Recent advances in the In-Medium SRG

Titus Morris

May 20th, 2015

Outline

- Brief review of In-Medium SRG
  - Closed/Open Shell results
  - Challenges to meet
- Magnus Expansion
  - Computational Efficiency
  - Effective Observables
  - Approximations to 3 body induced effects

Similarity Renormalization Group

Basic Concept

continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given “uncorrelated” many-body basis

- flow equation for Hamiltonian $H(s) = U(s)HU^\dagger(s)$:

$$\frac{d}{ds}H(s) = [\eta(s), H(s)] \,, \quad \eta(s) = \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

- choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(s) = [H_d(s), H_{od}(s)]$$

  to suppress (suitably defined) off-diagonal Hamiltonian

- consistent evolution for all observables of interest

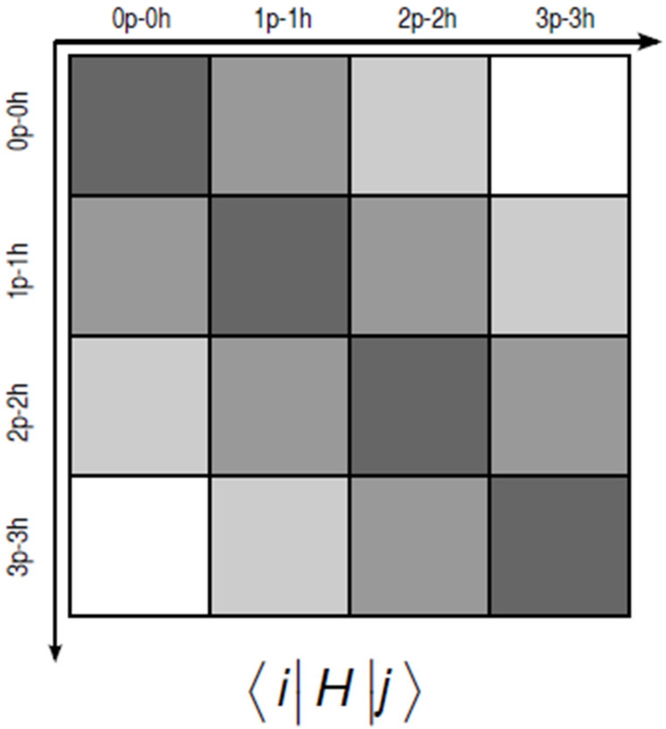
In-Medium SRG

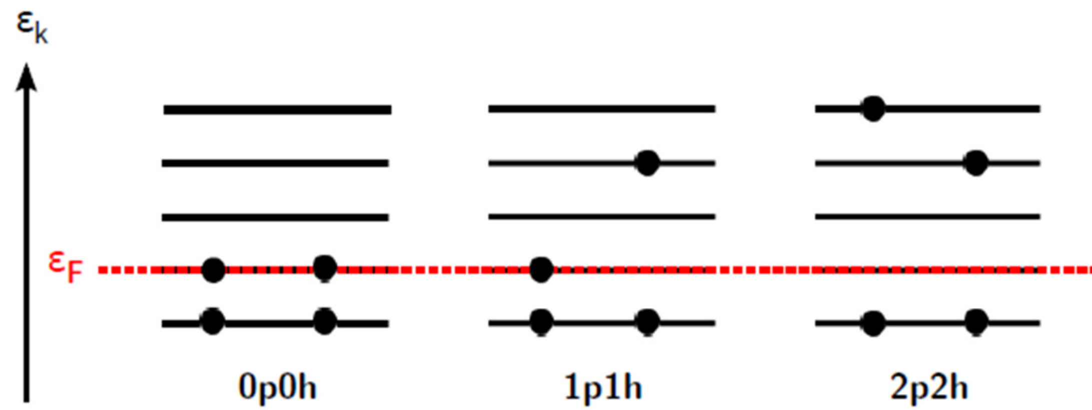
S. K. Bogner, H. H., T. Morris, A. Schwenk, and K. Tuskiyama, to appear in Phys. Rept.

H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013)

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

Decoupling in A-Body Space





excitations relative to reference state:
→ normal-ordering

Normal Ordering

- second quantization: $A^{k_1\dots k_N}_{l_1\dots l_N} = a^\dagger_{k_1}\dots a^\dagger_{k_N} a_{l_N}\dots a_{l_1}$
- particle- and hole density matrices:

$$\lambda^k_l = \langle\,\Phi\big|\,A^k_l\,\big|\Phi\,\rangle \longrightarrow n_k\delta^k_l\,,\quad n_k\in\{0,1\}$$
$$\xi^k_l = \lambda^k_l - \delta^k_l \qquad \longrightarrow -\bar{n}_k\delta^k_l \equiv -(1-n_k)\delta^k_l$$

- define normal-ordered operators recursively:

$$A^{k_1\dots k_N}_{l_1\dots l_N} = :A^{k_1\dots k_N}_{l_1\dots l_N}: + \lambda^{k_1}_{l_1}:A^{k_2\dots k_N}_{l_2\dots l_N}: + \text{singles}$$
$$+\left(\lambda^{k_1}_{l_1}\lambda^{k_2}_{l_2} - \lambda^{k_1}_{l_2}\lambda^{k_2}_{l_1}\right):A^{k_3\dots k_N}_{l_3\dots l_N}: + \text{doubles} + \dots$$

- algebra is simplified significantly because

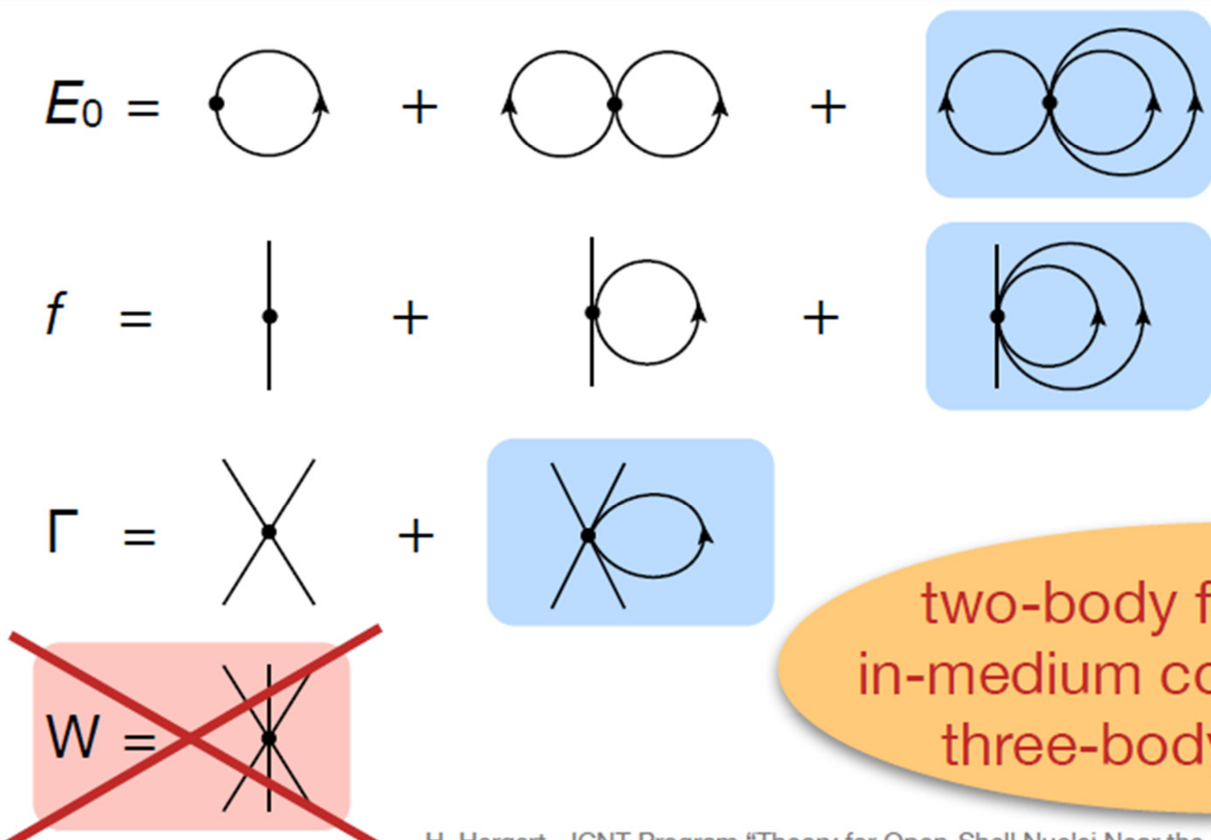
$$\langle\,\Phi\big|:A^{k_1\dots k_N}_{l_1\dots l_N}:\big|\Phi\,\rangle = 0$$

- Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

Normal-Ordered Hamiltonian

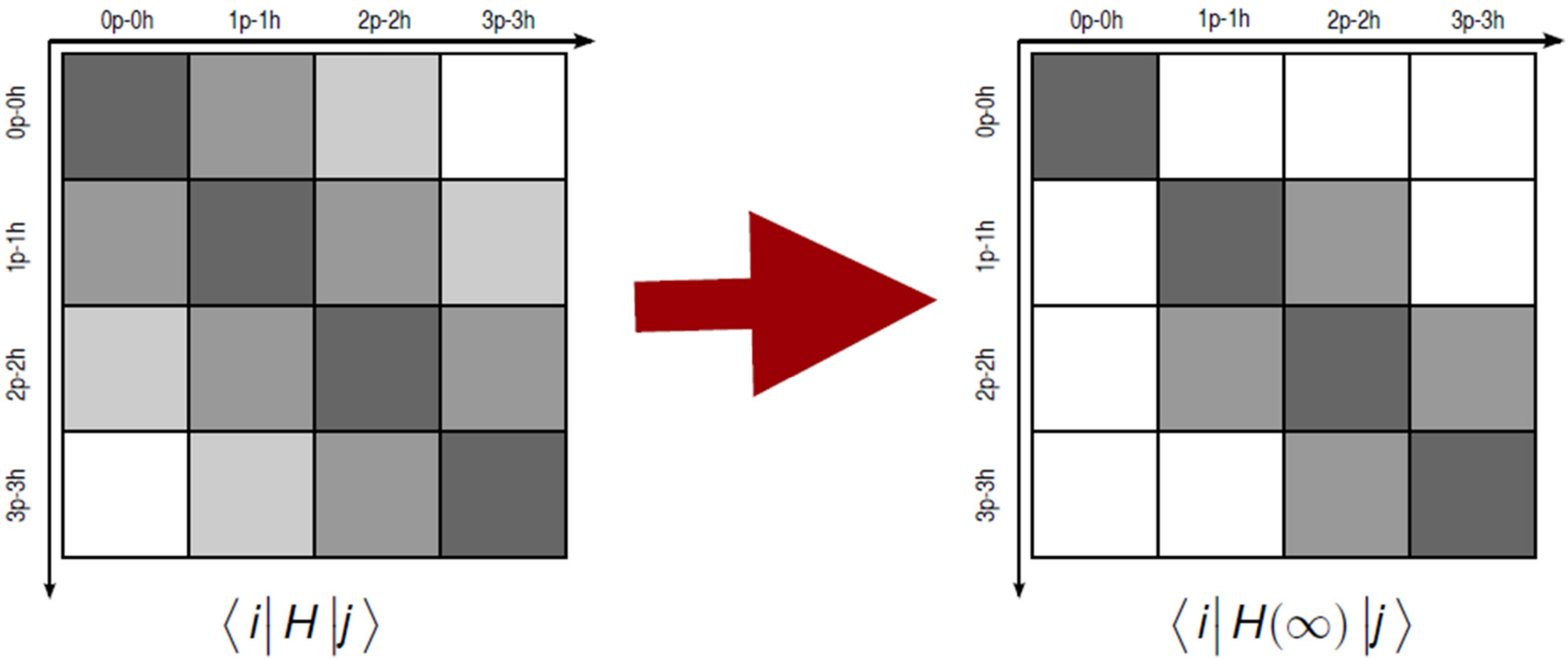
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f^k_l : A^k_l : + \frac{1}{4} \sum_{klmn} \Gamma^{kl}_{mn} : A^{kl}_{mn} : + \frac{1}{36} \sum_{ijklmn} W^{ijk}_{lmn} : A^{ijk}_{lmn} :$$



two-body formalism with in-medium contributions from three-body interactions

Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

Choice of Generator

- Wegner: $\eta^{I} = [H_d, H_{od}]$
- White: (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f^p_h}{\Delta^p_h} :A^p_h: + \frac{1}{4}\sum_{pp'hh'} \frac{\Gamma^{pp'}_{hh'}}{\Delta^{pp'}_{hh'}} :A^{pp'}_{hh'}: - \text{H.c.}$$

$\Delta^p_h, \Delta^{pp'}_{hh'}$: approx. 1p1h, 2p2h excitation energies

- "imaginary time": (Morris, Bogner)

$$\eta^{III} = \sum_{ph} \text{sgn}\left(\Delta^p_h\right) f^p_h :A^p_h: + \frac{1}{4}\sum_{pp'hh'} \text{sgn}\left(\Delta^{pp'}_{hh'}\right) \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: - \text{H.c.}$$

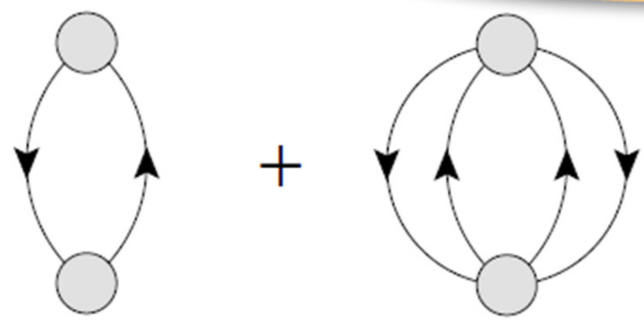
- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta| s}$ (imaginary time)
- g.s. energies ($s \to \infty$) differ by $\ll 1\%$

IM-SRG(2) Flow Equations

0-body Flow

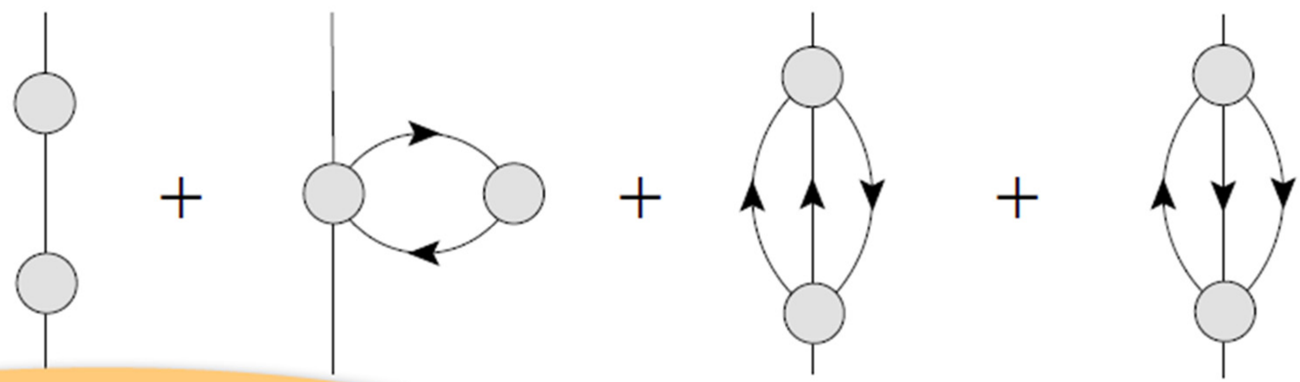
~ 2nd order MBPT for *H(s)*

$$\frac{dE}{ds} =$$



1-body Flow

$$\frac{df}{ds} =$$



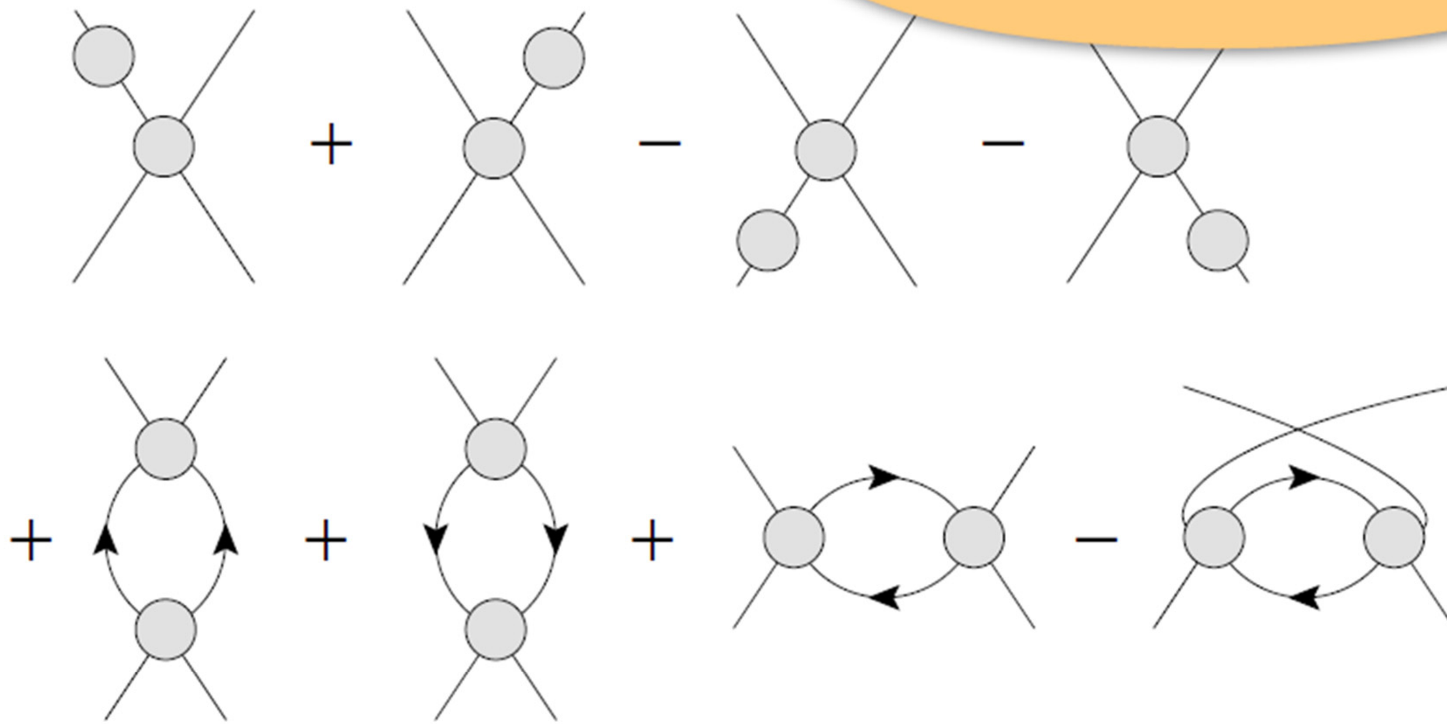
IM-SRG(2): truncate ops. at two-body level

IM-SRG(2) Flow Equations

O(N⁶) scaling
(before particle/hole distinction)

2-body Flow

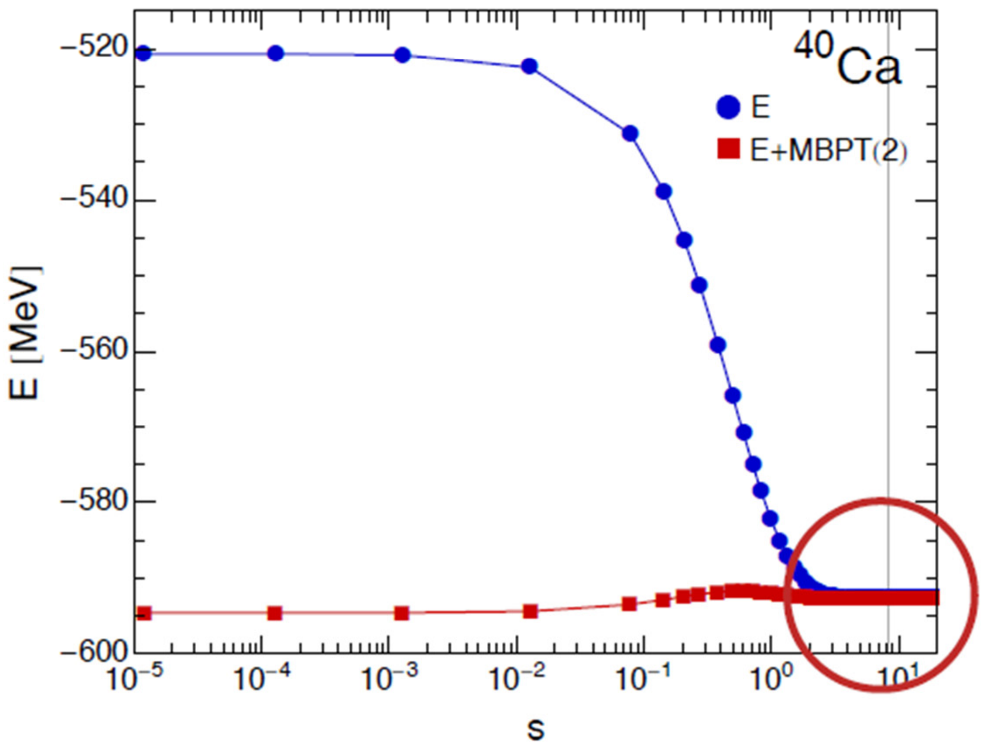
$$\frac{d\Gamma}{ds} =$$

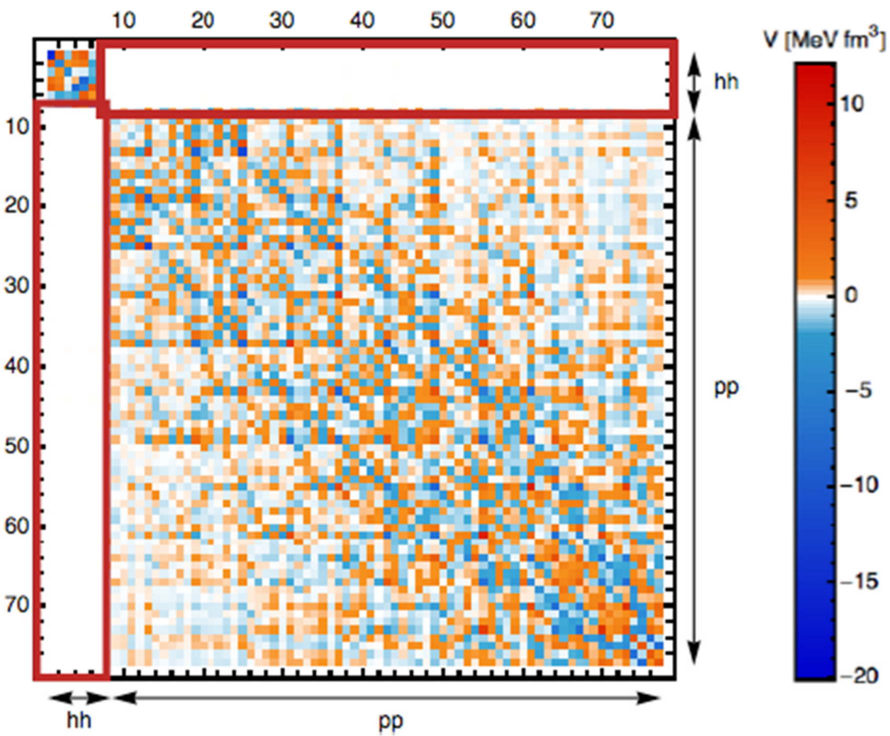


s channel — ladders

t channel, *u* channel — rings

Decoupling



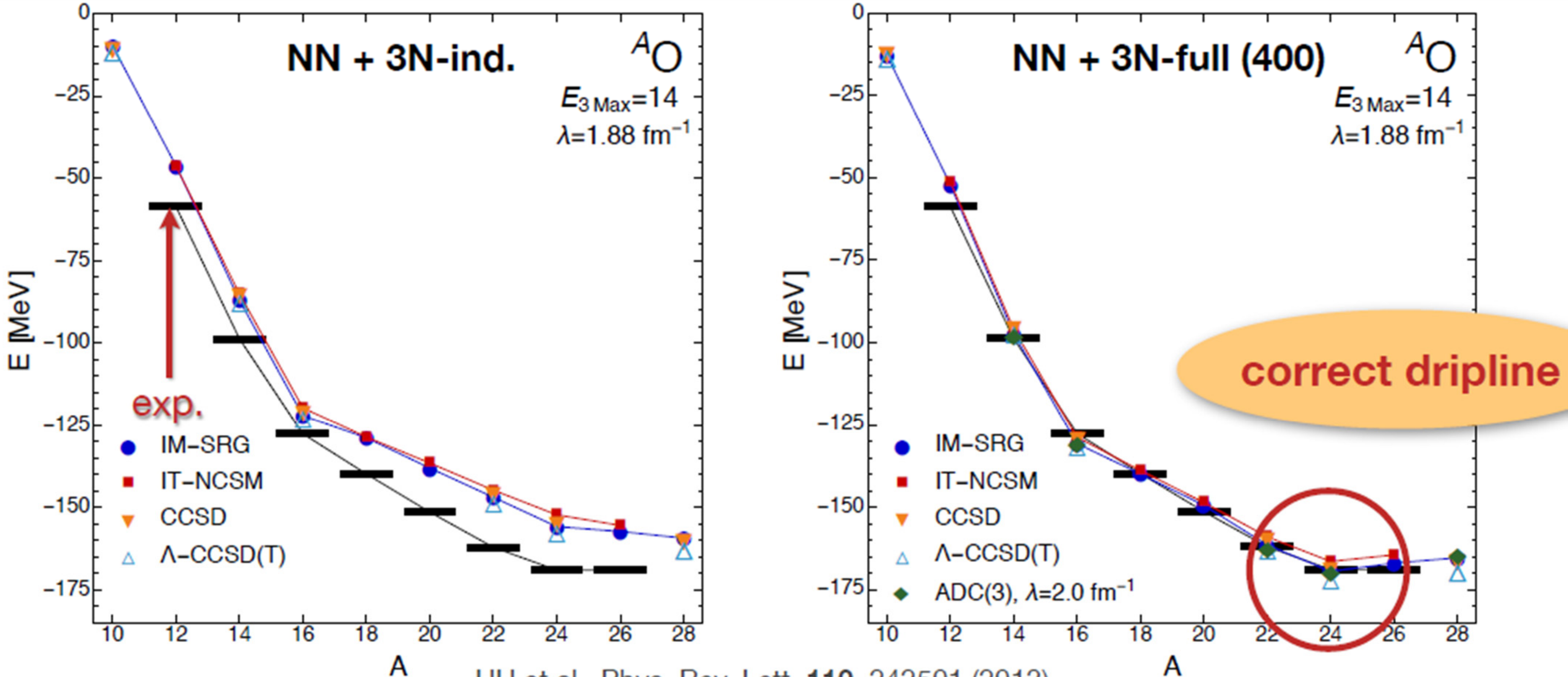


N3LO, $\lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

non-perturbative resummation of MBPT series (correlations)

off-diagonal couplings are rapidly driven to zero

Results: Oxygen Chain



HH et al., Phys. Rev. Lett. **110**, 242501 (2013)

ADC(3): A. Cipollone et al., Phys. Rev. Lett. **111**, 242501 (2013)

- Multi-Reference IM-SRG with number-projected Hartree-Fock-Bogoliubov as reference state (pairing correlations)
- consistent results from different many-body methods

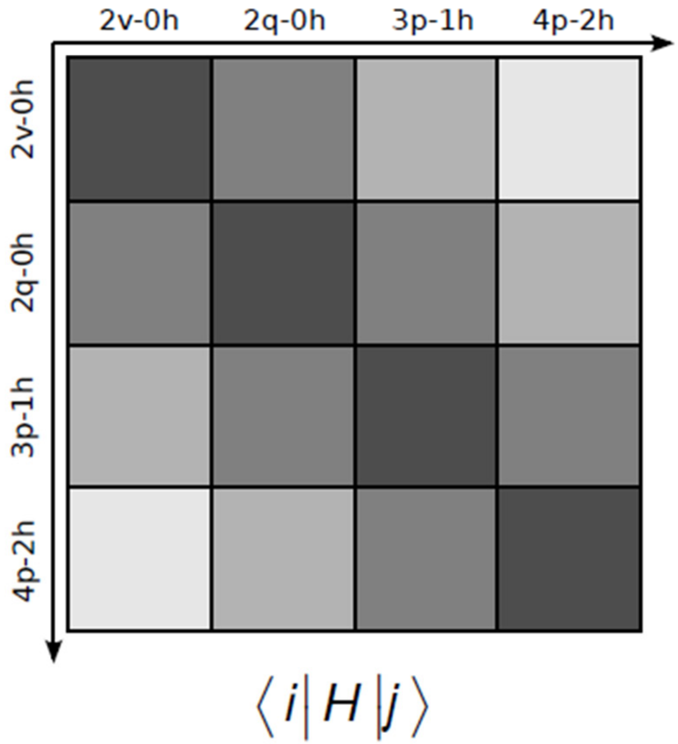
IM-SRG Interactions for the Shell Model

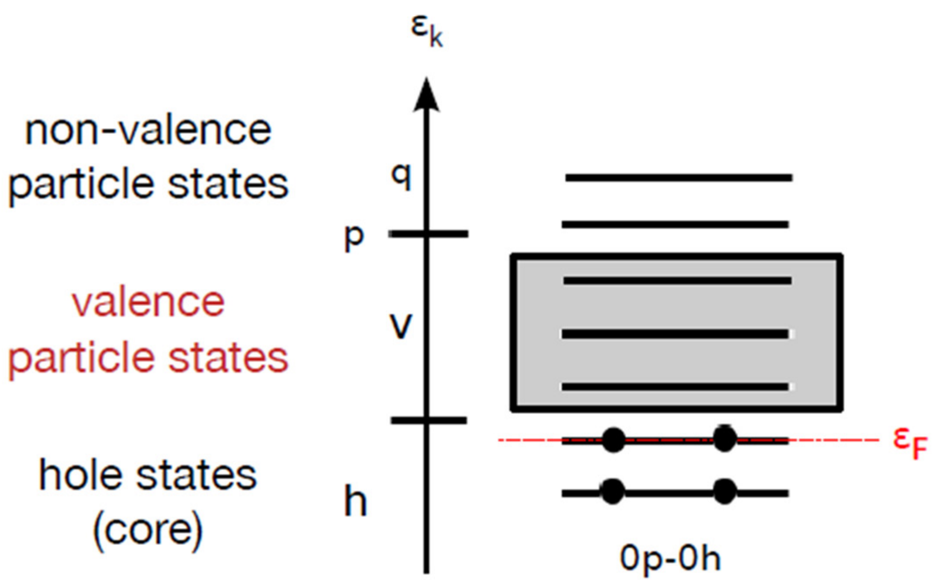
S. K. Bogner, H. H., J. D. Holt, A. Schwenk, in preparation

S. K. Bogner, H. H., J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. Lett. 113, 142501 (2014)

K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304(R) (2012)

Valence Space Decoupling





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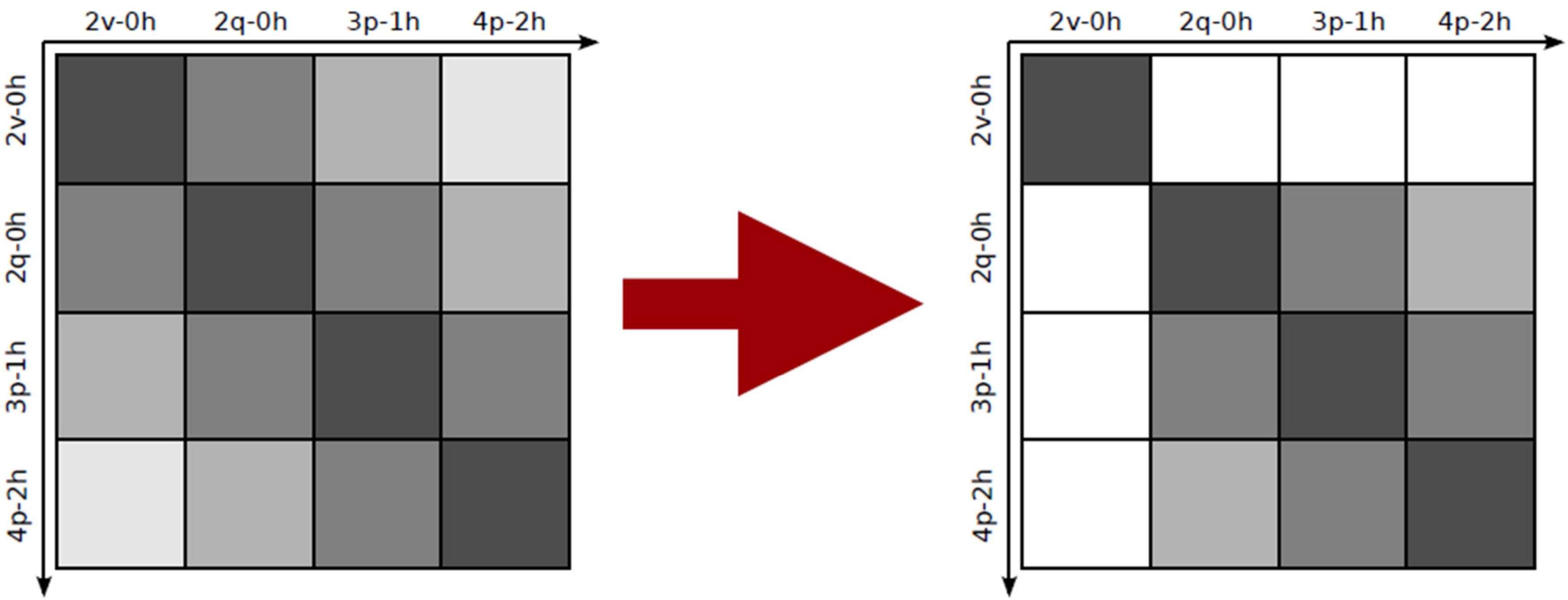
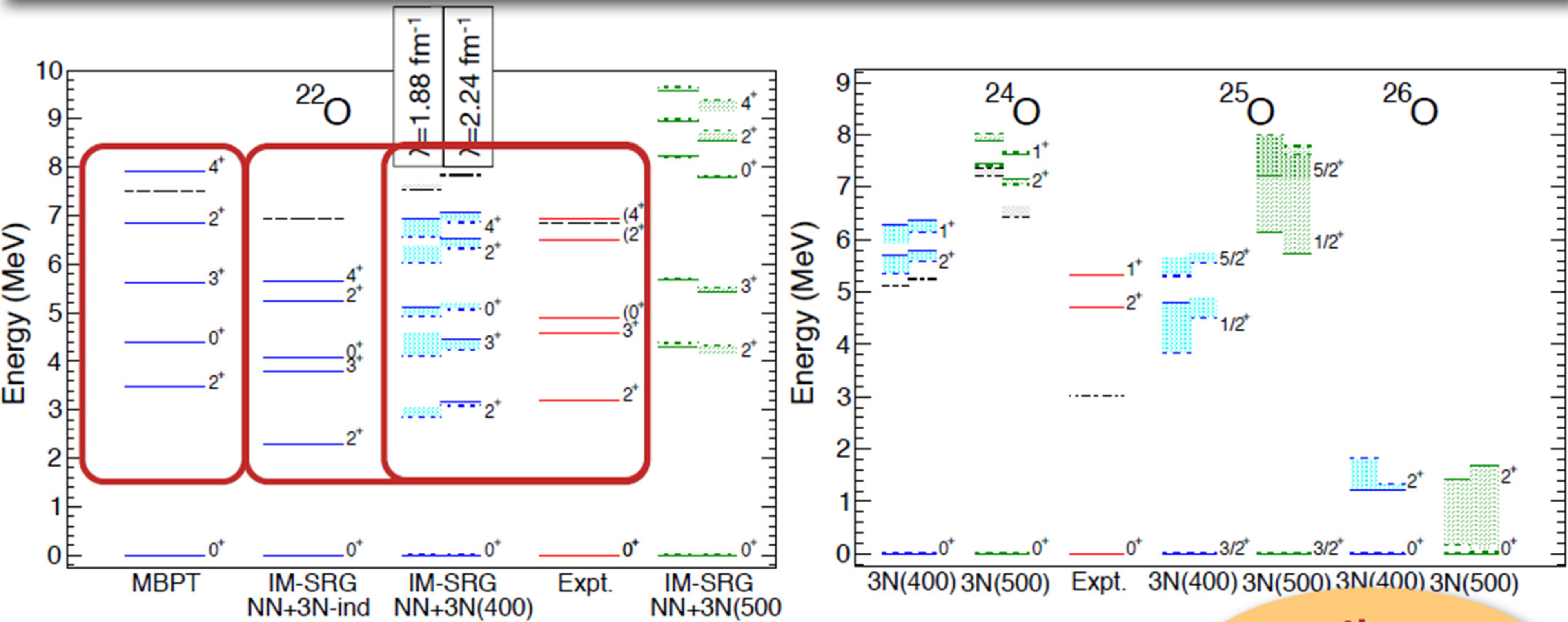


$\langle i | H | j \rangle$ $\quad\quad$ $\langle i | H(\infty) | j \rangle$

- construct generator from off-diagonal Hamiltonian

$$\left\{ H^{od} \right\} = \{ f^{h}_{h'}, f^{p}_{p'}, f^{p}_{h}, f^{q}_{v}, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma^{pq}_{vv'} \} \text{ \& H.c.}$$

From Oxygen...



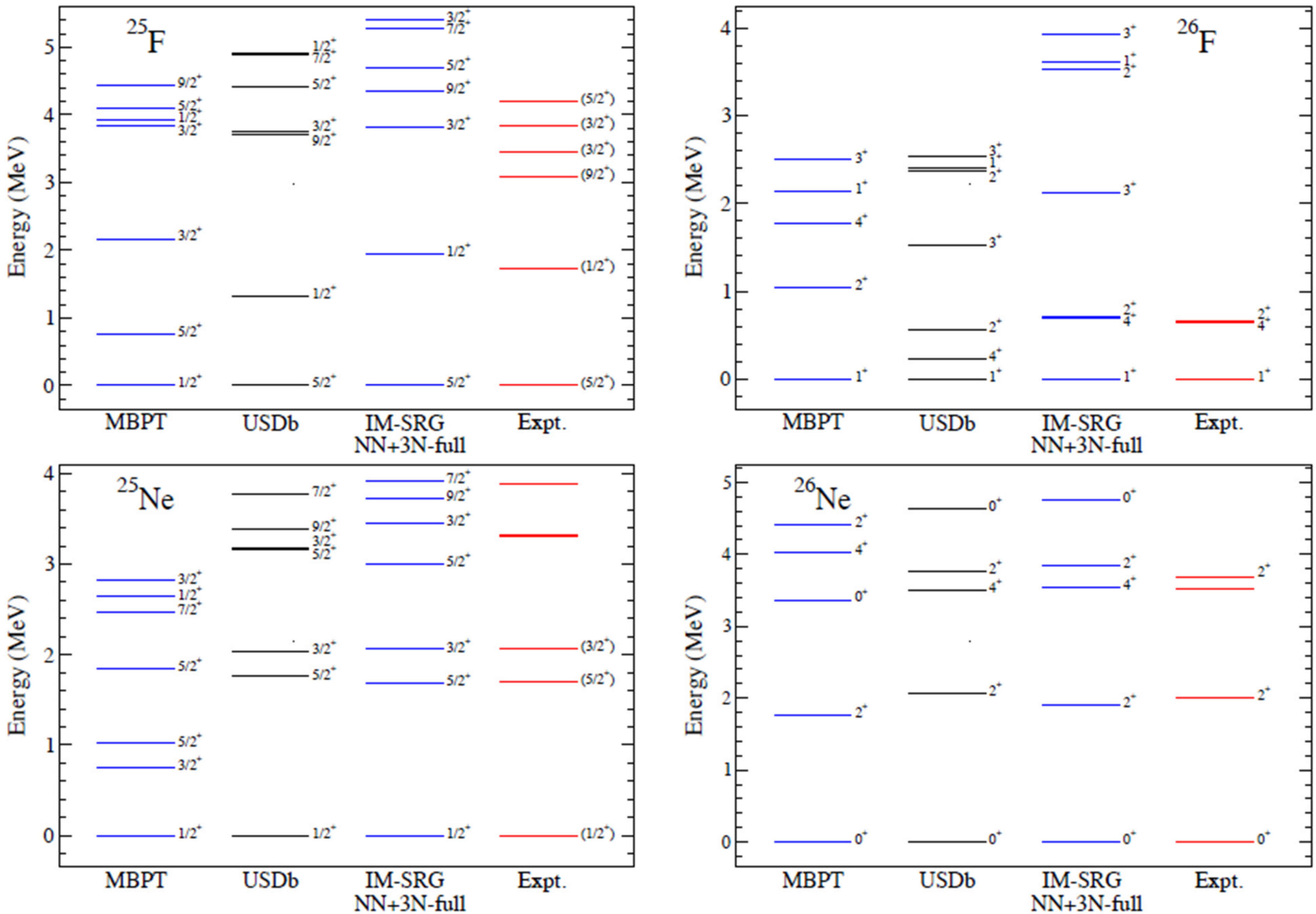
shading: $\hbar\Omega$ variation

Phys. Rev. Lett. **113**, 142501 (2014)

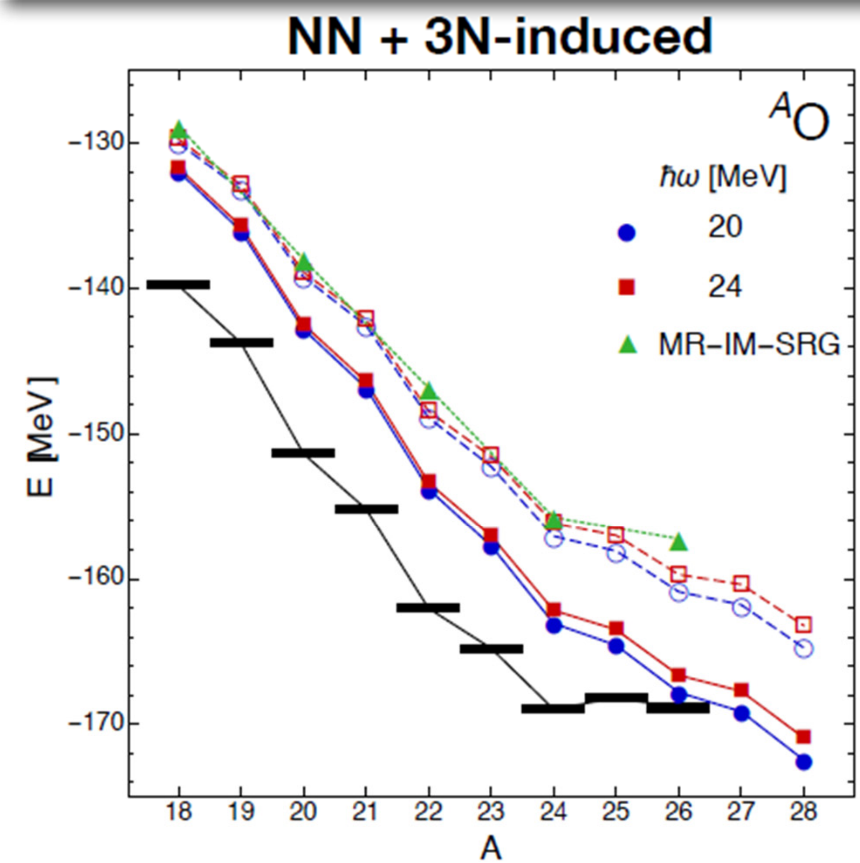
continuum lowers states by <1 MeV

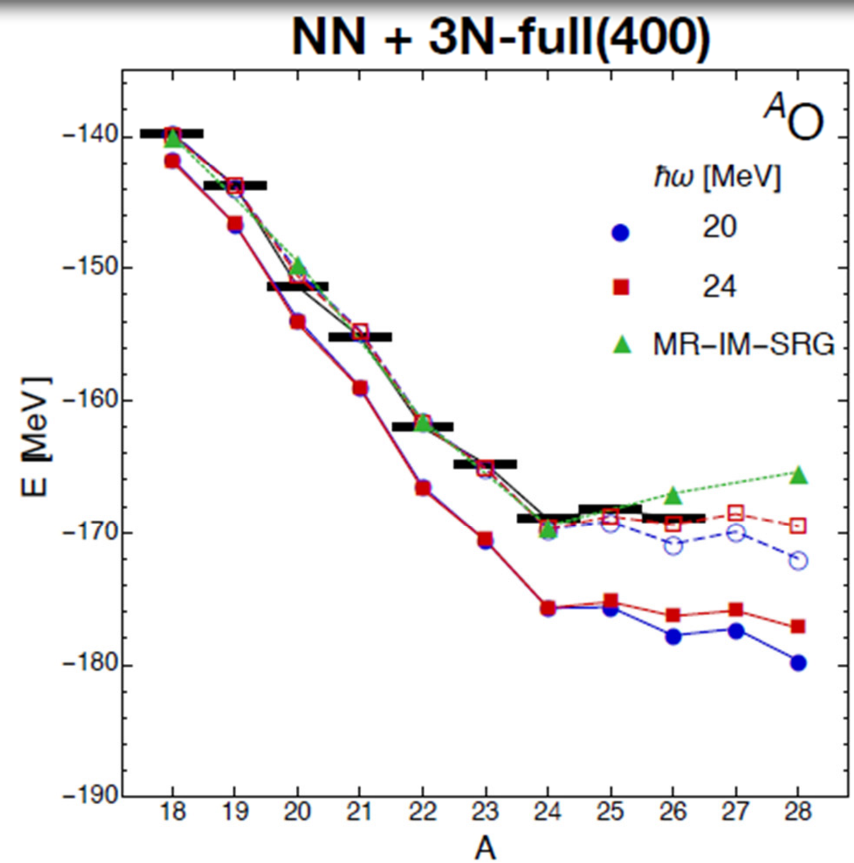
- **3N forces crucial**
- IM-SRG improves on finite-order MBPT effective interaction
- competitive with phenomenological calculations

... Into the *sd*-Shell...



Open Issue





- looks like simple shift: $\Delta E \approx \frac{A_v}{A} \cdot \text{const.}$ …
- … but it's more complicated; take more information on target into account (occupation of states, etc.) ?

Challenges within IM-SRG(2)

- Evolving H is technical and expensive itself

- Consistent but expensive evolution of observables

$$\frac{d}{ds}O = [\eta, O]$$

- No handle on induced 3-(higher body) forces

Magnus expansion within the IM-SRG

T.D.M., N. Parzuchowski, S.K. Bogner, in preparation
W. Magnus. *Comm. Pure and Appl. Math.*, VII:649–673, 1954.
F. Evangelista. J. Chem. Phys. **141**, 054109 (2014)

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continuous unitary transformation of the Hamiltonian to band-diagonal form w.r.t. a given "uncorrelated" many-body basis

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SRG Unitary Transformation

$$\frac{dU_s}{ds} = \eta_s U_s \quad \Rightarrow \quad U_s = \mathcal{S}\exp\left(\int_0^s \eta_{s'} ds'\right)$$

$$= 1 + \int_0^s \eta_{s'} ds' + \int_0^s \eta_{s'} \int_0^{s'} \eta_{s''} \, ds' ds'' + \ldots$$

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Kehrein calls attempting to form U “both difficult and not helpful.”

SRG Unitary Transformation

Magnus Expansion W. Magnus. *Comm. Pure and Appl. Math.*, VII:649–673, 1954.

$$U_s = \exp(\Omega_s)$$

$$\frac{d\Omega_s}{ds} = \eta_s + \frac{1}{2}[\Omega_s, \eta_s] + \frac{1}{12}[\Omega_s, [\Omega_s, \eta_s]] + \cdots \equiv \sum_{k=0}^{\infty} \frac{B_k}{k!} ad^k_{\Omega_s}(\eta_s)$$

$$ad^k_\Omega(\eta) = [\Omega, ad^{k-1}_\Omega(\eta)] \qquad B_k = \text{Bernoulli numbers}$$

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$$
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$$

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$$

$$
\begin{aligned}
H_s &= \exp(\Omega_s) H \exp(-\Omega_s) = H + [\Omega_s, H] + \frac{1}{2}[\Omega_s, [\Omega_s, H]] + \dots \\
O_s &= \exp(\Omega_s) O \exp(-\Omega_s) = O + [\Omega_s, O] + \frac{1}{2}[\Omega_s, [\Omega_s, O]] + \dots
\end{aligned}
$$

SRG Unitary Transformation

$H_s\,,\eta_s\,,\Omega_s$ truncated to N-ordered 2-body terms

$$
\begin{aligned}
\frac{d\Omega_s}{ds} &= \eta_s + \frac{1}{2}[\Omega_s,\eta_s]_{2B} + \frac{1}{12}\big[\Omega_s,[\Omega_s,\eta_s]_{2B}\big]_{2B} + \cdots \\
H_s &= H + [\Omega_s, H]_{2B} + \frac{1}{2}\big[\Omega_s,[\Omega_s,H]_{2B}\big]_{2B} + \cdots
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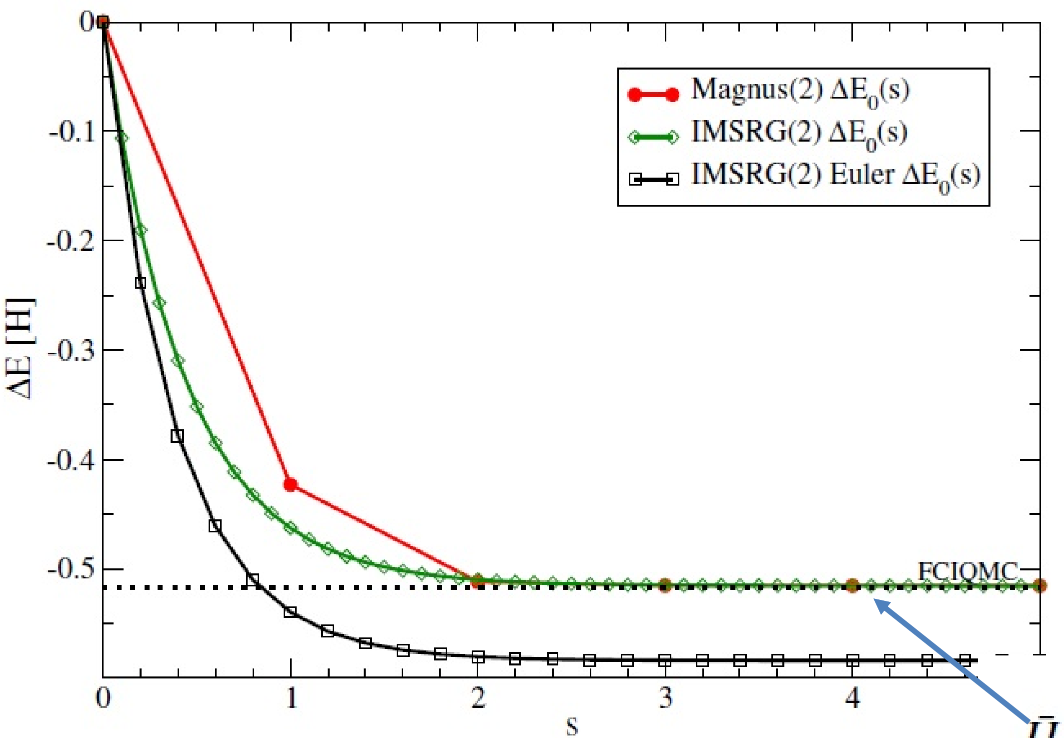
\end{aligned}
$$

Denote this as Magnus(2) for the remainder of this talk

Magnus(2) PBC Electron Gas



$$\frac{dU^\dagger}{ds} = \eta U^\dagger$$

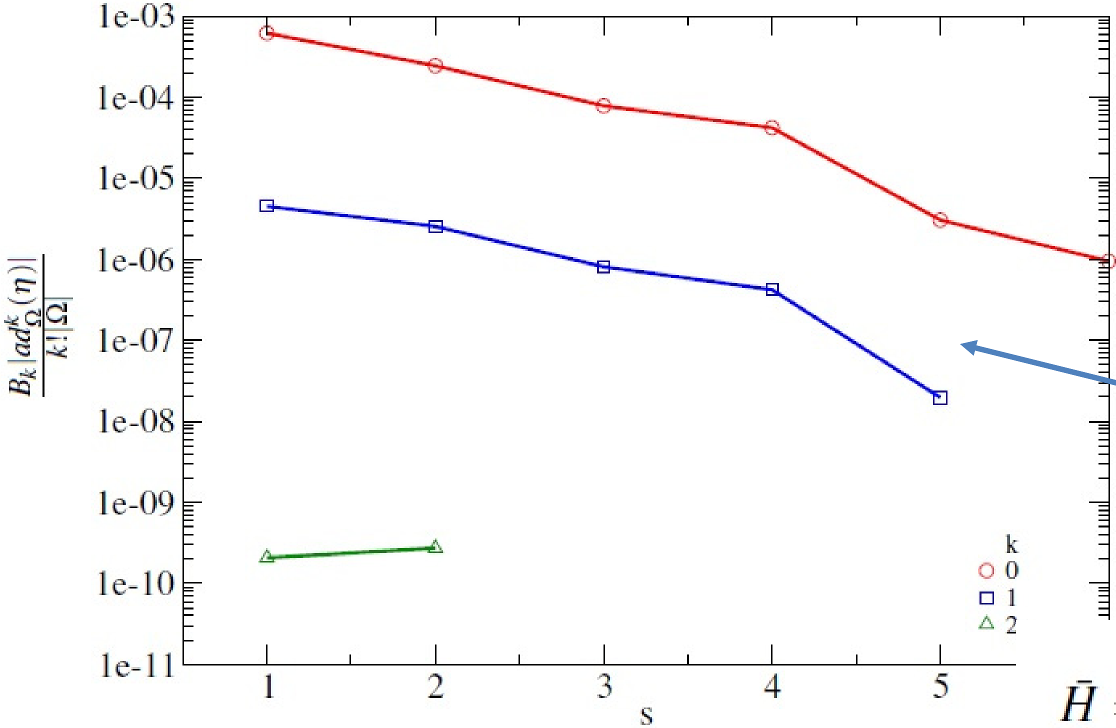
$$U^\dagger = exp(\Omega)$$

$$\frac{d\Omega}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^{k}(\eta)$$

$$\bar{H} = exp(\Omega) H \, exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(H)$$

J.J. Shepherd, G.H. Booth, A. Alavi, J. Chem. Phys. **136**, 244101 (2012)

Magnus(2) PBC Electron Gas



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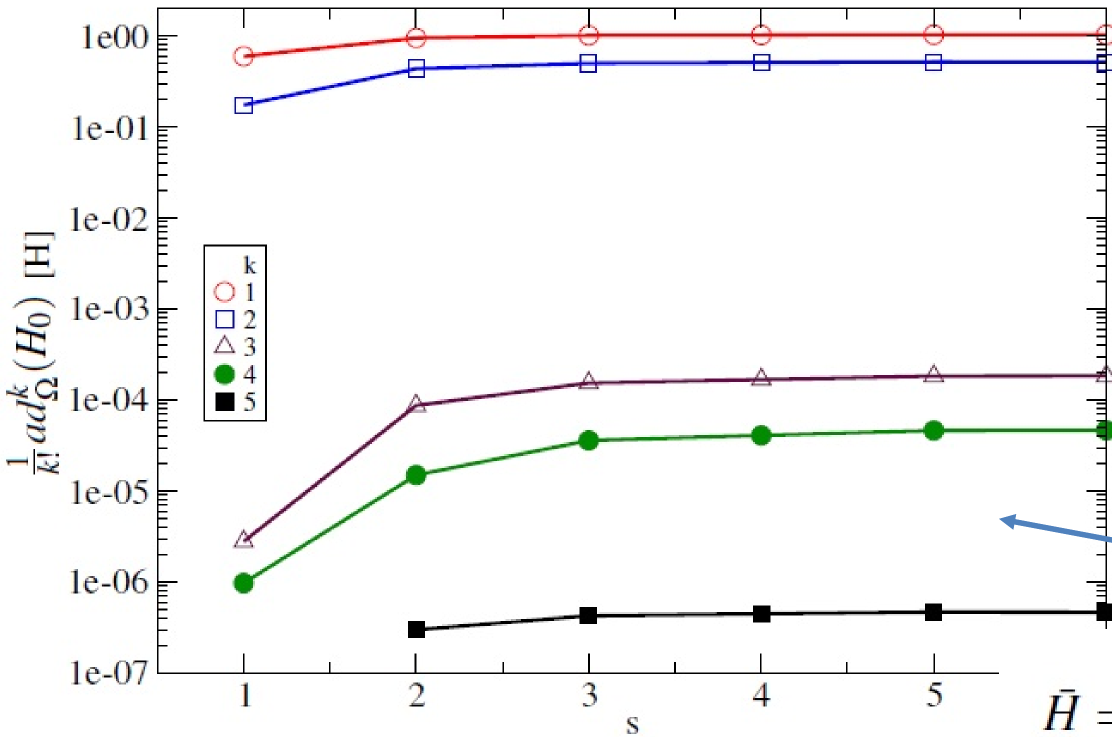

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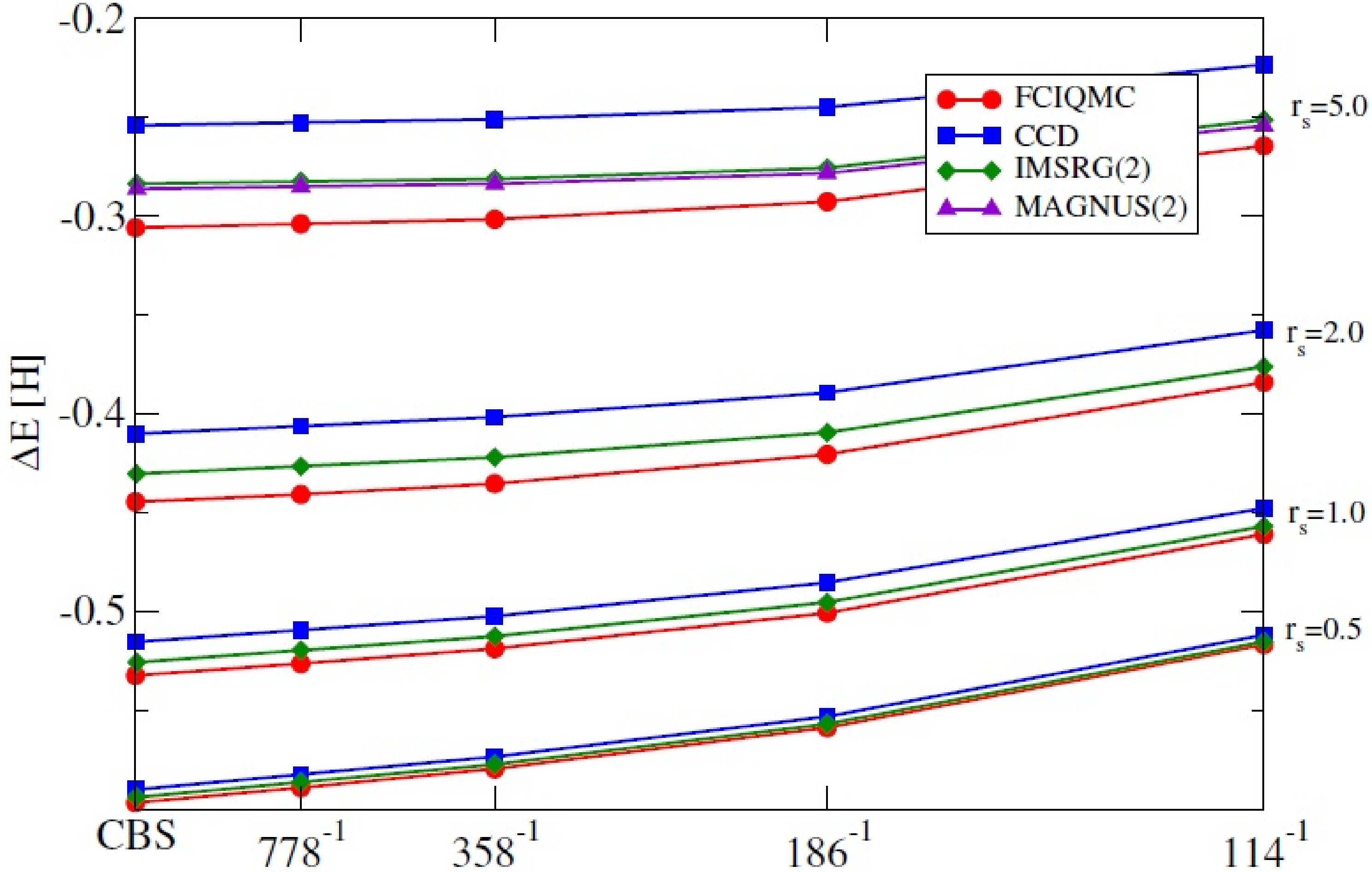
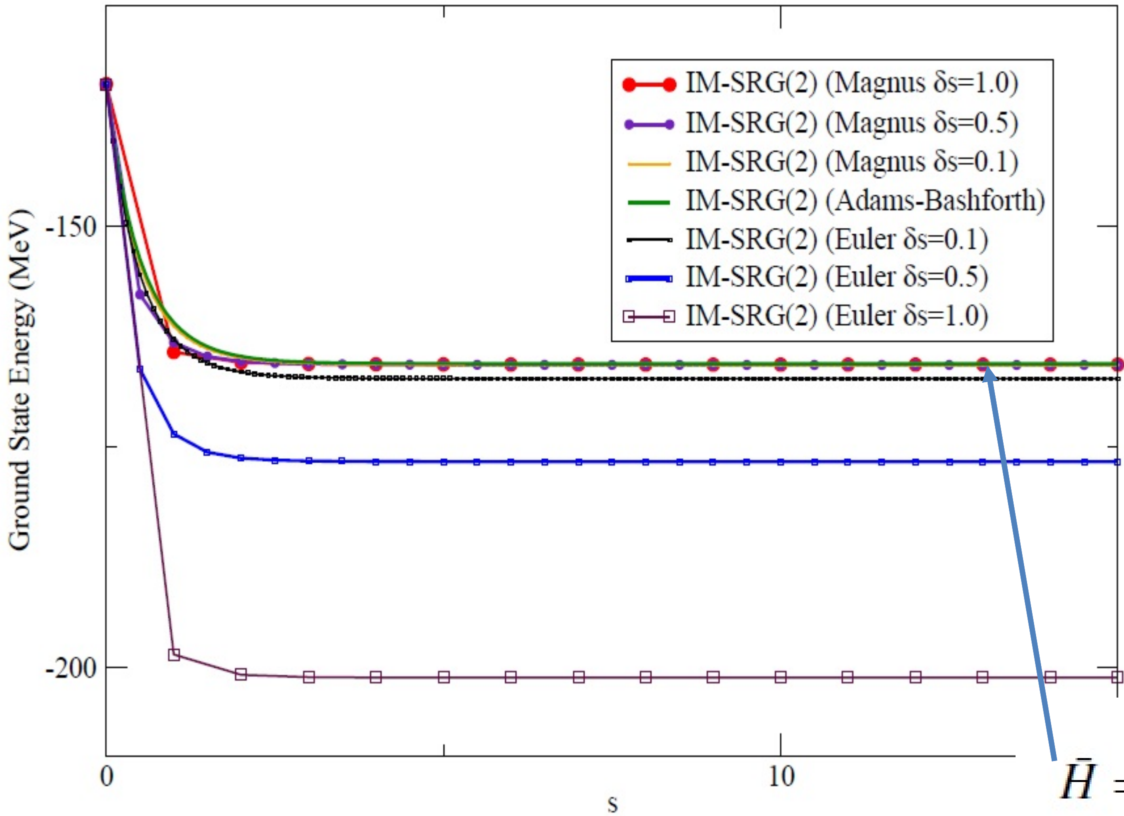


J.J. Shepherd, G.H. Booth, A. Alavi, J. Chem. Phys. **136**, 244101 (2012)

Magnus(2) ^{16}O



N3LO E.M. NN $\lambda = 2.0$, emax=8

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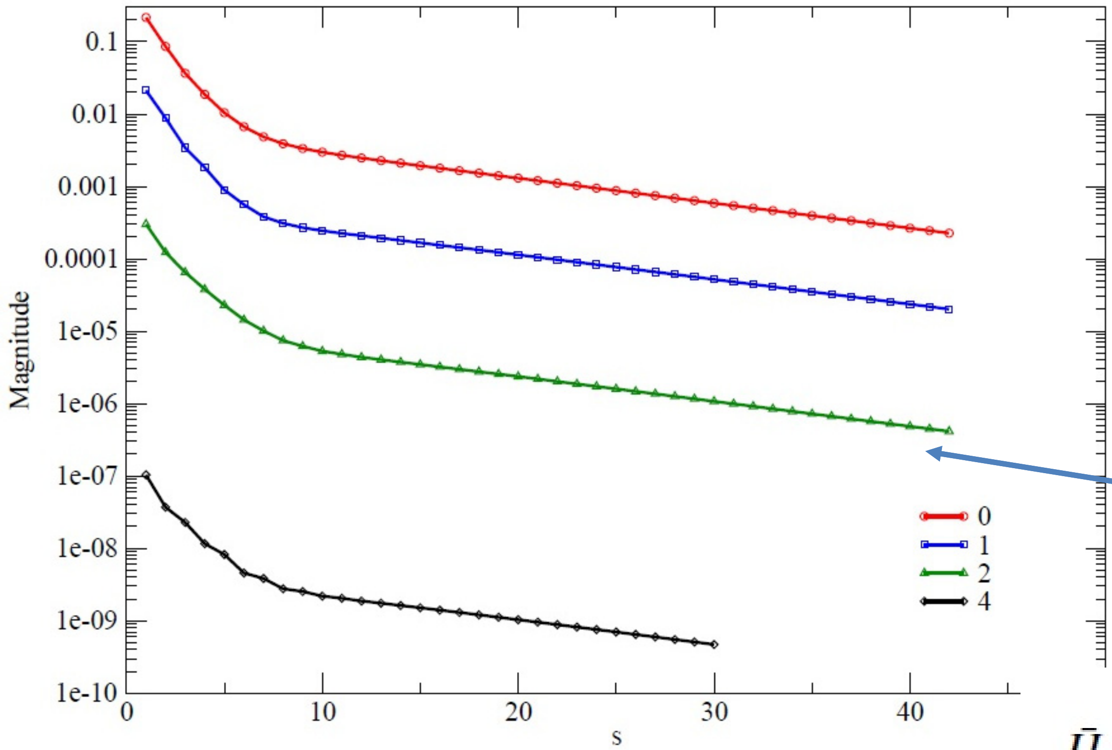

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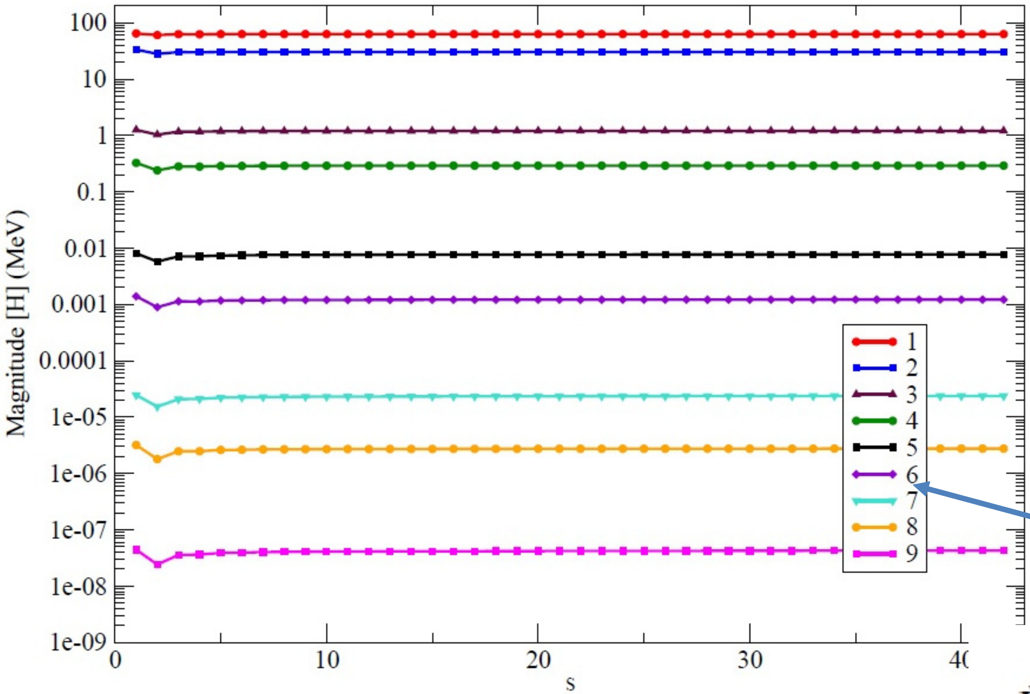

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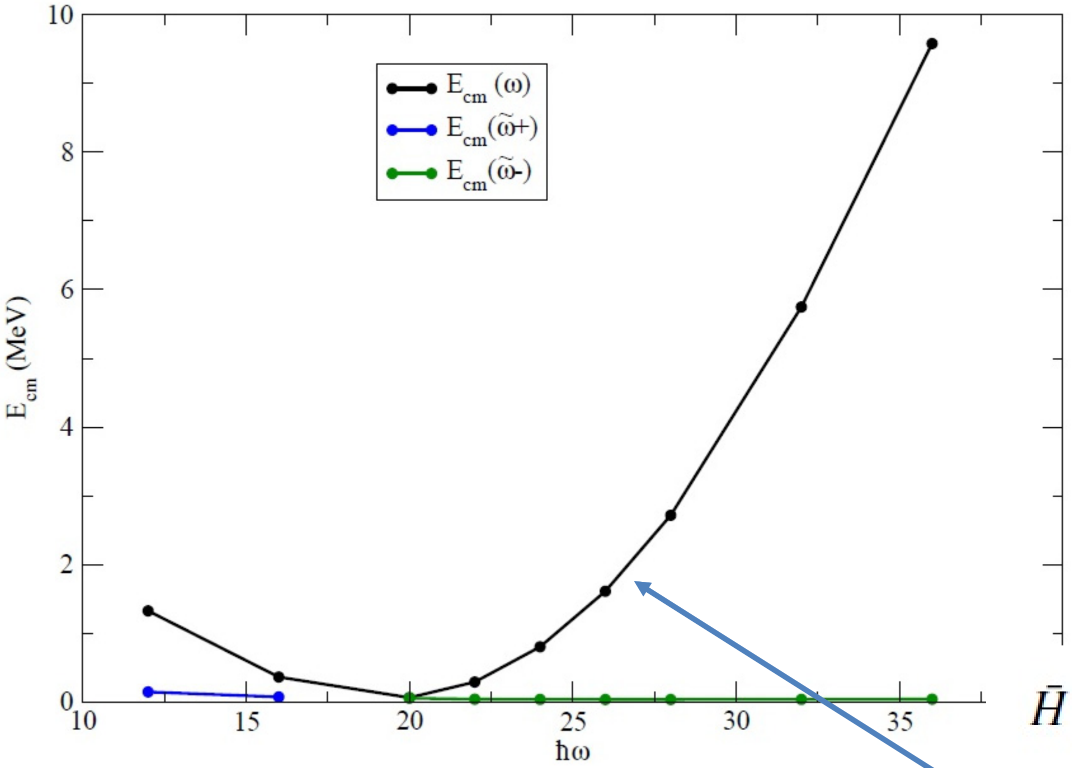
Magnus(2) ^{16}O C.O.M. Diagnostic



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$$\bar{H}_{cm} = exp(\Omega) H_{cm} \, exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_\Omega^k(H_{cm})$$

G. Hagen, T. Papenbrock, D. J. Dean, and M. Hjorth-Jensen, Phys. Rev. C **82**, 034330

Magnus(2) Observations

- G.S. decoupling, $\Omega \approx T - T^\dagger$
- CPU time, Magnus(2)≤IMSRG(2)
- $\bar{O}$ has similar cost as one timestep
  - Can be done after calculation
  - This is especially useful for Shell Model (R. Stroberg)
- MR-MAGNUS(2) is similarly successful
- Allows for approximation of Magnus(3)

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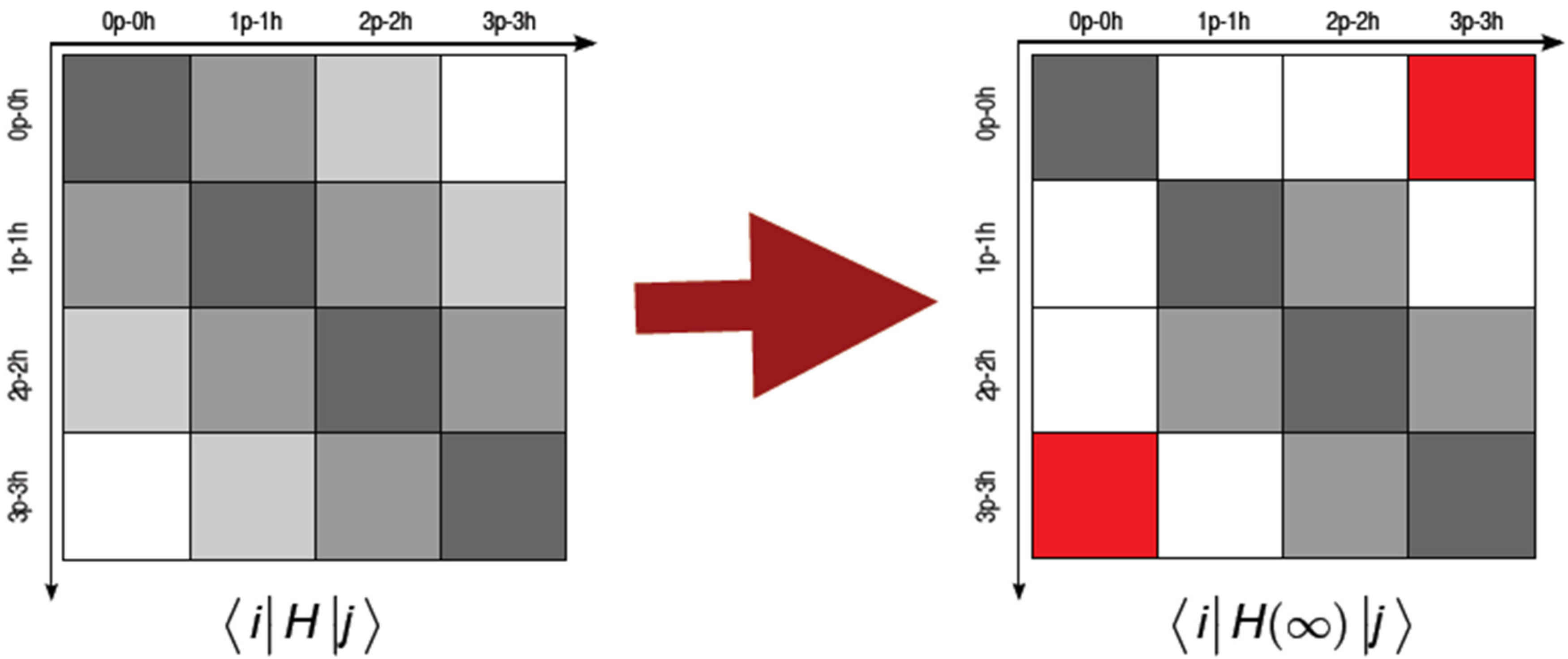
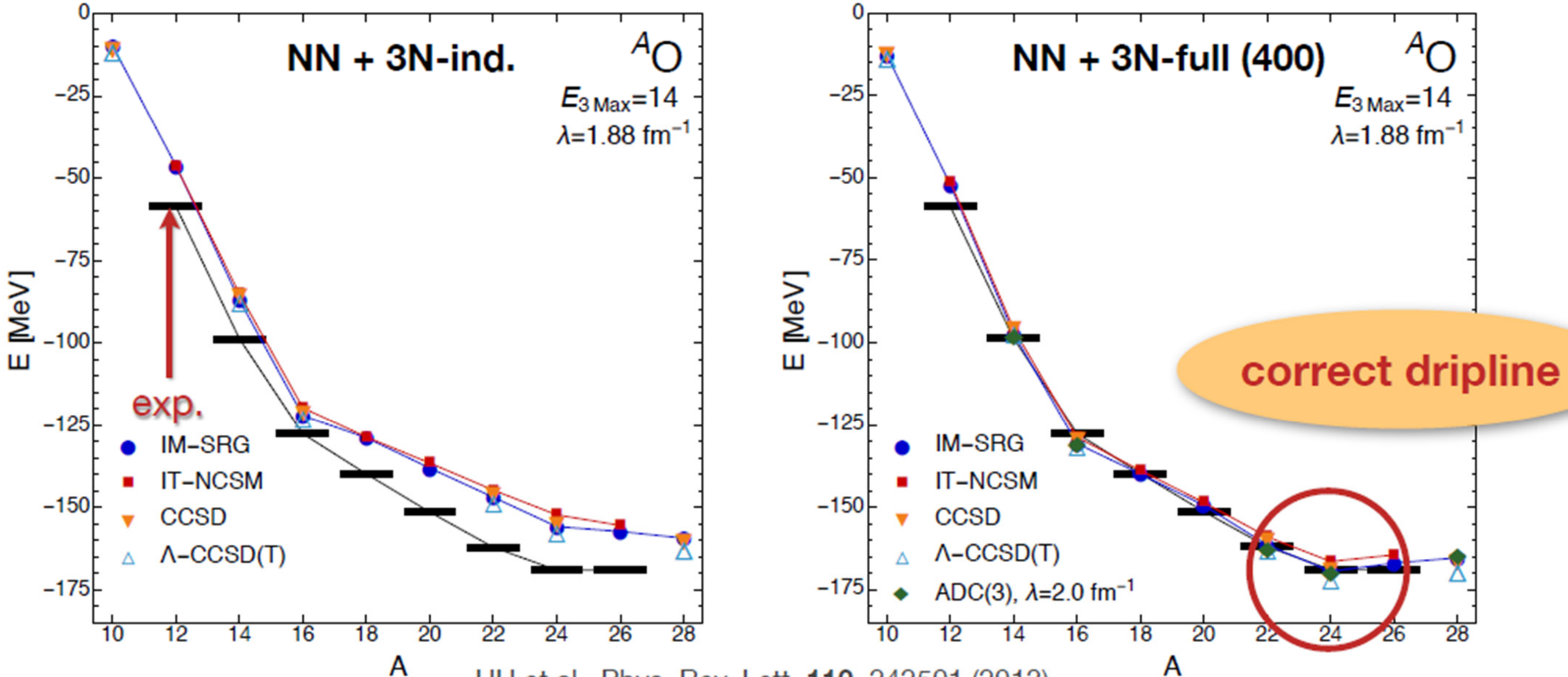
  - This is especially useful for Shell Model (R. Stroberg)
- MR-MAGNUS(2) is similarly successful
- Allows for approximation of Magnus(3)
  - What separates Magnus(2) from Magnus(3)?

Decoupling in A-Body Space



aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

Results: Oxygen Chain



HH et al., Phys. Rev. Lett. **110**, 242501 (2013)

ADC(3): A. Cipollone et al., Phys. Rev. Lett. **111**, 242501 (2013)

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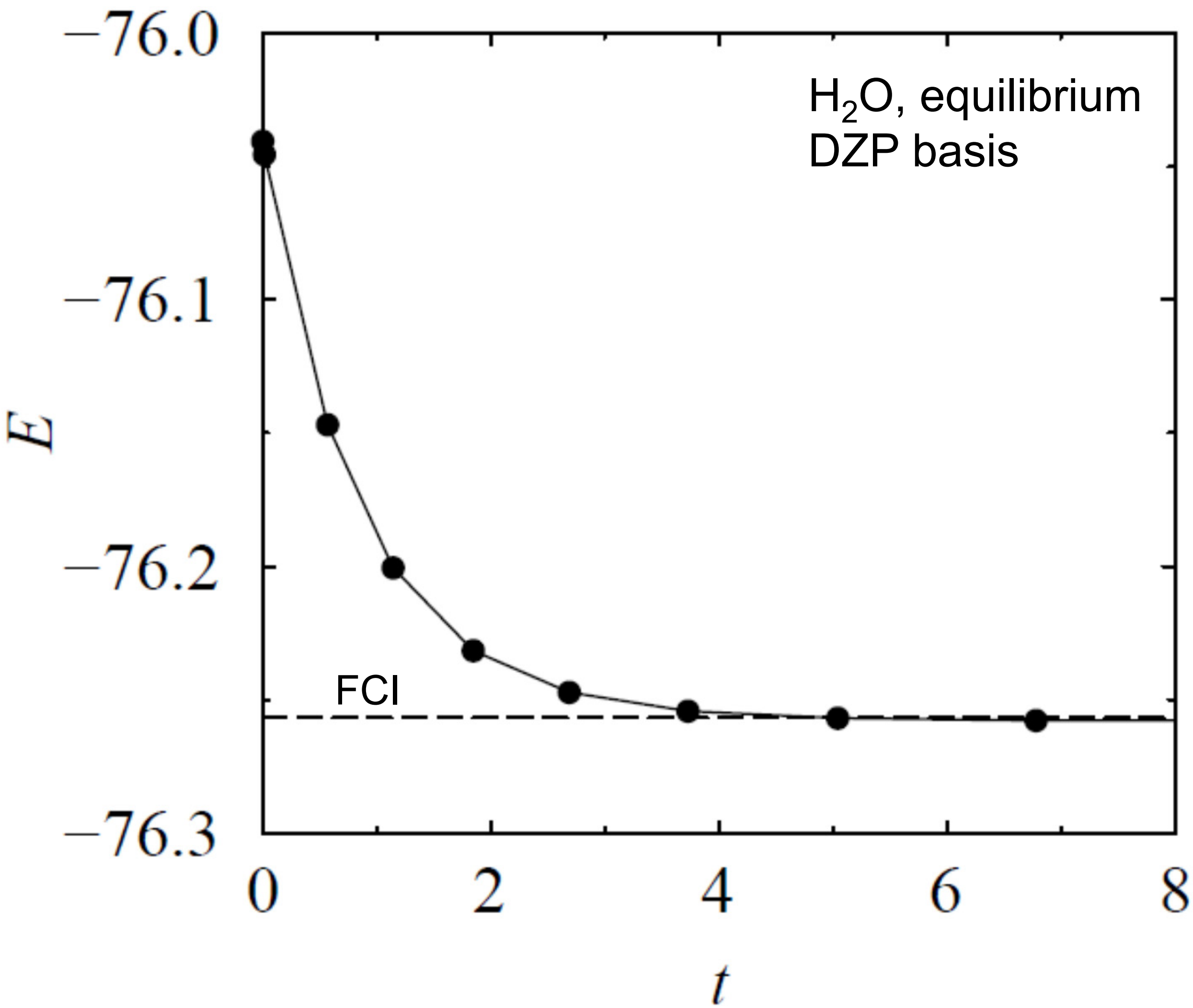
- consistent results from different many-body methods

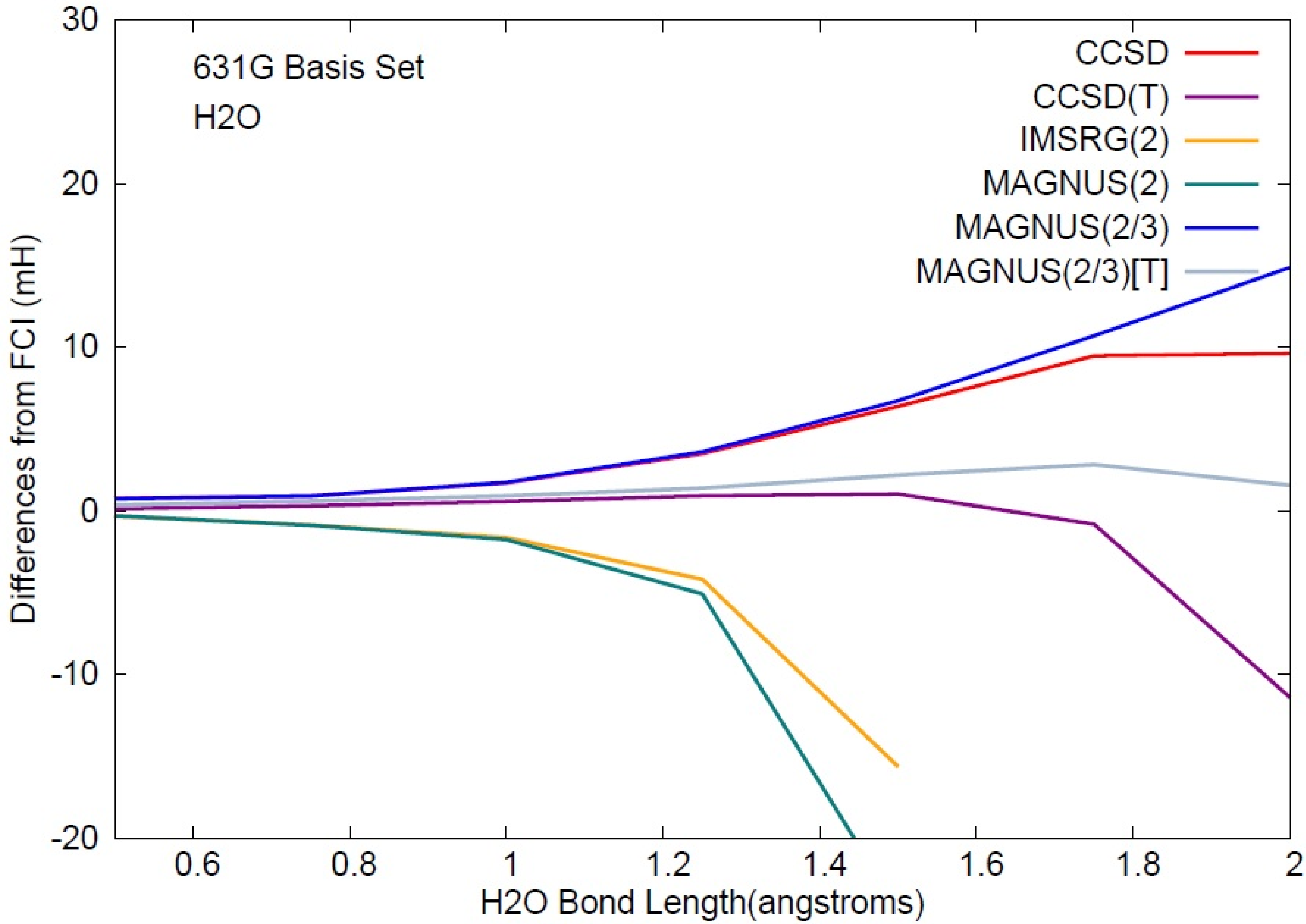
Puzzling Chemistry results



S.R. White, J. Chem. Phys. 117, 7472 (2002)

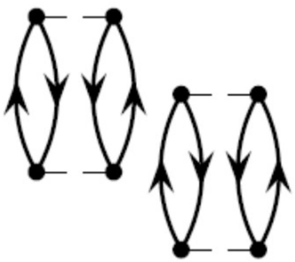
This result is actually dramatically overbound by chemistry standards!

Puzzling Chemistry results



M.E./M.B. results calculated with Psi4

Fixing Missing MBPT4



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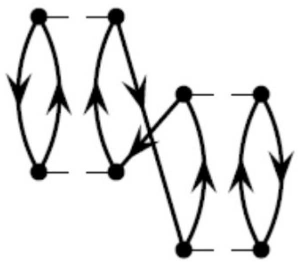
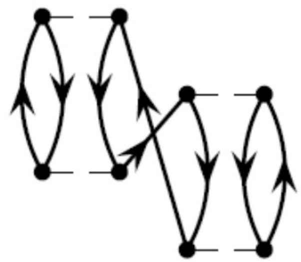


34



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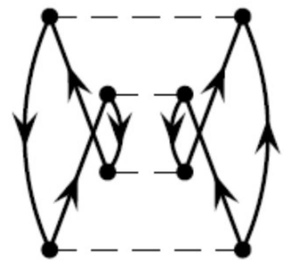

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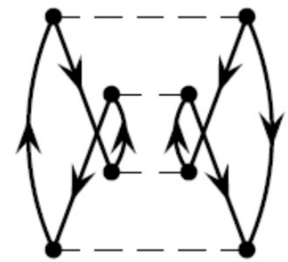

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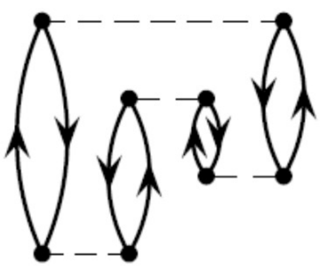

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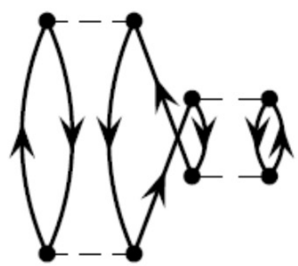

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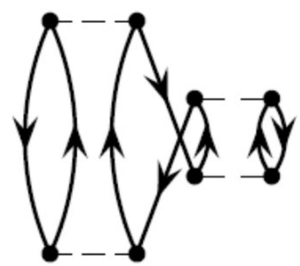

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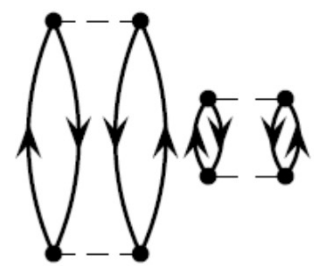
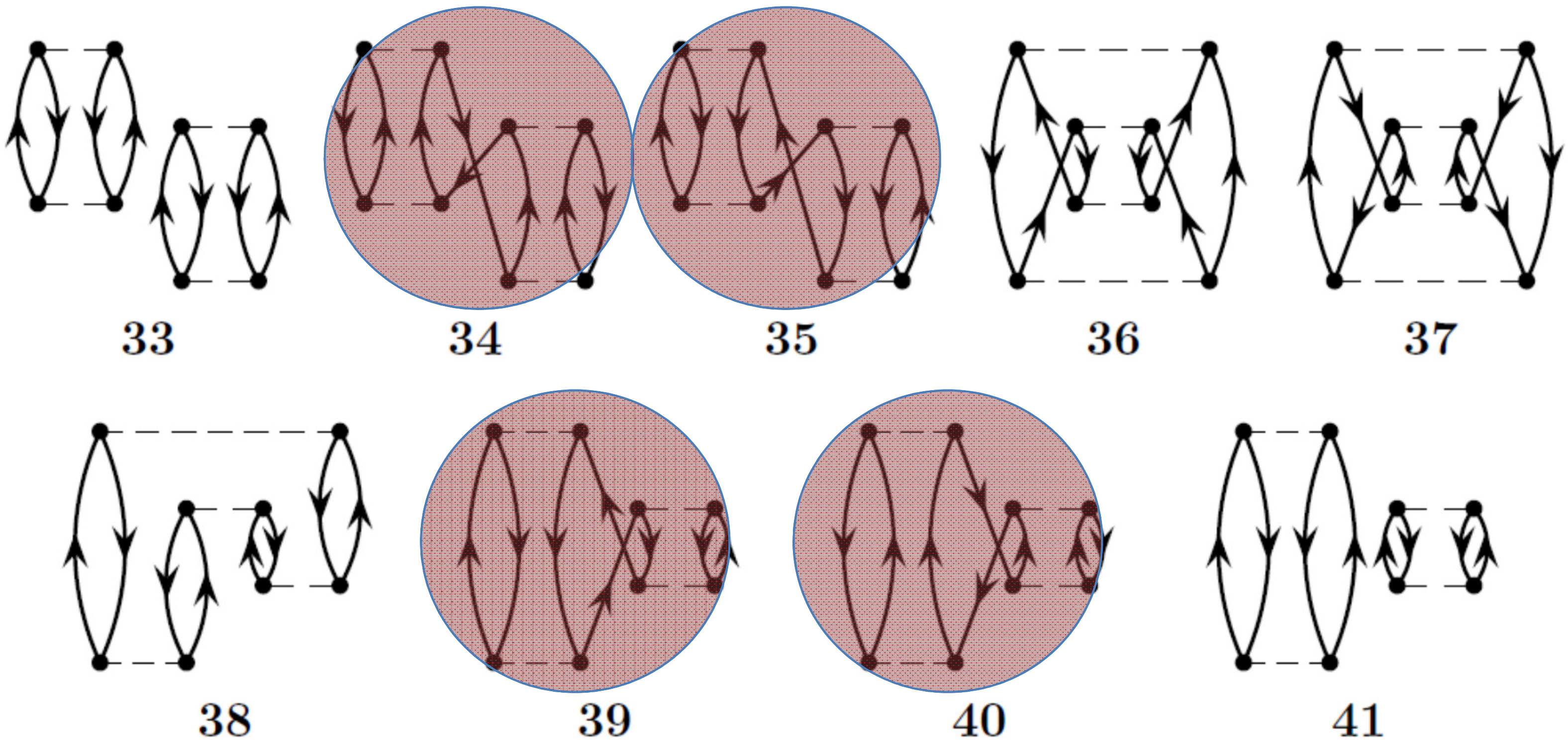


41

Fixing Missing MBPT4



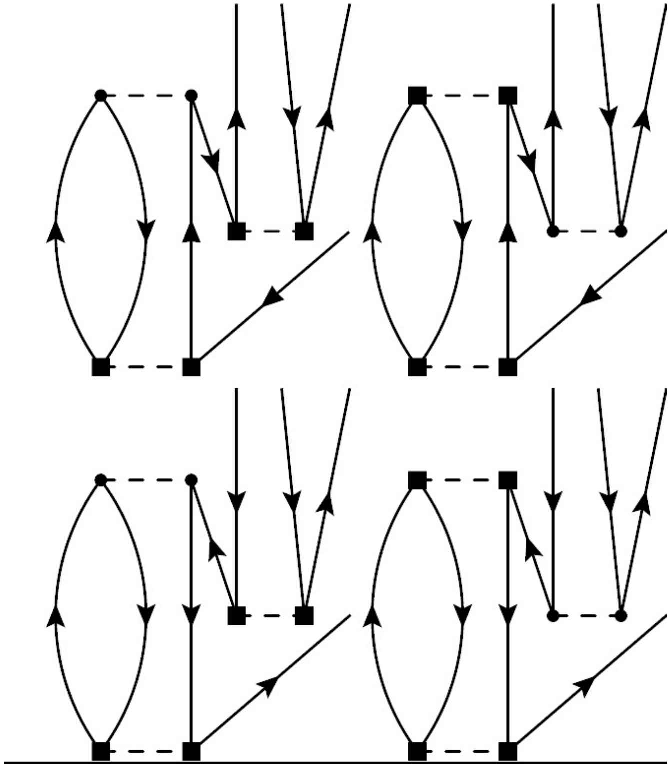
$$\frac{1}{2}(\Delta E_{34} + \Delta E_{35} + \Delta E_{39} + \Delta E_{40}) \subset \Delta E_{IMSRG(2)}, \Delta E_{MAGNUS(2)}$$

Missing MBPT(4) content

$$\bar{H} = exp(\Omega)H\,exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(H)$$

$$[\Omega, [\Omega, X]_{3B}]_{2B}$$

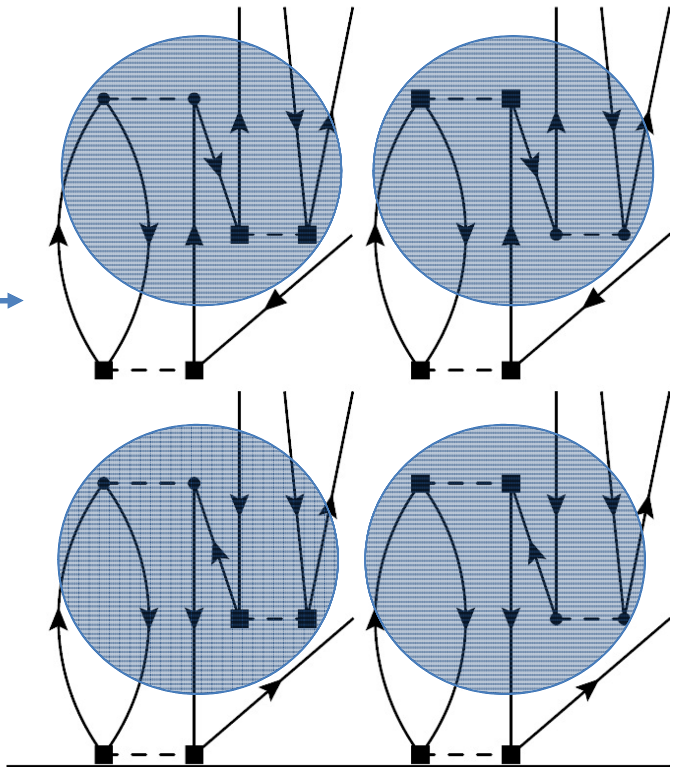
Restoring this term to all commutators makes the method Magnus(2/3) agree with CCSD!



Missing MBPT(4) content

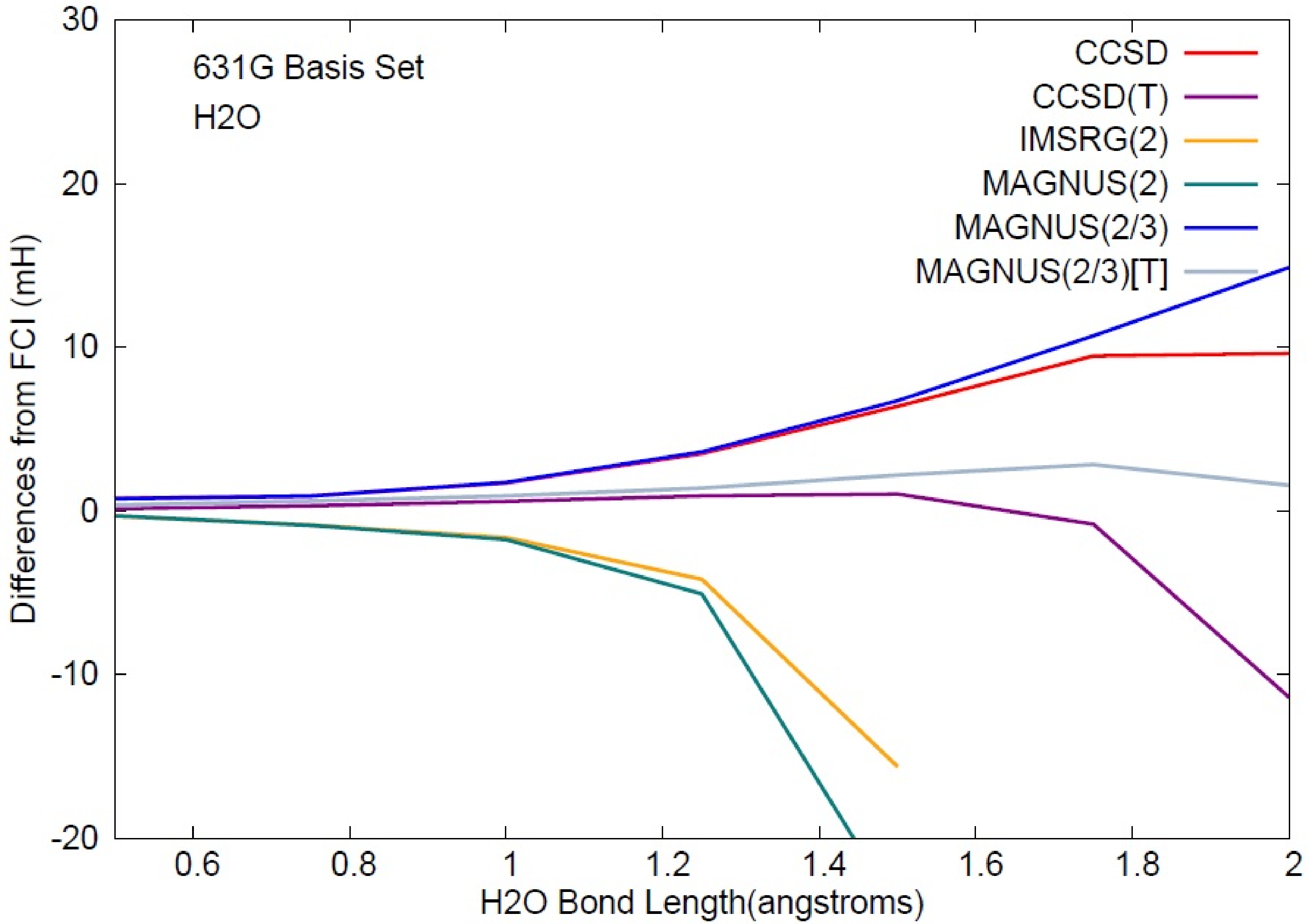
$$\bar{H} = exp(\Omega)H\,exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(H)$$

$$[\Omega, [\Omega, X]_{3B}]_{2B}$$



Restoring this term to all commutators makes the method Magnus(2/3) agree with CCSD!

Magnus(2/3) solves puzzle



M.E./M.B. results calculated with Psi4

Magnus(2/3)[T]

$$\bar{H} = exp(\Omega) H \, exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(H)$$

$$\bar{W} \approx [\Omega, H]_{3B} \qquad \Omega_{p_1 p_2 p_3 h_1 h_2 h_3} = \frac{\bar{W}_{p_1 p_2 p_3 h_1 h_2 h_3}}{\Delta_{p_1 p_2 p_3 h_1 h_2 h_3}}$$

$$\Delta E_T = \frac{1}{2} [\Omega^{(3)}, [\Omega^{(2)}, H]_{3B}]_{0B}$$

Magnus(2/3)[T]

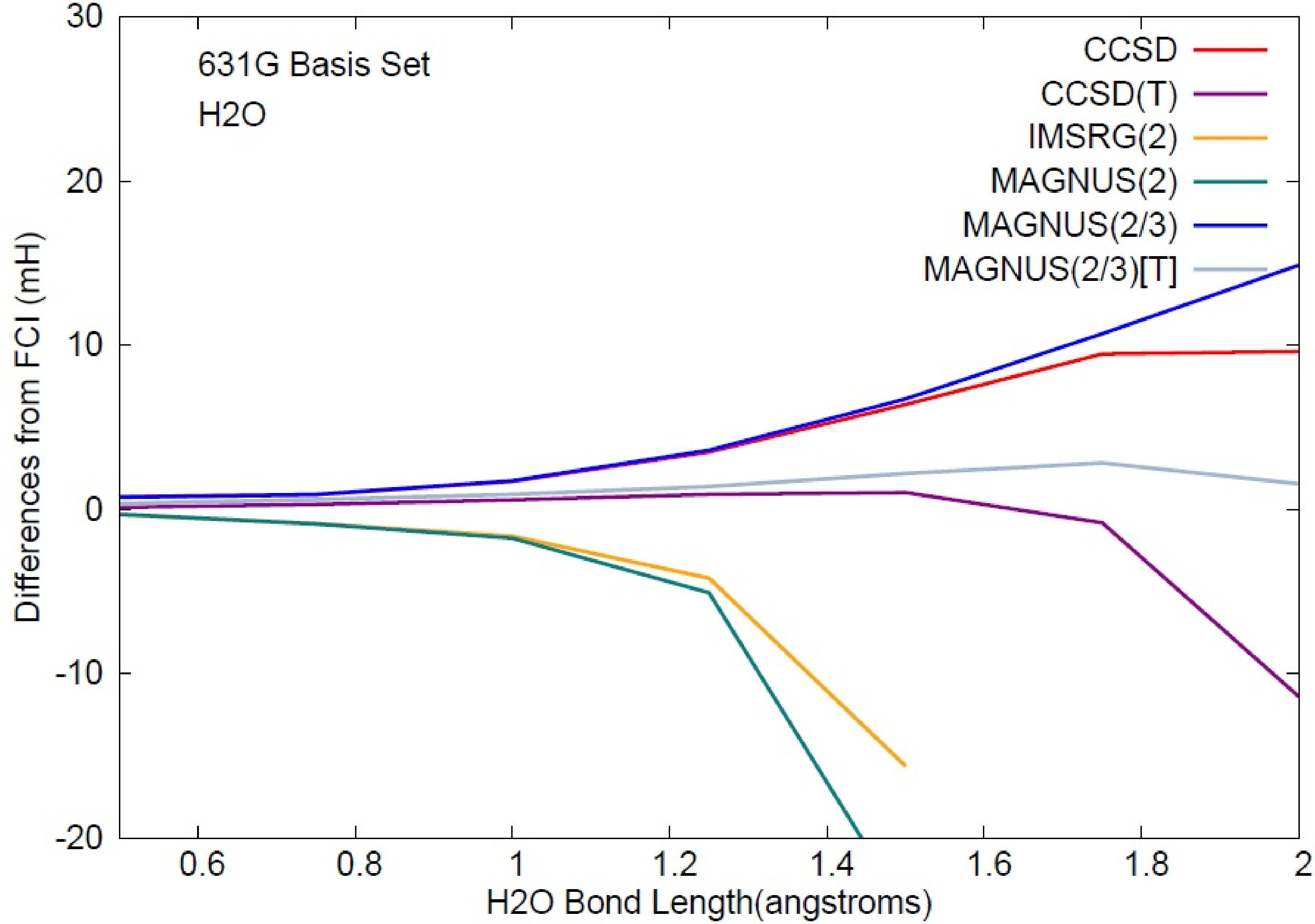
$$\bar{H} = exp(\Omega) H \, exp(-\Omega) = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(H)$$

$$\bar{W} \approx [\Omega, H]_{3B} \qquad \Omega_{p_1 p_2 p_3 h_1 h_2 h_3} = \frac{\bar{W}_{p_1 p_2 p_3 h_1 h_2 h_3}}{\Delta_{p_1 p_2 p_3 h_1 h_2 h_3}}$$

$$\Delta E_T = \frac{1}{2}[\Omega^{(3)}, [\Omega^{(2)}, H]_{3B}]_{0B}$$

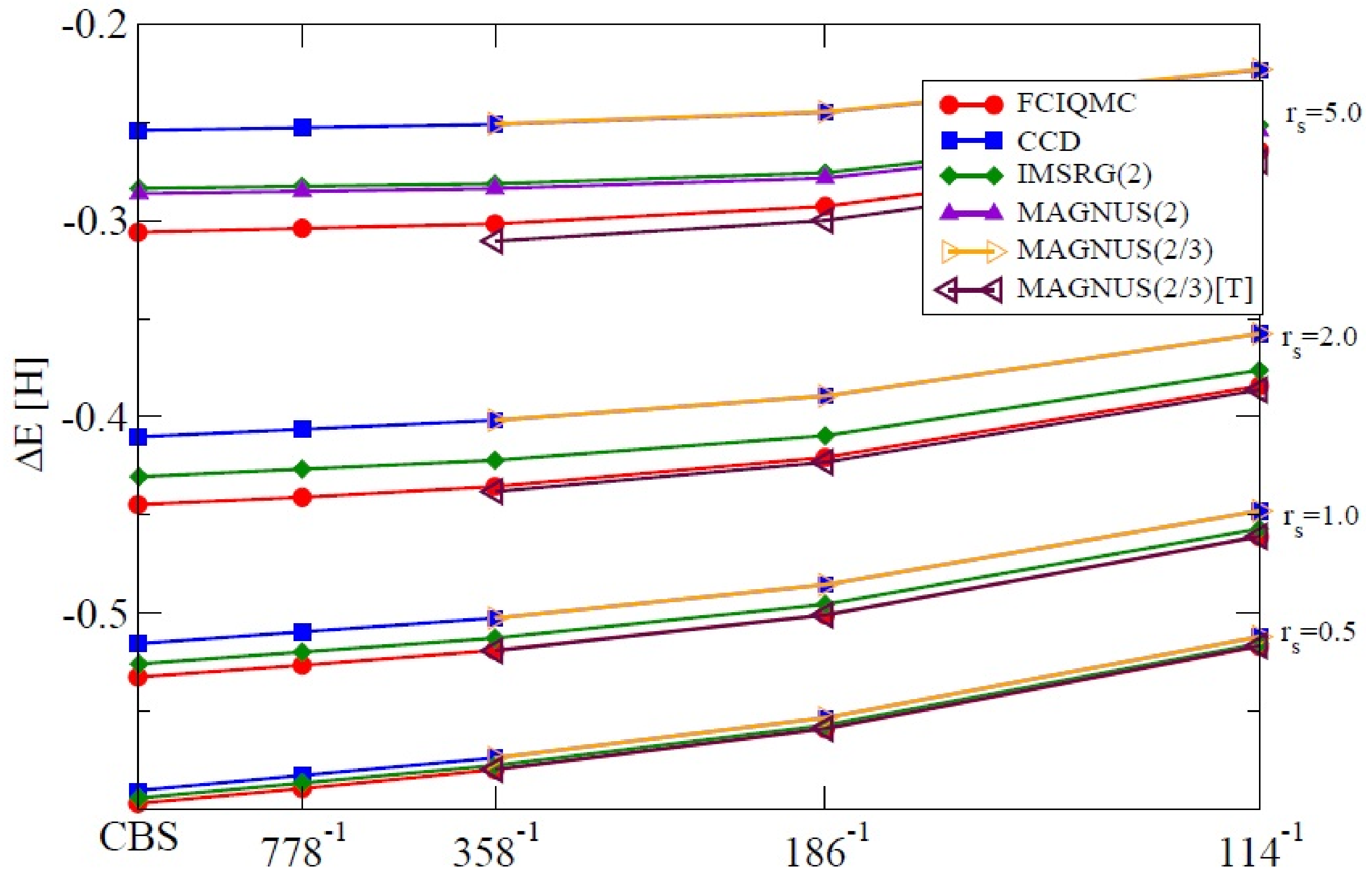
Get same expression using MBPT2 with W. But using commutator, these corrections can be carried out for observables as well with minimal change in code! **Maybe** applicable MR-MAGNUS!

Magnus(2/3)[T]



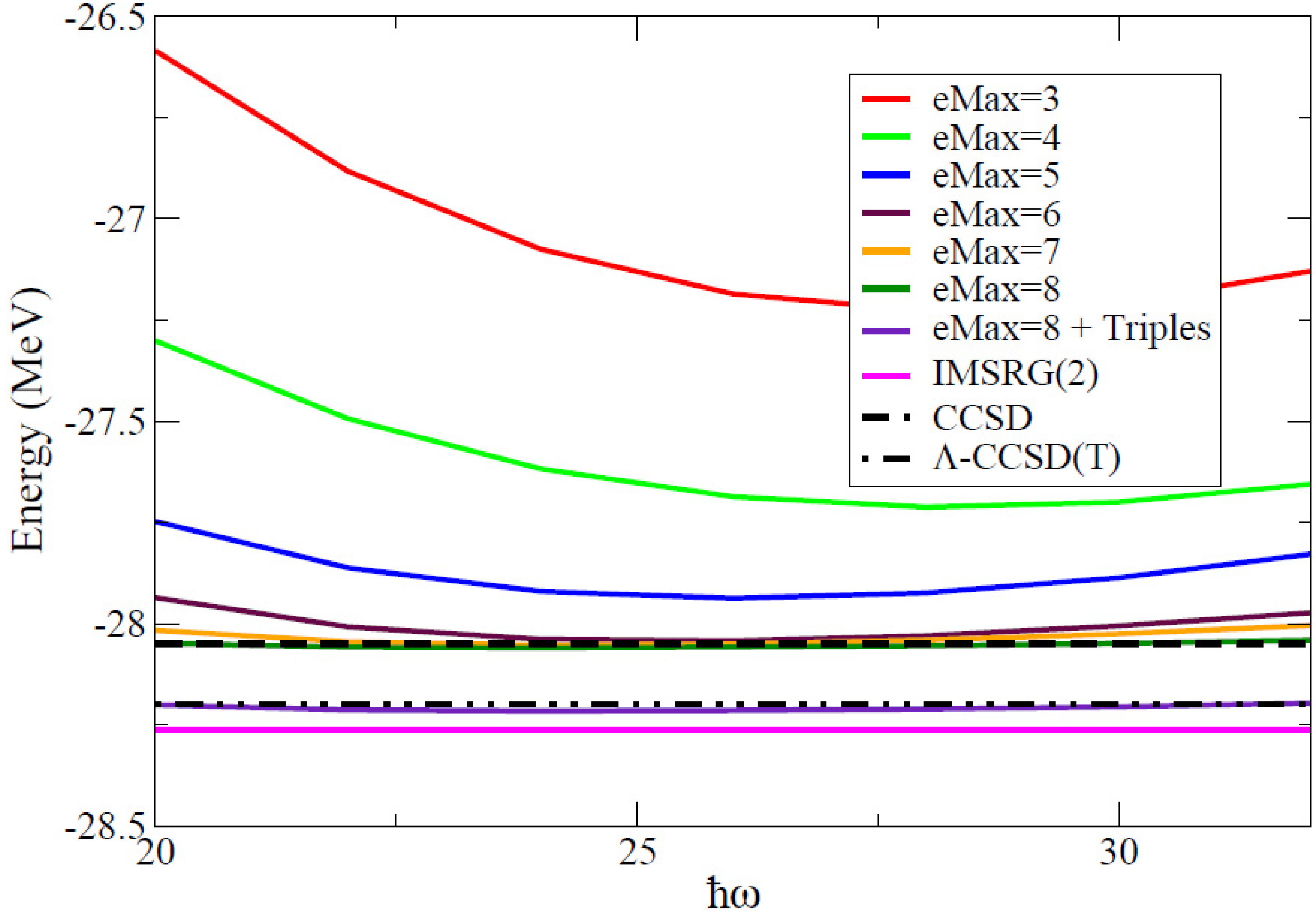
M.E./M.B. results calculated with Psi4

Magnus(2/3)[T]



-0.2
-0.3
-0.4
-0.5
ΔE [H]
CBS
778^-1
358^-1
186^-1
114^-1
FCIQMC
CCD
IMSRG(2)
MAGNUS(2)
MAGNUS(2/3)
MAGNUS(2/3)[T]
r_s=5.0
r_s=2.0
r_s=1.0
r_s=0.5

Magnus(2/3)[T] ^{4}He



N3LO E.M. NN $\lambda = 2.0$

Magnus(2/3)[T] Observations

- CCSD[T] cost
- More robust than CCSD[T] in chemistry
- PT analysis for shell model?
- Scuseria et al. $$\frac{1}{\Delta_{p1p2p3h1h2h3}} = -\int_0^\infty e^{-x\Delta_{p1p2p3h1h2h3}} dx$$
  - MR-MAGNUS(2/3)[T] computed at N^6
- All results are applicable to generic operators
- Past triple zero body

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