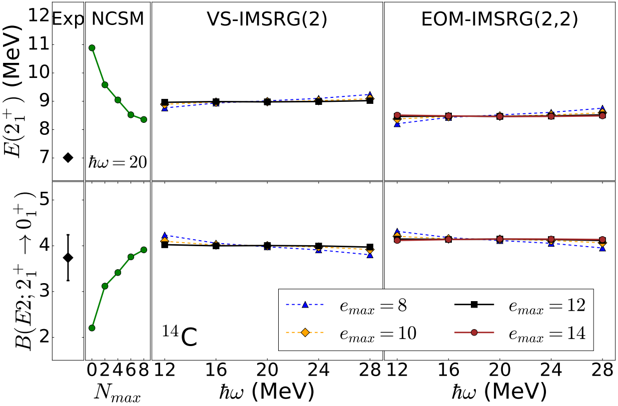
$$\frac{d\Omega}{ds} = \eta + [\Omega, \eta] - \frac{1}{2}[\Omega, [\Omega, \eta]] + \cdots$$

Effective operators from Baker-Campbell-Hausdorff:

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

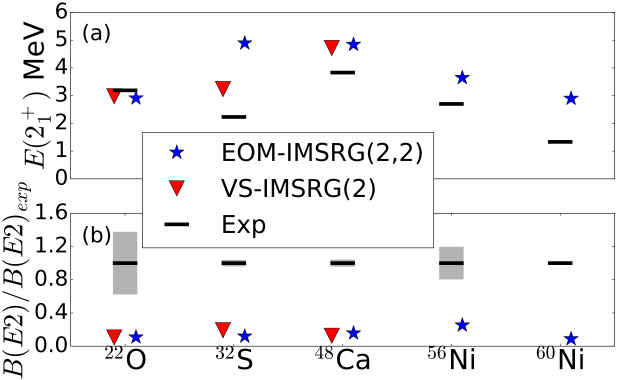
Morris, Parzuchowski, and Bogner, Phys. Rev. C **92**, 034331 (2015).

Electromagnetic Observables: ^{14}C



Parzuchowski, *et. al.*, Phys. Rev. C **96**, 034324 (2017).

Underestimated Quadrupole Transition Strengths



Parzuchowski, *et. al.*, Phys. Rev. C **96**, 034324 (2017).

Adding Static Correlation: General Reference States

- Single-ref methods: EOM-IMSRG, VS-IMSRG, Coupled Cluster...

  $$|\Phi\rangle = |\Phi_{HF}\rangle \,.$$

  Dynamic correlations built on top of one Slater determinant.

- Multireference methods: MR-IMSRG, config. interaction...

  $$|\Phi\rangle = \sum_{I \in \mathbf{R}} C_I |\Phi_I\rangle \,.$$

  Static correlations built into reference state.
  Dynamic correlations incorporated by many-body method.

Multireference IMSRG (MR-IMSRG)

- Generalized Wick's theorem defines contractions dependent on 1-,2-,...,A-body irreducible density matrices.

Kutzelnigg, Mukherjee J. Chem. Phys. **107**, 432 (1997). Hergert et. al. Phys. Rev. C **90**, 041302 (1997).

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- Particle-hole excitations are non-orthogonal,

$$\langle\Phi|\{a^\dagger_h a_p\}\{a^\dagger_{p'} a_{h'}\}|\Phi\rangle = \lambda_{hpp'h'} + \delta_{pp'}\lambda_{hh'} - \lambda_{hh'}\lambda_{pp'} \,.$$

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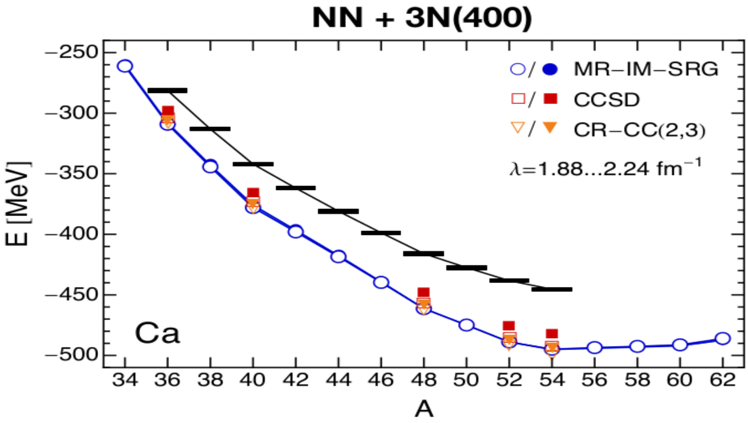
- Leads to near-singular systems of equations for CC theory, EOM methods.
- IMSRG flow equation not affected by additional spurious eigenvalues, which are far removed from the low-lying spectrum.

Kutzelnigg, Mukherjee J. Chem. Phys. **107**, 432 (1997). Hergert et. al. Phys. Rev. C **90**, 041302 (1997).

Benefits of Generalized Normal Ordering

HH et al., PRL **110**, 242501 (2013), ADC(3): A. Cipollone et al., PRL **111**, 242501 (2013)



How to do equations-of-motion?

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- Work-around: undo normal ordering.

$$H = E_0 + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j^\dagger a_l a_k\}$$

$$\to H = \tilde{E}_0^\rho + \sum_{ij} \tilde{T}_{ij}^\rho a_i^\dagger a_j + \frac{1}{4} \sum_{ijkl} \tilde{V}_{ijkl}^\rho a_i^\dagger a_j^\dagger a_l a_k$$

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- Next step: Multireference configuration interaction.

Multireference Configuration Interaction (MR-CI)

- Nucleus is described well by some general reference state

$$|\Phi\rangle = \sum_{I \in \mathbf{R}} C_I |\Phi_I\rangle \, .$$

Datta, Nooijen. J. Chem. Phys. **137**, 204107 (2012). Sherrill, Schaefer. Adv. Q. Chem. **34**, 143 (1999).

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Multireference Configuration Interaction (MR-CI)

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$$|\Phi\rangle = \sum_{I \in \mathbf{R}} C_I |\Phi_I\rangle \,.$$

- Disregard coefficients and focus on reference *space* **R**.
- Consider all particle-hole excitations from **R**:

MR-CIS:

$$|\Psi_\nu\rangle = \sum_{I \in \mathbf{R}} D_I |\Phi_I\rangle + \sum_{I \in \mathbf{R}} \sum_{ij} D_I^{ij} a_i^\dagger a_j |\Phi_I\rangle \,.$$

MR-CISD:

$$|\Psi_\nu\rangle = \sum_{I \in \mathbf{R}} D_I |\Phi_I\rangle + \sum_{I \in \mathbf{R}} \sum_{ij} D_I^{ij} a_i^\dagger a_j |\Phi_I\rangle + \sum_{I \in \mathbf{R}} \sum_{ijkl} D_I^{ijkl} a_i^\dagger a_j^\dagger a_l a_k |\Phi_I\rangle \,.$$

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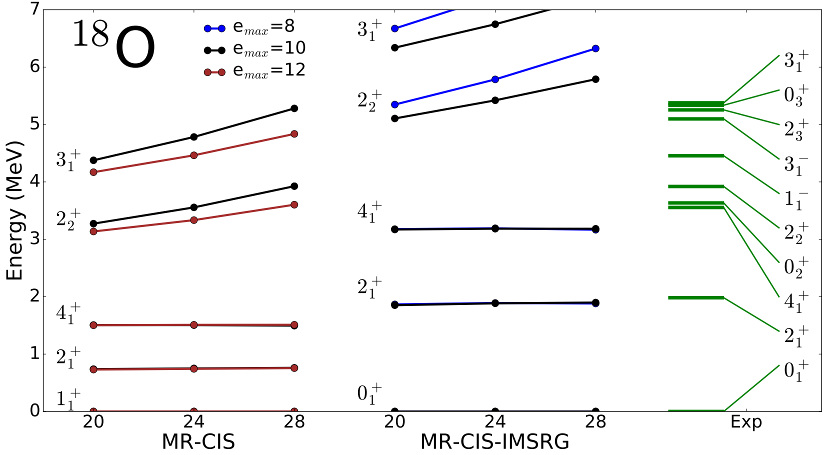
Open Shell Spectra



PRELIMINARY. N^{3}LO NN(500) + NNLO NNN(400). Exp: ENSDF.

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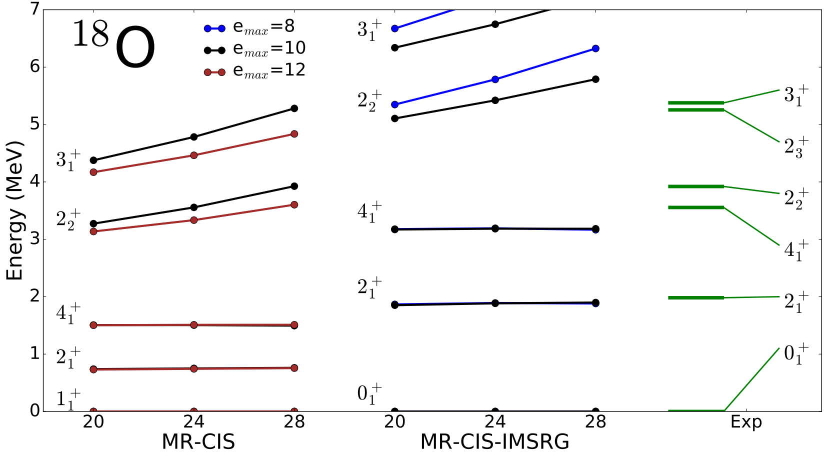

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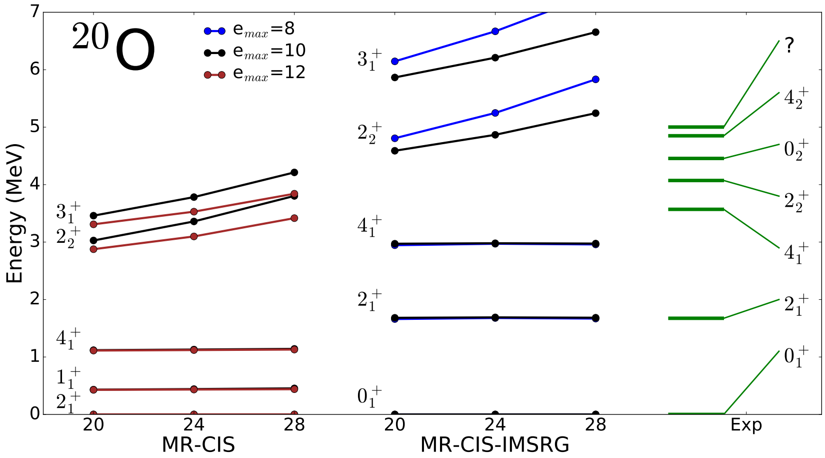

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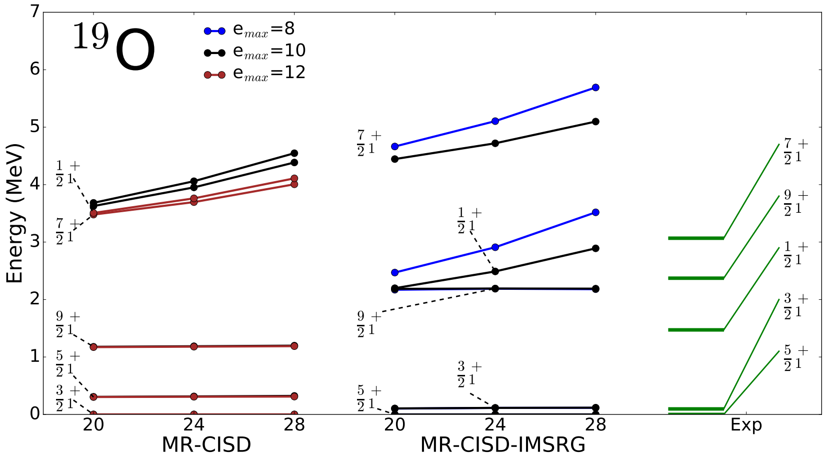

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Summary/Outlook

Summary

- New Method:
  Multireference IMSRG + Configuration Interaction.
- Lightweight tool for computing spectra for all nuclei (in principle).
- Both components of the method are systematically improvable.

Outlook

- Experiment with different reference states, decoupling strategies.
- Implement transition operators in MR-IMSRG: EM response, Gamow-Teller, $0\nu\beta\beta$?
- Corrections to CI?

Thank you!

Also thanks to:

IMSRG at MSU:
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Heiko Hergert
Fei Yuan
Kevin Fossez

IMSRG at Reed:
Ragnar Stroberg

IMSRG at ORNL
Titus Morris???

Gaute Hagen (EOM-CC results)
Petr Navratil (NCSM results)
Jason Holt

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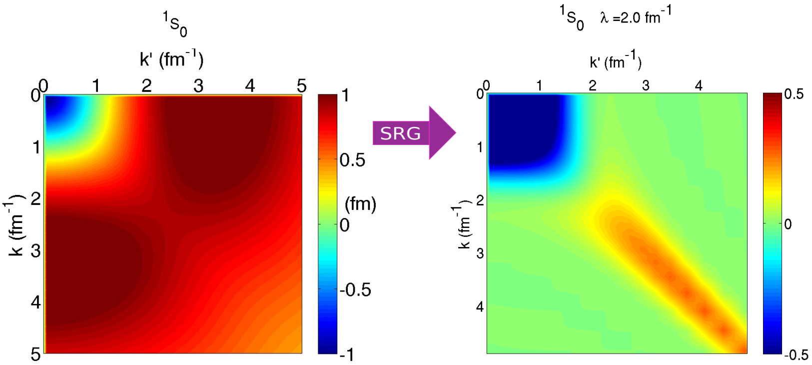
THE OHIO STATE UNIVERSITY

Similarity Renormalization Group (SRG)



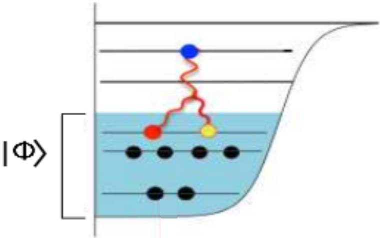
Figures from R. Furnstahl.

In-Medium Forces

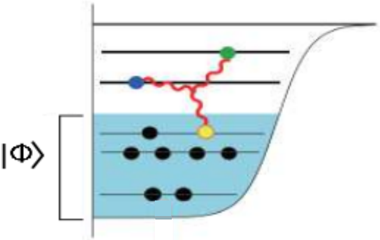
Hamiltonian "normal-ordered" with respect to reference state

$$H = E_0 + \sum_{pq} f_{pq} A^p_q + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} A^p_r A^q_s + \frac{1}{36} \sum_{pqrs} W_{pqrstu} A^p_s A^q_t A^r_u$$

In-medium
one-body force



In-medium
two-body force



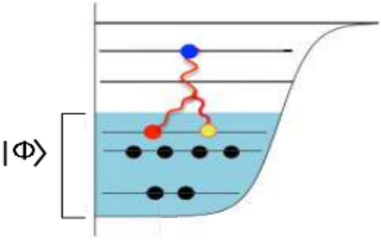
Figures: J. Holt.

In-Medium Forces

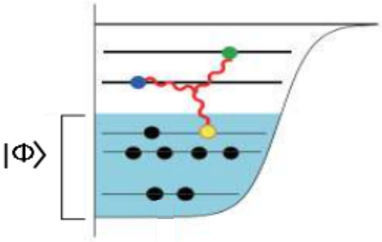
Hamiltonian "normal-ordered" with respect to reference state

$$H = E_0 + \sum_{pq} f_{pq} A^p_q + \frac{1}{4}\sum_{pqrs} \Gamma_{pqrs} A^p_r A^q_s + \frac{1}{36}\sum_{pqrs} W_{pqrstu} A^p_s A^q_t A^r_u$$

In-medium
one-body force



In-medium
two-body force



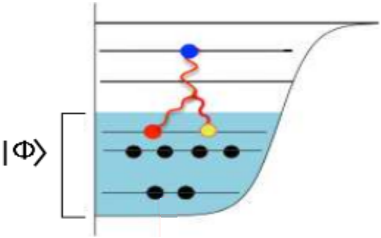
Figures: J. Holt.

In-Medium Forces

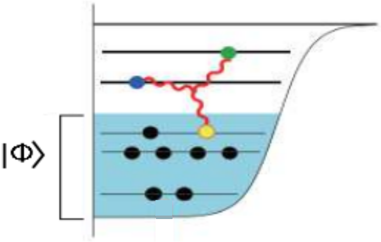
Hamiltonian "normal-ordered" with respect to reference state

$$H \approx E_0 + \sum_{pq} f_{pq} A^p_q + \frac{1}{4} \sum_{pqrs} \Gamma_{pqrs} A^p_r A^q_s$$

In-medium
one-body force



In-medium
two-body force



Figures: J. Holt.

Approximate 4th Order Exactness in MBPT

$\bar{H}(s)$ is calculated with the Baker-Campbell-Hausdorff Expansion.

$$\bar{H}(s) = e^{\Omega(s)} H e^{-\Omega(s)} = H + [\Omega(s), H] + \frac{1}{2}[\Omega(s), [\Omega(s), H]] + \cdots$$

4th Order Quadruples Correction (Mag(2*)):

$$\frac{1}{2}[(\Omega(s))_{2b}, [\Omega(s), H]_{3b}]_{2b}$$

4th Order Triples Correction (Mag(2*,3)):

$$\frac{1}{36} \sum_{ijkabc} \frac{W_{ijkabc} W_{abcijk}}{\Delta^{ijk}_{abc}} \qquad W \equiv [\Omega(s), H]_{3b}$$

MBPT(4) diagrams

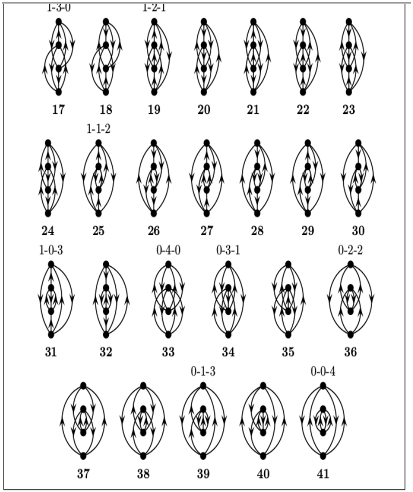
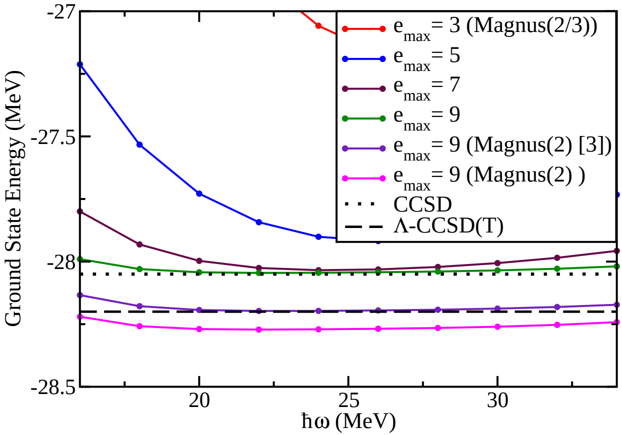


Fig. 5.6. Hugenholtz diagrams for the principal term of $E^{(4)}$ for canonical HF.

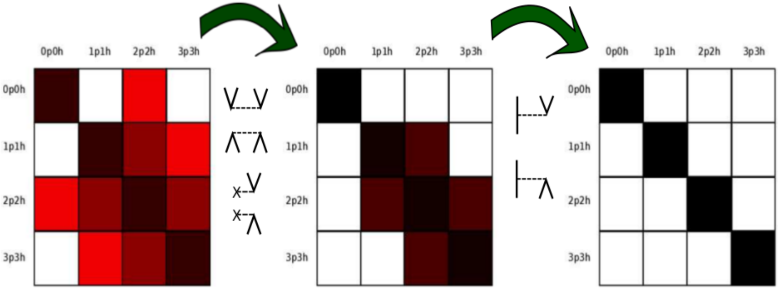
Corrections to IMSRG(2) with ^{4}He



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

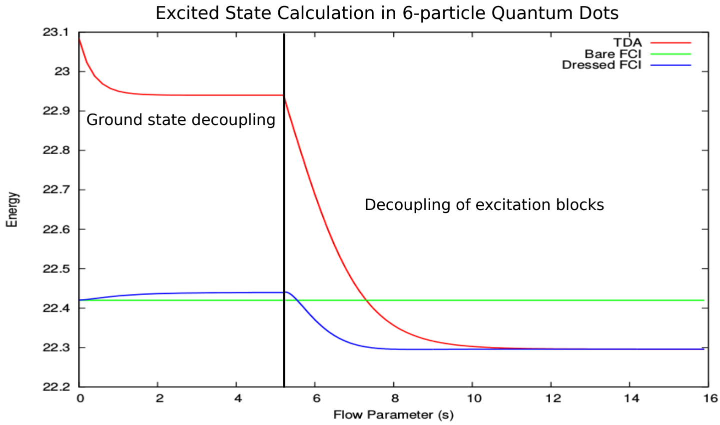
Additional Decoupling: TDA-IMSRG

Could we decouple sub-blocks and diagonalize individually?
Matrix dimensions more manageable than shell model.
1p1h diagonalization: Tamm-Dancoff Approximation (TDA)



Not so fast...

IMSRG(2) truncation breaks unitarity badly for large rotations



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 IMSRG:

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

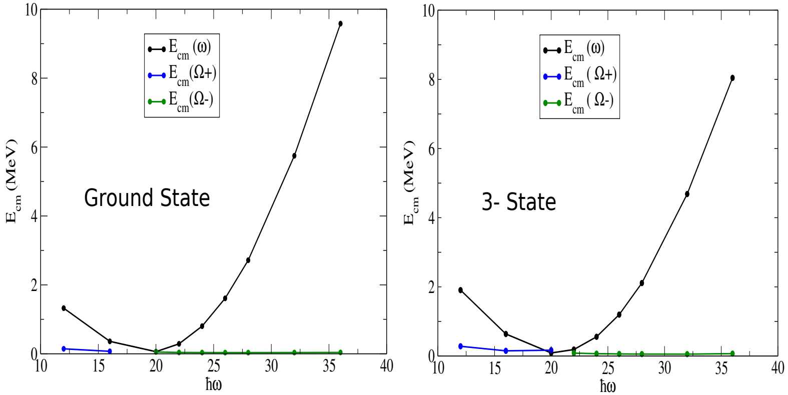
CoM frequency Ω calculated in the manner of Hagen et. al.

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

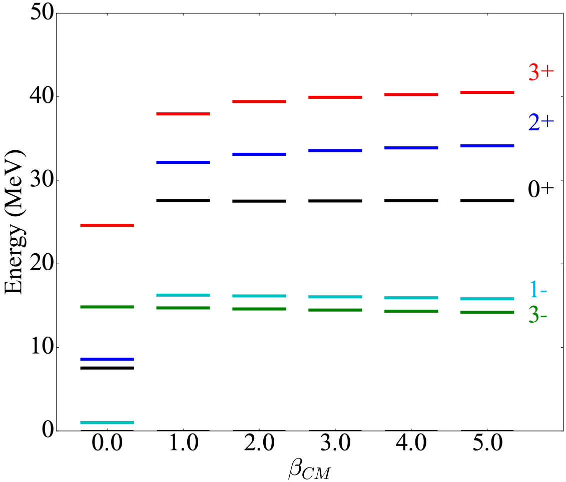
G. Hagen, T. Papenbrock, and D. J. Dean,
Phys. Rev. Lett. 103, 062503 (2009).

CoM diagnostic for ^{16}O 3- state

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



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



Solving the IMSRG equations

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

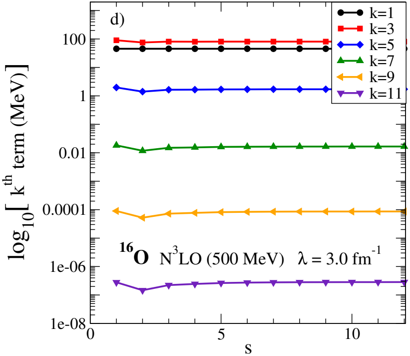
- Transform operators via flow equation.
  - requires very precise ODE solver
  - small step sizes in s needed for convergence
- Construct the unitary transformation explicitly.
  - Magnus expansion

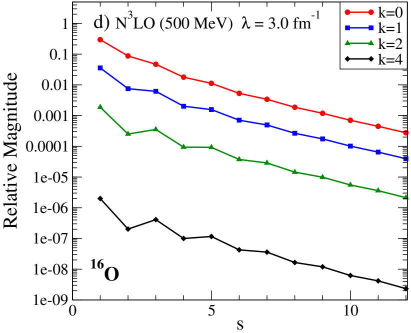
$$U(s) = e^{-\Omega(s)}$$

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

  - less precision needed, larger step sizes

Numerical tests of Magnus





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

Full Triples (2,3): $\mathcal{O}(N_u^5 N_o^3)$:

$$\bar{X}_\nu^\dagger = \sum_{ph} \bar{x}_h^p a_p^\dagger a_h + \frac{1}{4} \sum_{pp'hh'} \bar{x}_{hh'}^{pp'} a_p^\dagger a_{p'}^\dagger a_{h'} a_h + \frac{1}{36} \sum_{\substack{pp'p'' \\ hh'h''}} \bar{x}_{hh'h''}^{pp'p''} a_p^\dagger a_{p'}^\dagger a_{p''}^\dagger a_{h''} a_{h'} a_h$$

Perturbative Triples (2,{3}): $\mathcal{O}(N_u^4 N_o^3)$:

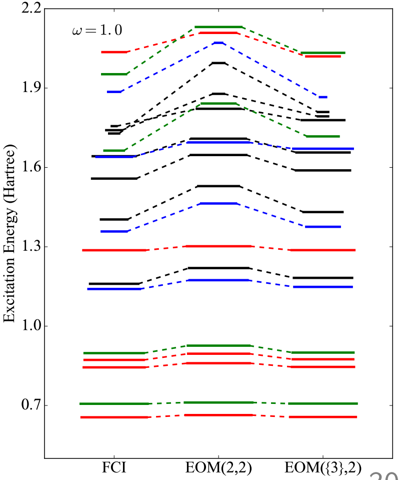
$$\bar{X}_\nu^\dagger = \sum_{ph} \bar{x}_h^p a_p^\dagger a_h + \frac{1}{4} \sum_{pp'hh'} \bar{x}_{hh'}^{pp'} a_p^\dagger a_{p'}^\dagger a_{h'} a_h$$

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

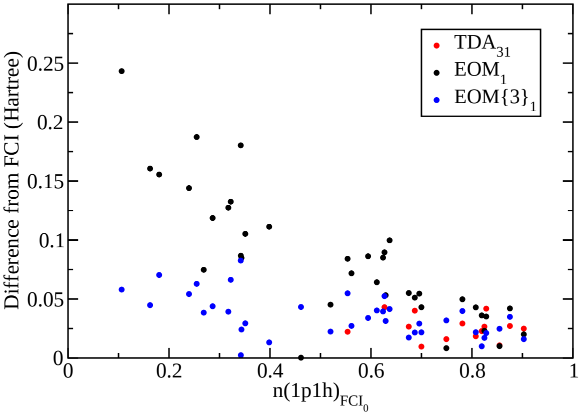
Method Comparison in 2D Quantum Dots

RMS Errors (Hartree)

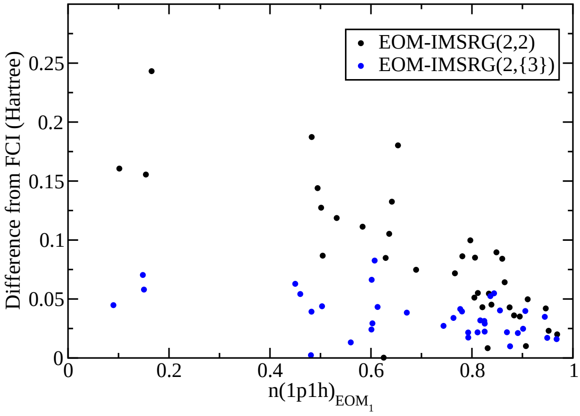
Method	FCI_0
FCI_1	
(2,2)	0.095
(2,{3})-MP	0.066
(2,{3})-EN	0.031



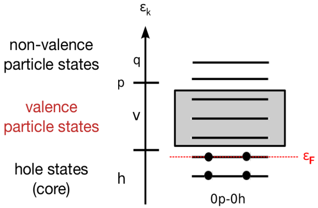
Error w.r.t. FCI_0 calculation

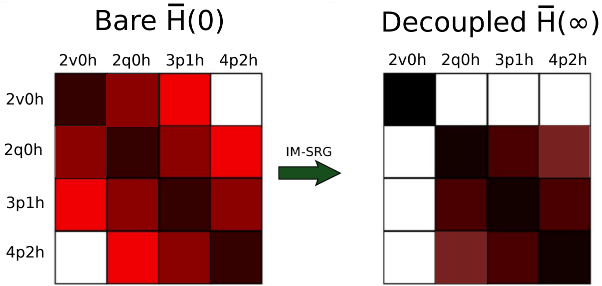


EOM 1p1h Partial Norm with Triples



Coupling to the Shell Model





Valence-Space Decoupling with Shell Model

S. R. Stroberg, H. Hergert, J. D. Holt, S. K. Bogner, and A. Schwenk
Phys. Rev. C 93, 051301(R) (2016)