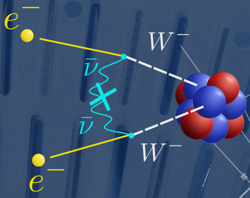
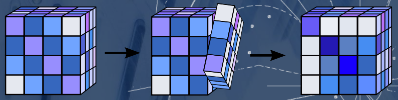
Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Neutrinoless Double Beta Decay with the Valence Space IMSRG

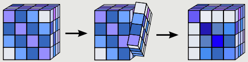




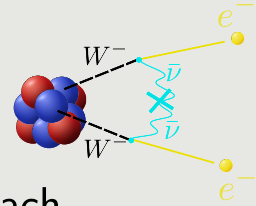
Ragnar Stroberg

TRIUMF

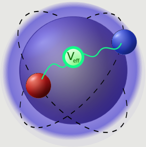
Neutrinoless Double Beta Decay
INT Program INT-17-2a
Seattle, Washington
June 20, 2017



Outline



1. Arguments for a valence space approach
2. Valence space IMSRG
3. Consistent evolution of operators
4. First $0\nu\beta\beta$ matrix elements and outlook



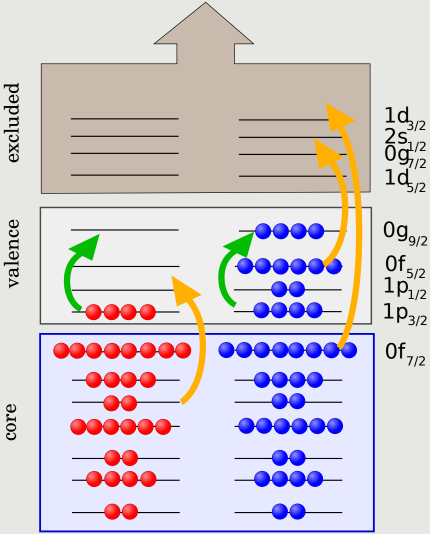
In collaboration with: A. Calci, J. Holt, P. Navrátil, C. Payne, S. Bogner, H. Hergert, N. Parzuchowski, K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf, G. Hagen, T. Morris, and J. Engel

	DFT	GCM	RPA	IBM	SM	CC	MR-IMSRG	NCSM	QMC
χ_{EFT}	✗	?	✗	✗	✔	✔	✔	✔	✔
p-shell	✗	✗	✗	✗	✔	✔	✔*	✔	✔
^{48}Ca	✔	✔	✔	✔	✔	✔	✔	?	?
^{76}Ge	✔	✔	✔	✔	✔	✗	?	✗	✗
^{82}Se	✔	✔	✔	✔	✔	✗	?	✗	✗
^{96}Zr	✔	✔	✔	✔	✔	✗	?	✗	✗
^{100}Mo	✔	✔	✔	✔	?	✗	?	✗	✗
^{116}Cd	✔	✔	✔	✔	?	✗	?	✗	✗
^{124}Sn	✔	✔	✔	✔	✔	✗	?	✗	✗
^{130}Te	✔	✔	✔	✔	✔	✗	?	✗	✗
^{136}Xe	✔	✔	✔	✔	✔	✗	?	✗	✗
^{150}Nd	✔	✔	✔	✔	✗	✗	?	✗	✗

Shell model / valence space approach

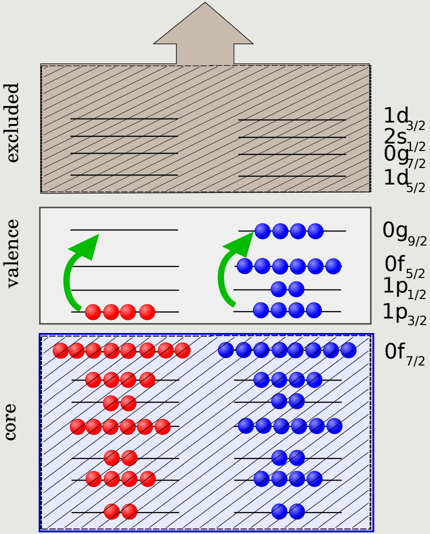
- Most $0\nu\beta\beta$ candidates are accessible
- Compatible with χ_{EFT} interactions $\Rightarrow$ consistent $0\nu\beta\beta$ operator (w/SRCs)
- Applicable in light systems $\Rightarrow$ benchmark with exact NCSM/QMC results
- Pairing/deformation/shell effects are incorporated
- Many other observables: energies, radii, single β decay, $E0$, EM moments/transitions
- Quantified unceraintities?

Shell model / valence space approach

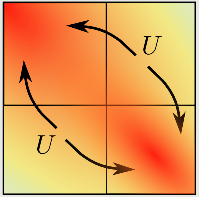


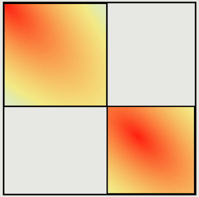
Renormalized interaction

- Phenom. adjustments
- Perturbation theory
- Non-pert. methods



Magnus IMSRG (Canonical transformation)





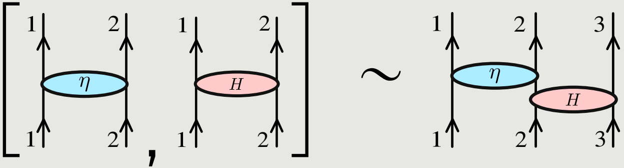
$$\underbrace{H|\Psi_n\rangle = E_n|\Psi_n\rangle}_{\text{Large space}} \qquad \underbrace{\tilde{H}|\Phi_n\rangle = E_n|\Phi_n\rangle}_{\text{Valence space}}$$

$$\begin{aligned}\tilde{H} &= UHU^\dagger = e^{\Omega}He^{-\Omega} \\ &= H + [\Omega, H] + \frac{1}{2!}[\Omega, [\Omega, H]] + \frac{1}{3!}[\Omega, [\Omega, [\Omega, H]]] + \ldots\end{aligned}$$

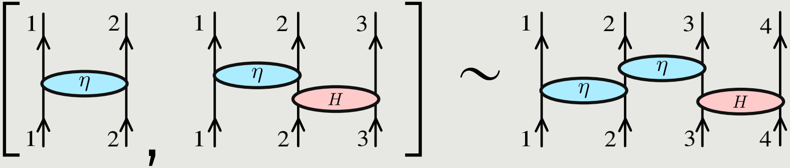
Glazek and Wilson 1994, Wegner 1994, Bogner, Furnstahl, and Perry 2007, Tsukiyama, Bogner, and Schwenk 2011; Tsukiyama, Bogner, and Schwenk 2012, Hergert et al. 2013, Bogner et al. 2014, Morris, Parzuchowski, and Bogner 2015...

Many-body forces

$$H + [\Omega, H] + \frac{1}{2!}[\Omega, [\Omega, H]] + \frac{1}{3!}[\Omega, [\Omega, [\Omega, H]]] + \dots$$



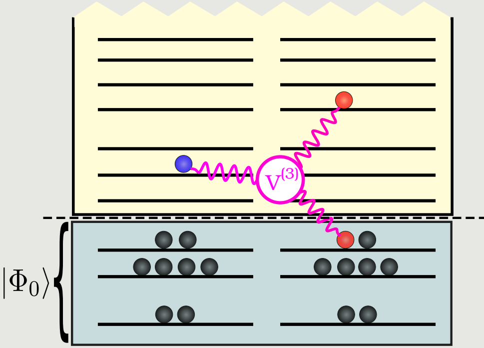
(Two-body) (Two-body) (Three-body)



(Two-body) (Three-body) (Four-body)

$$H = \underbrace{E_0}_{\text{0-body}} + \underbrace{\sum_{ij} H_{ij}\{a_i^\dagger a_j\}}_{\text{1-body}} + \underbrace{\frac{1}{4}\sum_{ijkl} H_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\}}_{\text{2-body}} + \underbrace{\frac{1}{36}\sum_{ijklmn} H_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}}_{\text{3-body}} + \ldots$$

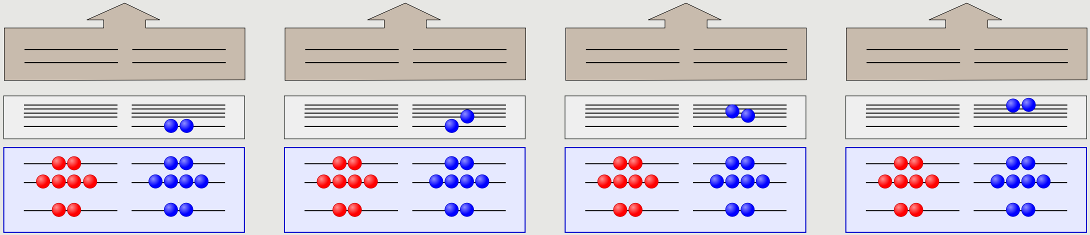
- Write H in terms of excitations out of reference $|\Phi_0\rangle$
- Normal ordering: $\langle\Phi_0|\{a_1^\dagger \ldots a_N^\dagger a_N \ldots a_1\}|\Phi_0\rangle = 0$
- If $|\Phi_0\rangle \approx |\Psi\rangle$, higher-body terms are negligible
- **Truncate all operators at 2 body level (NO2B)**



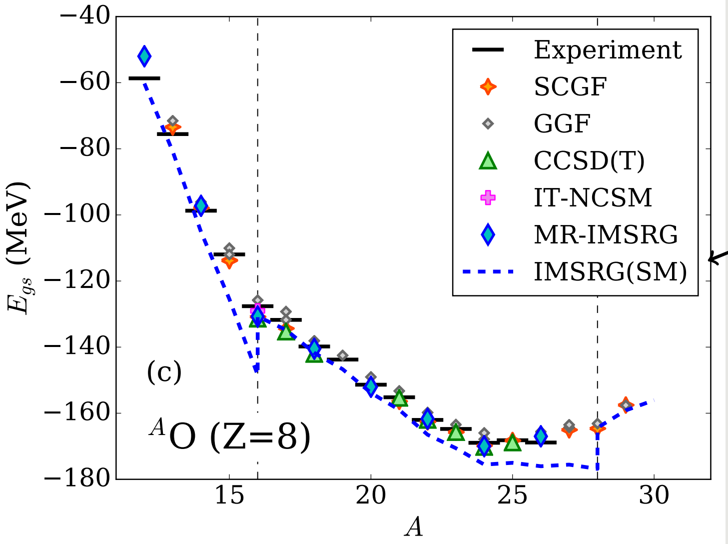
Tsukiyama, Bogner, and Schwenk 2011, Bogner et al. 2014

What reference should be used when decoupling a valence space?

(i.e. what is the "medium"?)



Obvious choice: the inert core, e.g. ^{16}O.

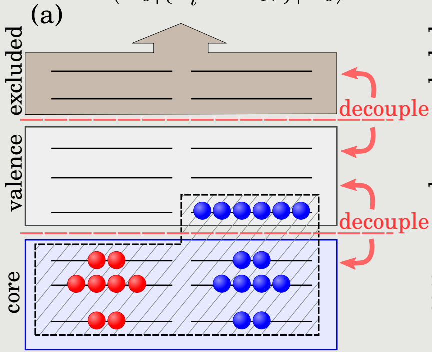


Reference: inert core

Somà et al. PRC (2013), Cipollone et al. PRC (2015), Jansen et al. PRL (2014), Roth et al. PRL (2012), Hergert et al. PRL (2013), Bogner et al. PRL (2014)

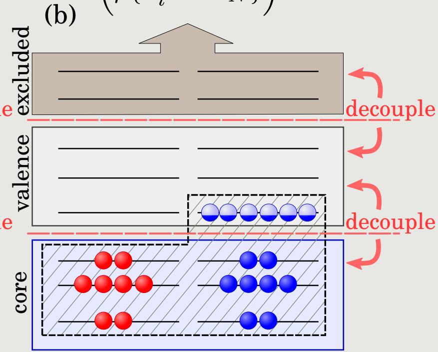
Ensemble normal ordering

$$\langle \Phi_0 | \{a_i^\dagger \dots a_N\} | \Phi_0 \rangle = 0$$

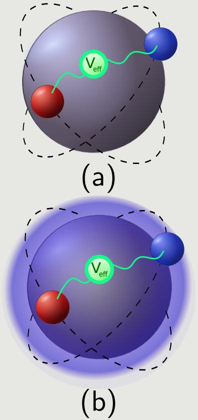


$$|\Phi_0\rangle = |^{22}\mathrm{O}\rangle$$

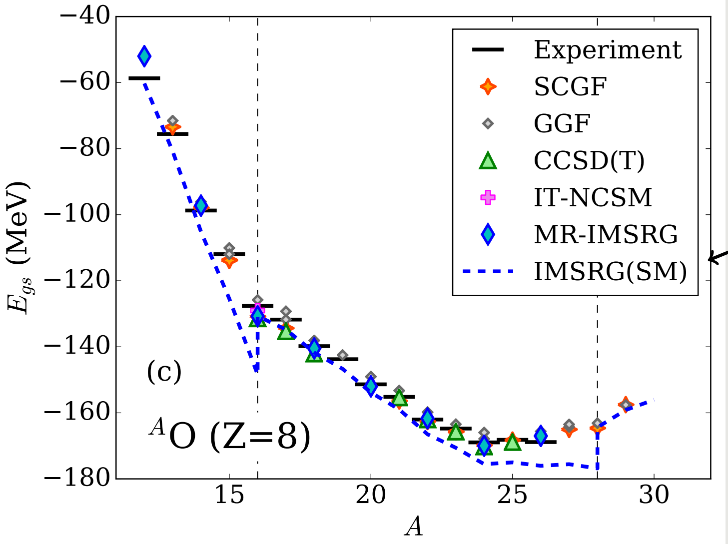
$$\mathrm{Tr}\left(\rho\{a_i^\dagger \dots a_N\}\right) = 0$$



$$\rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|$$

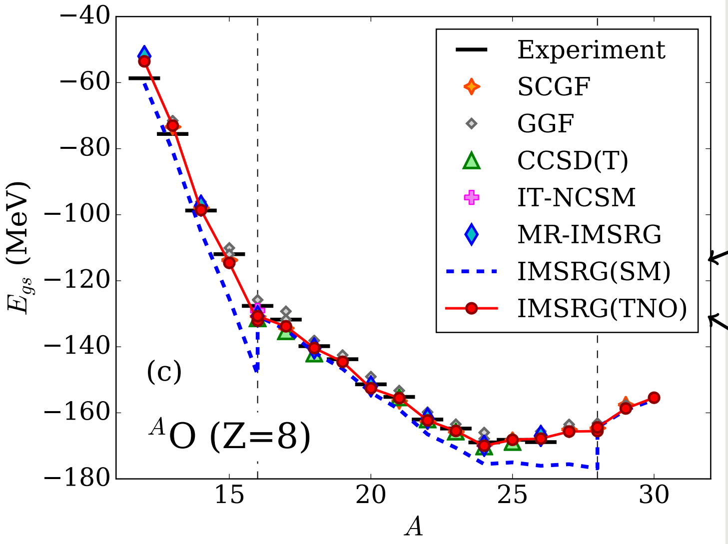


SRS(2015), SRS(2016)



Reference: inert core

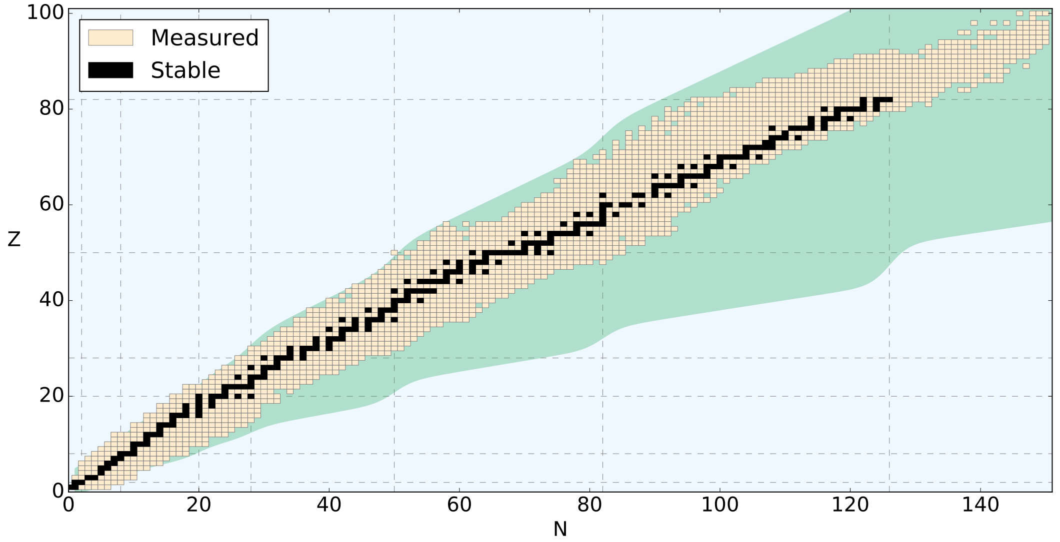
Ensemble normal ordering



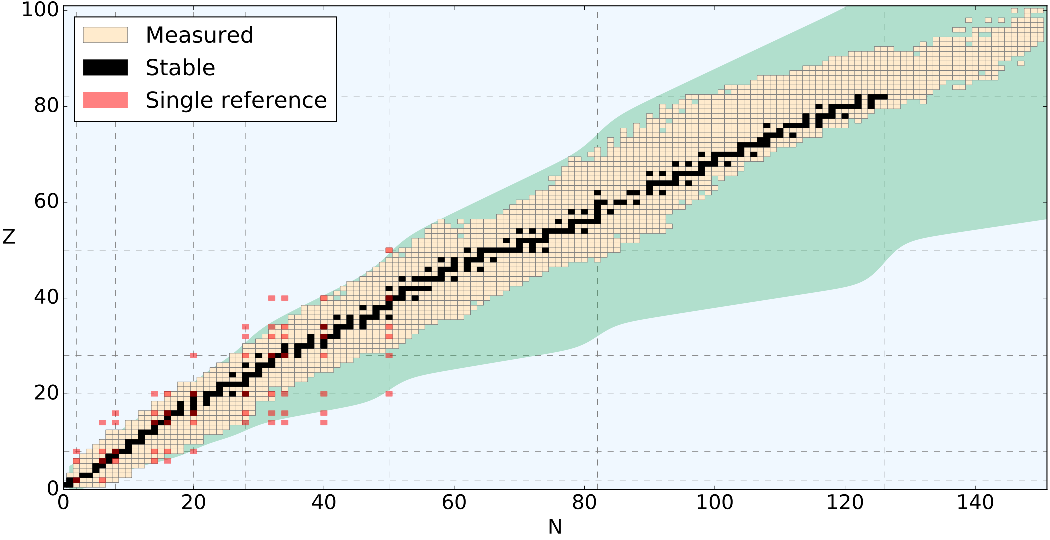
Reference: inert core

Ensemble reference

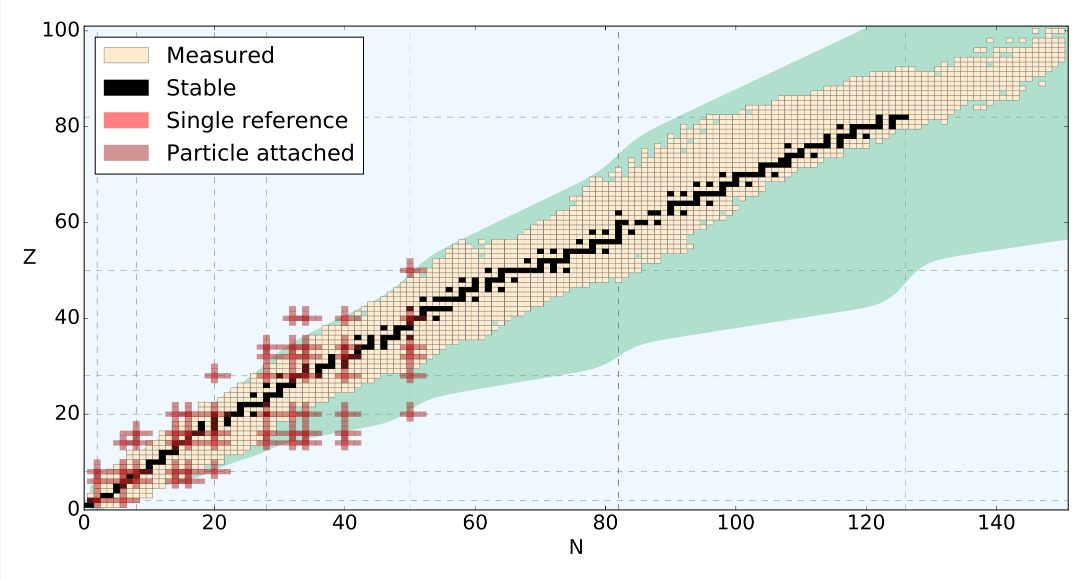
The reach of ab initio theory



The reach of ab initio theory



The reach of ab initio theory



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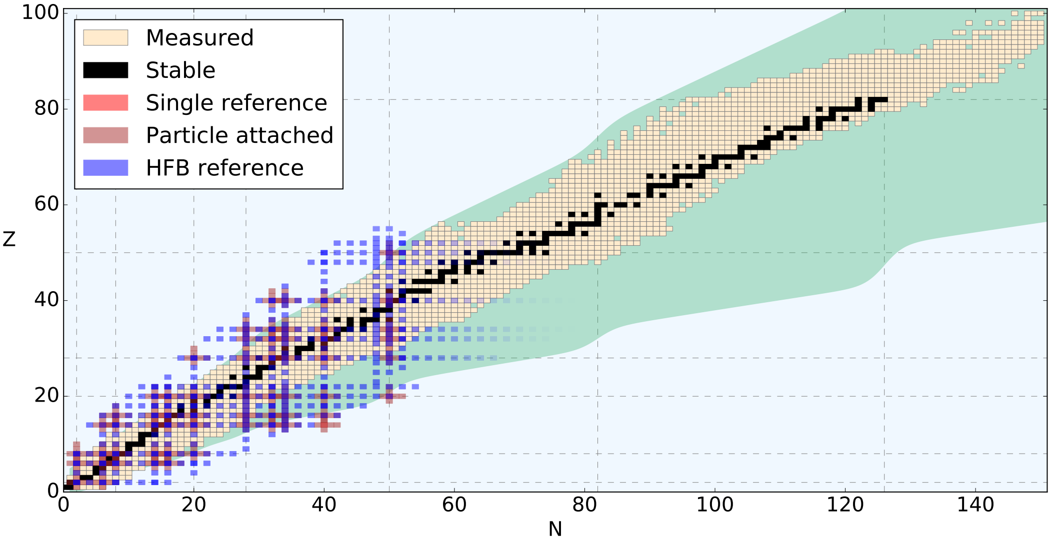

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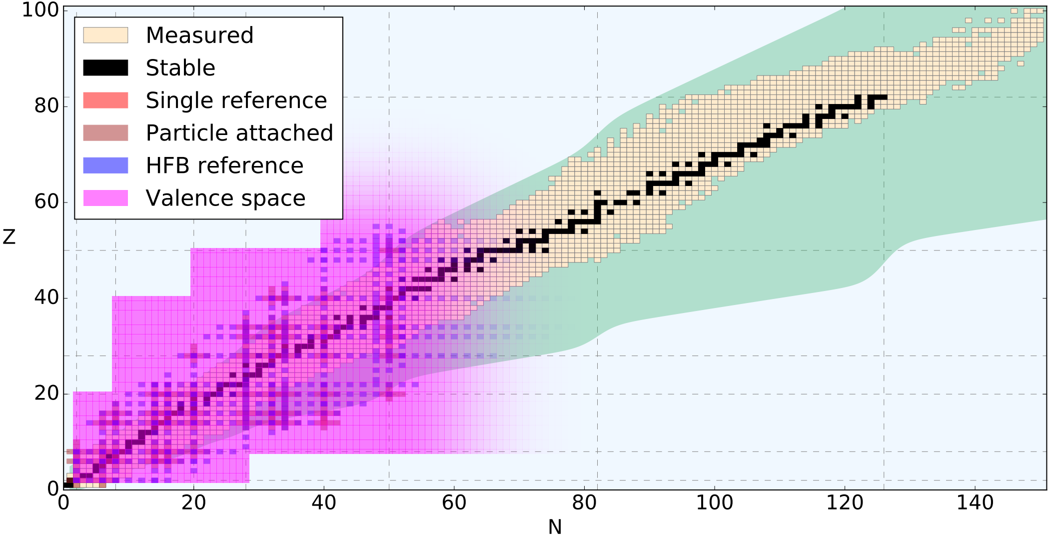

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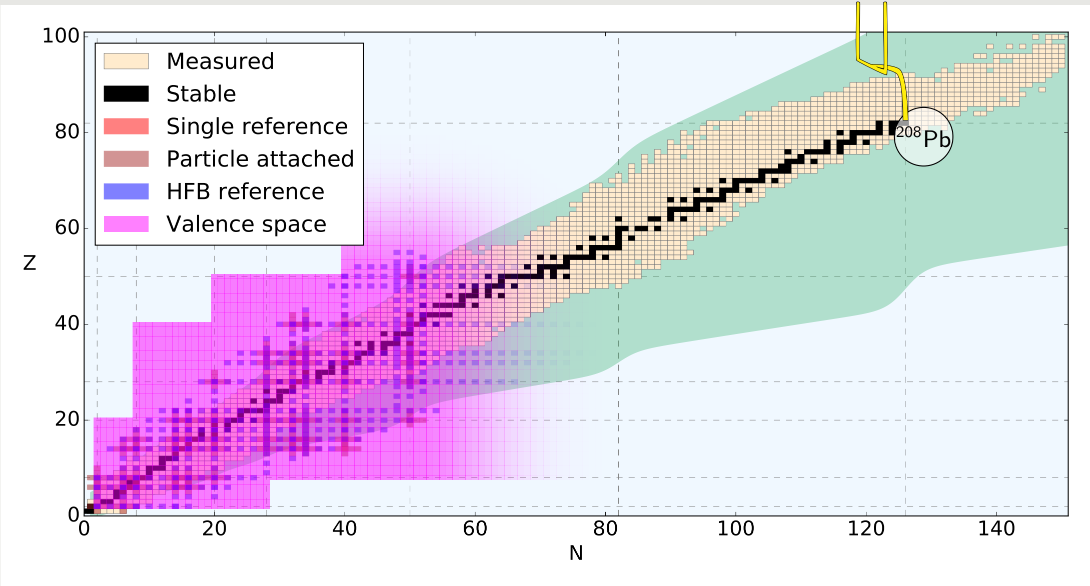

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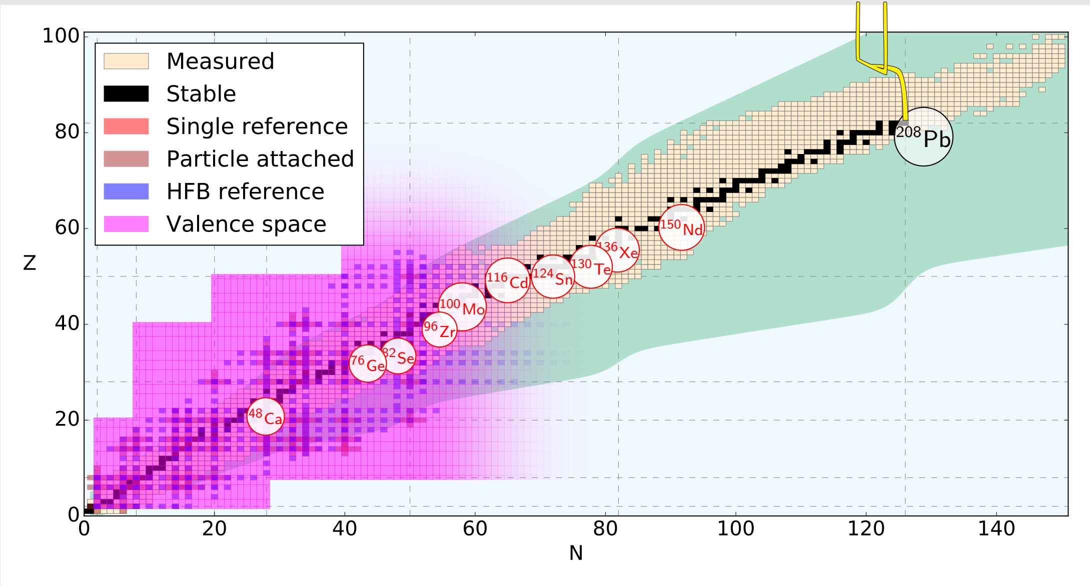
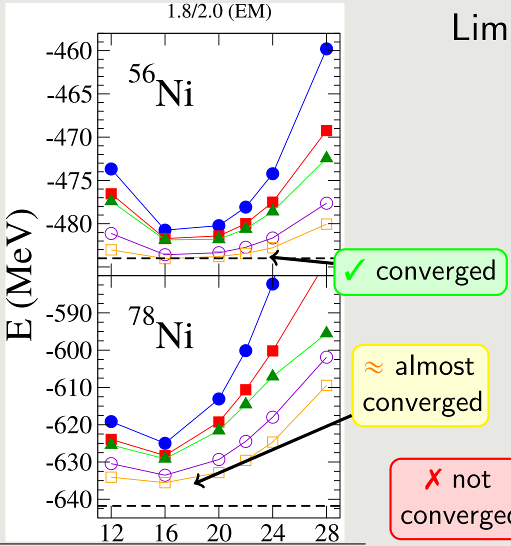
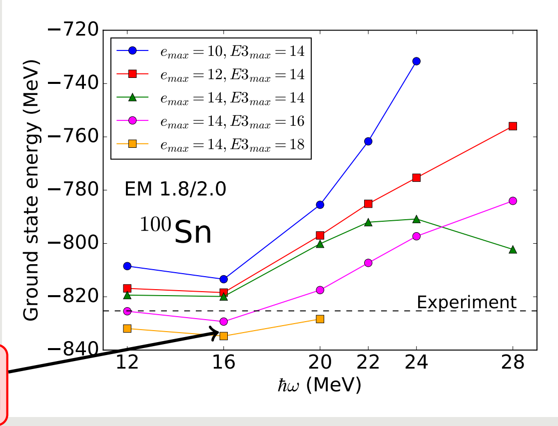




Limited by truncation of 3N matrix elements

$$E3_{max} = e_1 + e_2 + e_3$$



Simonis et al. (2017)

Limited by truncation of 3N matrix elements

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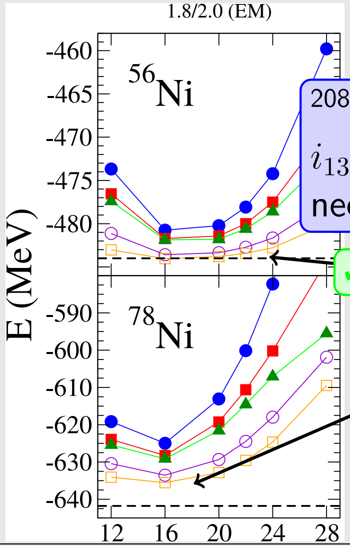


^{208}Pb:

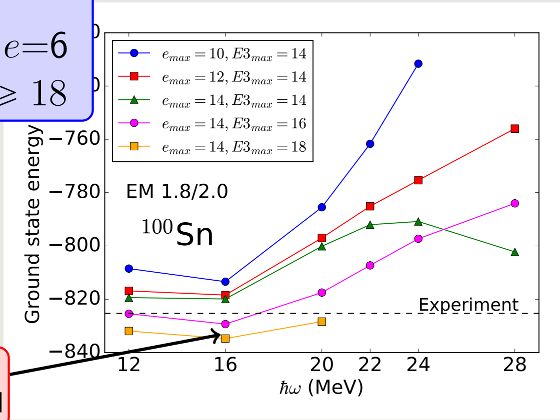
$i_{13/2}$ orbit $\to$ e=6

need $E3_{max} \geqslant 18$

✓ converged

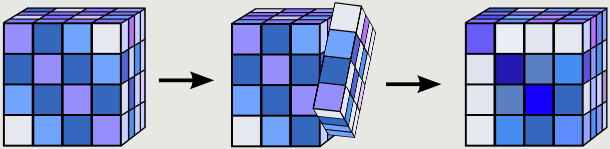
≈ almost converged

✗ not converged



Simonis et al. (2017)

Consistently evolved operators



Consistently evolved operators

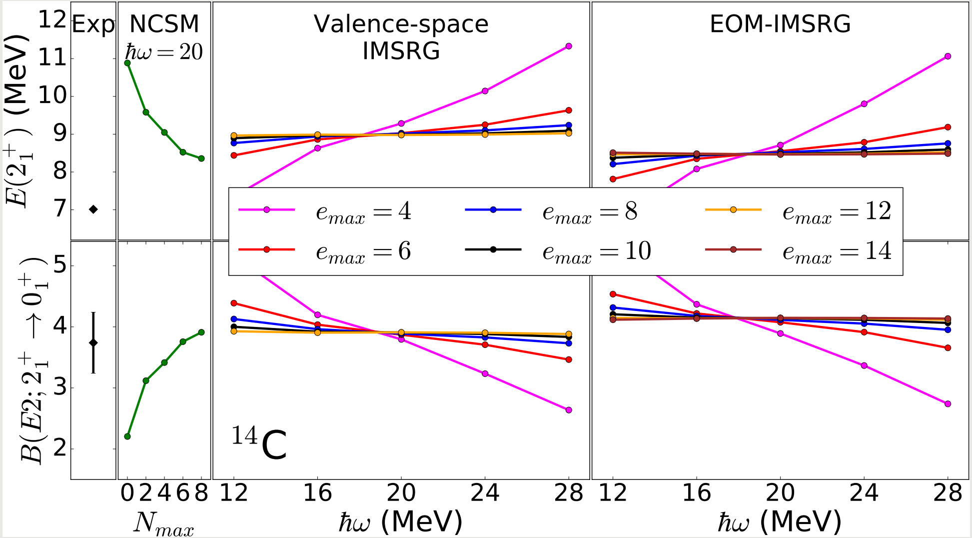
Hamiltonian:

$$\tilde{H} = UHU^{\dagger} = e^{\Omega} H e^{-\Omega}$$
$$= H + [\Omega, H] + \frac{1}{2!}[\Omega, [\Omega, H]] + \dots$$

Operator with tensor rank λ:

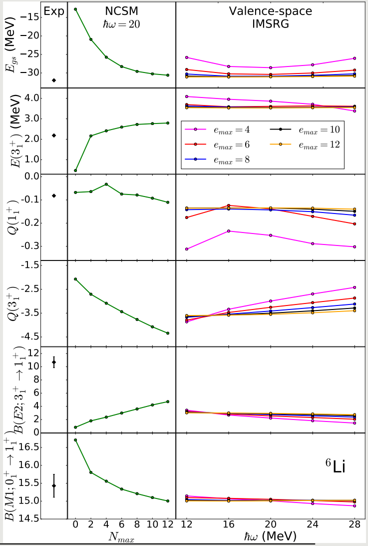
$$\tilde{\mathcal{O}}^{\lambda} = U\mathcal{O}^{\lambda}U^{\dagger} = e^{\Omega}\mathcal{O}^{\lambda}e^{-\Omega}$$
$$= \mathcal{O}^{\lambda} + [\Omega, \mathcal{O}^{\lambda}] + \frac{1}{2!}[\Omega, [\Omega, \mathcal{O}^{\lambda}]] + \dots$$

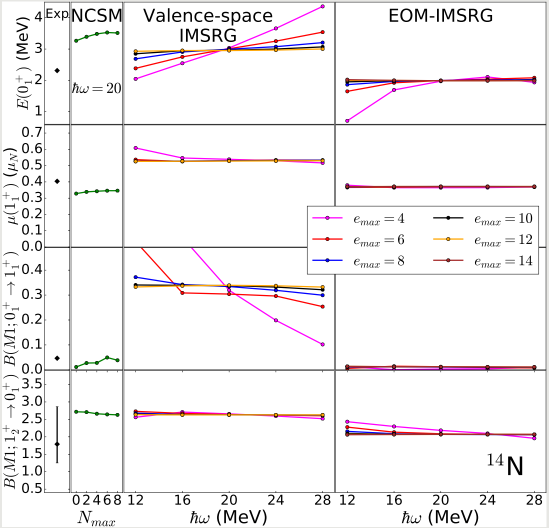
Consistently evolved operators: Benchmark with NCSM



Parzuchowski et. al (2017)

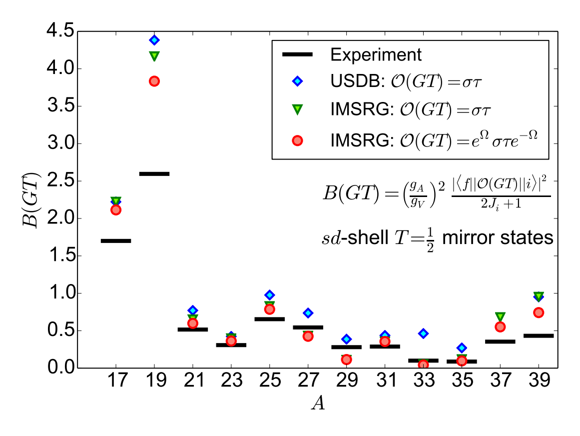
Consistently evolved operators: Benchmark with NCSM

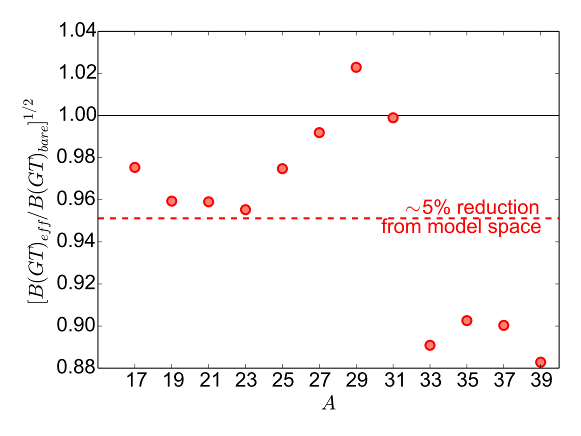




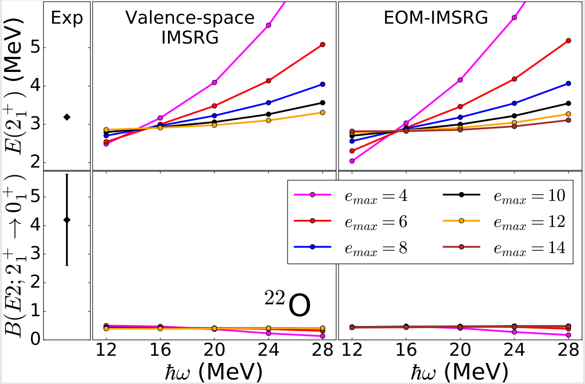
Parzuchowski et. al (2017)

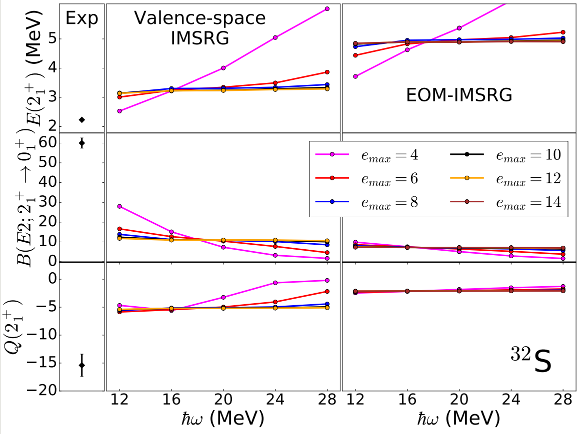
Consistently evolved operators: Corrections to GT operator





Consistently evolved operators: weak E2 strength





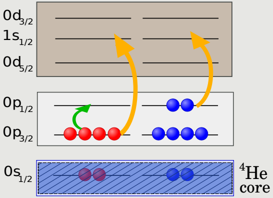
- Results converged w.r.t e_{max}, $\hbar\omega$
- Underpredicts experiment by 5-10×
- NO2B approximation?

Parzuchowski et. al (2017)

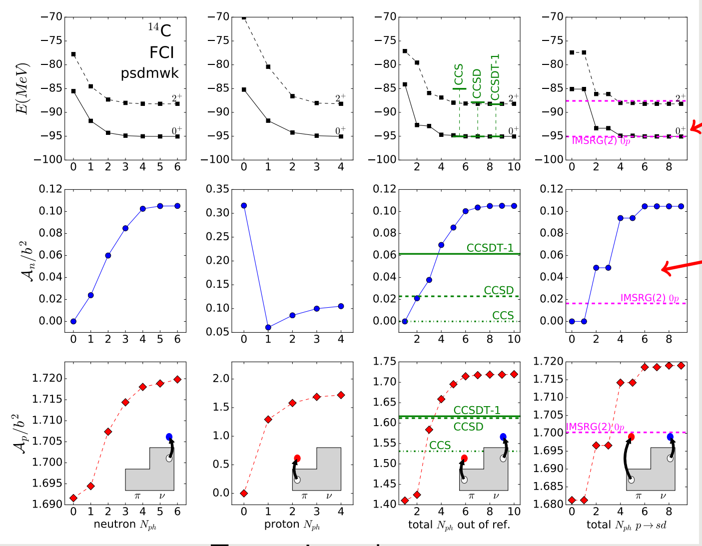
Missing E2 strength

Toy problem:

^{14}C in p-sd shell



- Diagonalize with various truncations
- Compare with results of CC & IMSRG

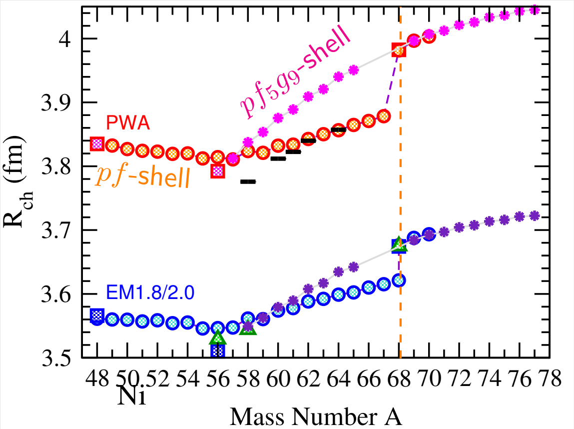


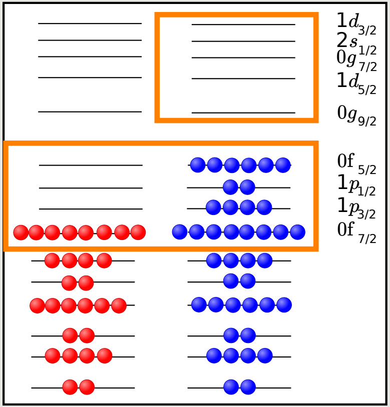
Truncation schemes →

Energy well-reproduced

Missing cross-shell excitations essential

Radii of Ni isotopes

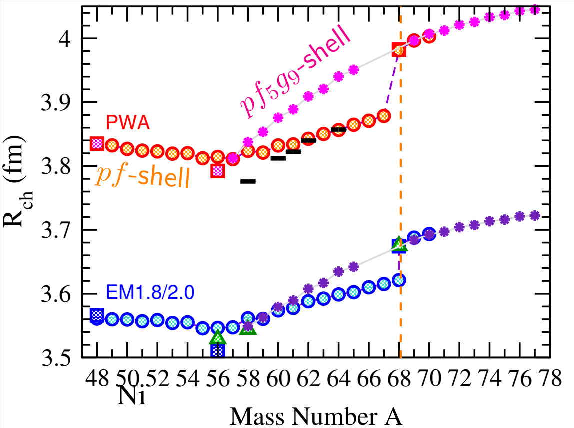


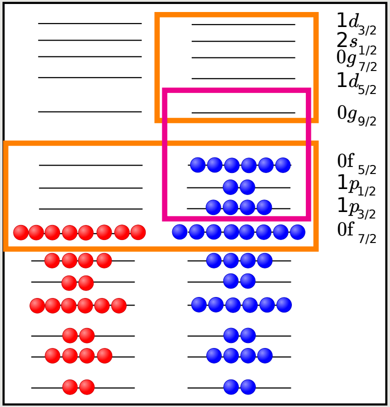


Changing the valence space changes the results!
Can't blame normal-ordering reference this time. . .

CC results from Gaute Hagen.

Radii of Ni isotopes





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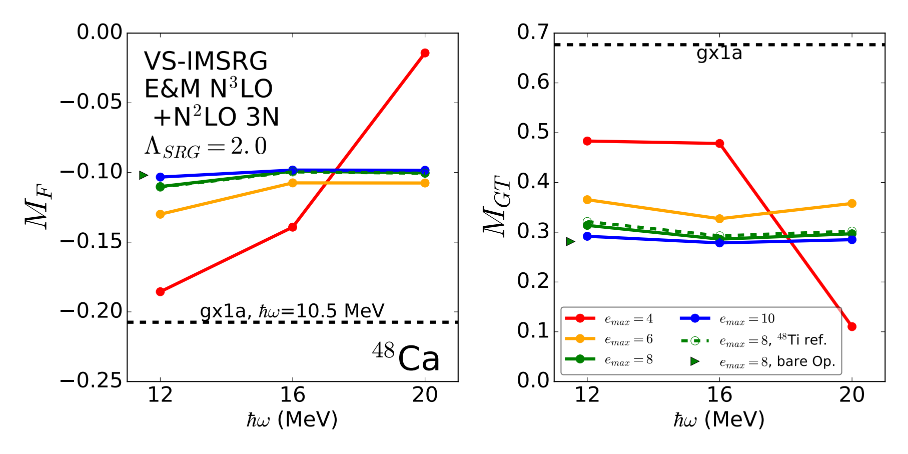
CC results from Gaute Hagen.

First $0\nu\beta\beta$ nuclear matrix elements from VS-IMSRG

Work done by Charlie Payne (UBC M.Sc. student)†



C.f. Iwata et al. 2016 full sdpf: $M_F \rightarrow -0.3$, $M_{GT} \rightarrow 1.0$

† With help from Jon Engel

$$U\mathcal{O}U^\dagger = e^{\Omega}\mathcal{O}e^{-\Omega} = \mathcal{O} + [\Omega,\mathcal{O}] + \frac{1}{2!}[\Omega,[\Omega,\mathcal{O}]] + \ldots$$

Valence space IMSRG

$$|^{76}\text{Ge}\rangle = U_{vs}^\dagger|^{76}\text{Ge}_{vs}\rangle$$

$$M_{\beta\beta} = \langle^{76}\text{Se}_{vs}|U_{vs}\mathcal{O}_{\beta\beta}U_{vs}^\dagger|^{76}\text{Ge}_{vs}\rangle$$

Multi-reference IMSRG

$$|^{76}\text{Ge}\rangle = U_{^{76}\text{Ge}}^\dagger|^{76}\text{Ge}_{\text{ref}}\rangle$$

$$M_{\beta\beta} = \langle^{76}\text{Se}_{\text{ref}}|U_{^{76}\text{Se}}\mathcal{O}_{\beta\beta}U_{^{76}\text{Ge}}^\dagger|^{76}\text{Ge}_{\text{ref}}\rangle$$

- In VS-IMSRG, bra and ket are expressed in the *same frame*.
- If all terms up to A-body are kept, VS-IMSRG is exact.
- But they're not kept. Normal ordering improves IMSRG(2) approximation.
- The *only* source of error is missing 3-,4-...body terms.
- This doesn't imply that this error is small or easy to estimate...

$$U\mathcal{O}U^\dagger = e^{\Omega}\mathcal{O}e^{-\Omega} = \mathcal{O} + [\Omega,\mathcal{O}] + \frac{1}{2!}[\Omega,[\Omega,\mathcal{O}]] + \dots$$

Valence space IMSRG

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- The *only* source of error is missing 3-,4-...body terms.
- This doesn't imply that this error is small or easy to estimate...

$$UOU^\dagger = e^{\Omega}\mathcal{O}e^{-\Omega} = \mathcal{O} + [\Omega,\mathcal{O}] + \frac{1}{2!}[\Omega,[\Omega,\mathcal{O}]] + \ldots$$

Valence space IMSRG

$$|^{76}\text{Ge}\rangle = U_{vs}^\dagger|^{76}\text{Ge}_{vs}\rangle$$

$$M_{\beta\beta} = \langle^{76}\text{Se}_{vs}|U_{vs}\mathcal{O}_{\beta\beta}U_{vs}^\dagger|^{76}\text{Ge}_{vs}\rangle$$

Multi-reference IMSRG

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Sources of many-body error

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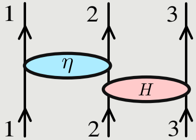
For the (not-too-distant) future

- Quantification of many-body uncertainty
  - Perturbative estimation of omitted 3,4...-body terms
  - Full IMSRG(3): Include 3-body terms throughout the calculation
  - Invariant trace?



- Heavy-mass frontier
  - Improve handling of 3N forces
- Decoupling arbitrary valence spaces
  - How does the choice of reference affect the IMSRG(2) approximation?
  - How does the choice of valence space affect the IMSRG(2) approximation?
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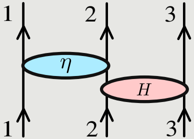

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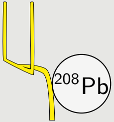

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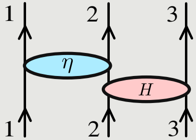

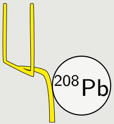

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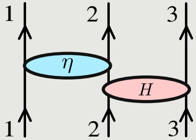

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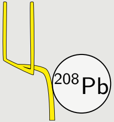

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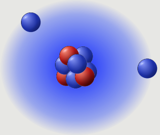
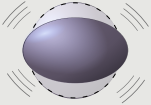
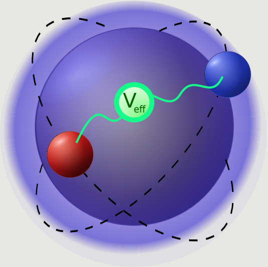




Thank you



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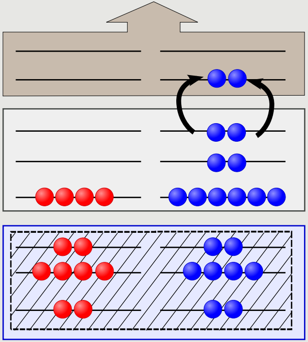
NSCL/MSU S. Bogner, H. Hergert, N. Parzuchowski

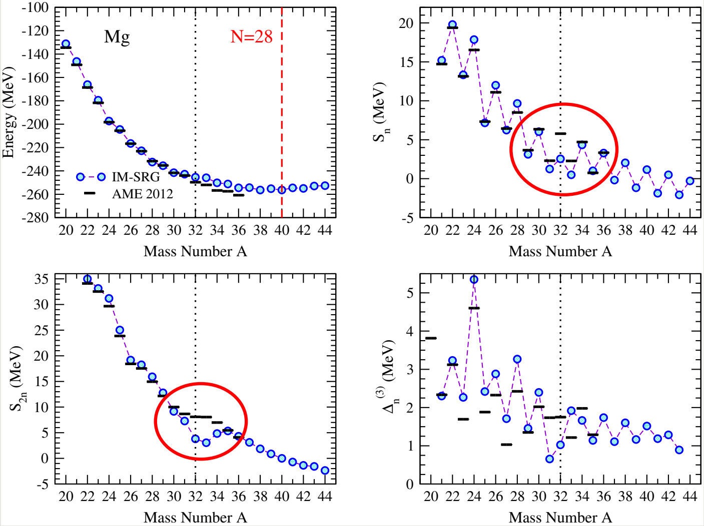
TU Darmstadt K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf

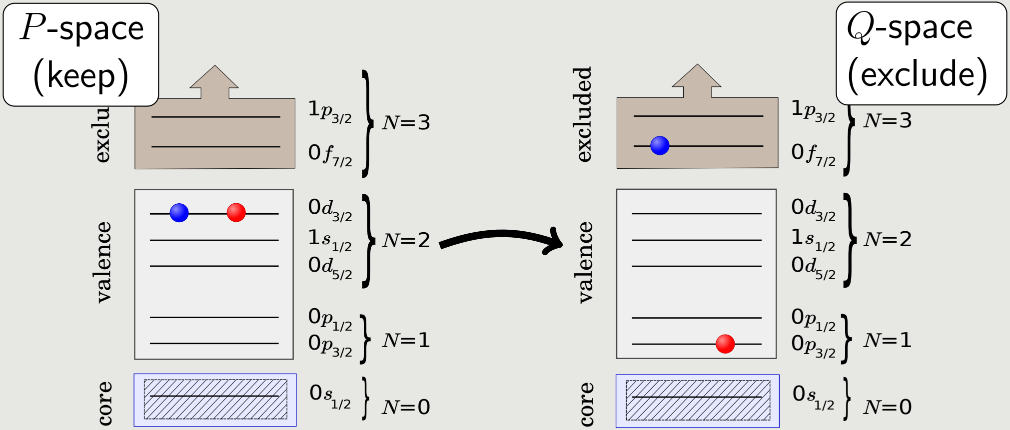
ORNL/UT G. Hagen, T. Morris

Backup slides

Non-standard valence spaces





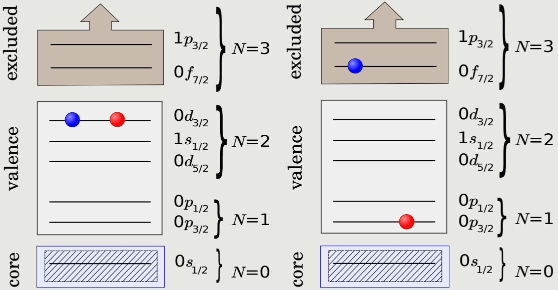


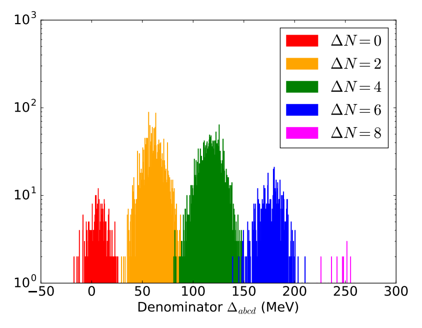
$$\eta_s = \frac{1}{2}\text{atan}\left(\frac{2H_{qp}(s)}{H_{qq}(s)-H_{pp}(s)}\right) - h.c.$$

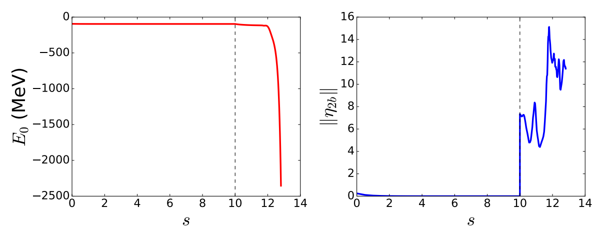
Q-space configuration lower in energy.

$\Delta N = 0 \rightarrow$ **negative denominators**

psd space, ^{16}O reference

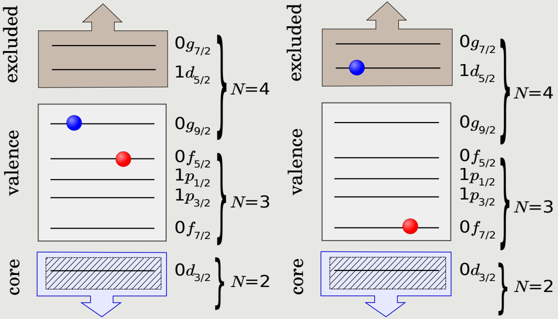


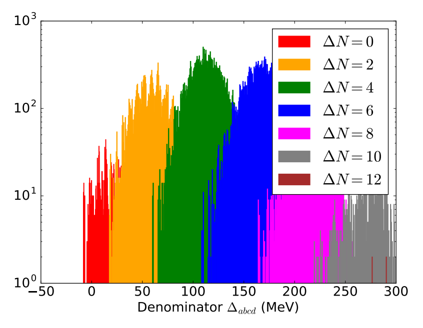


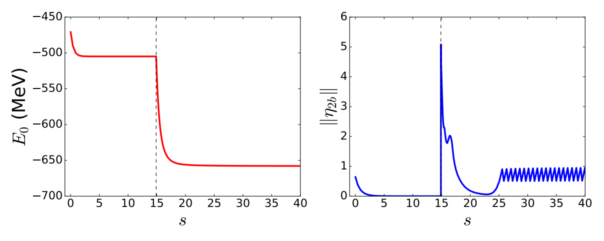


Non-standard valence spaces

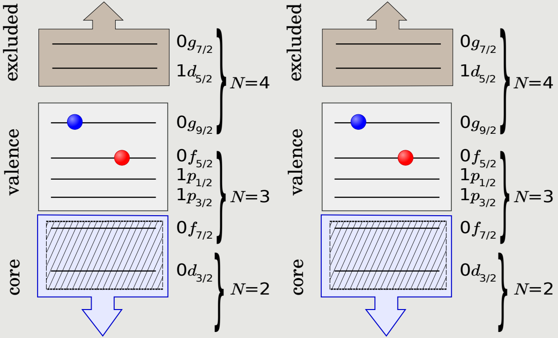
pfg_9 space, ^{76}Ge reference

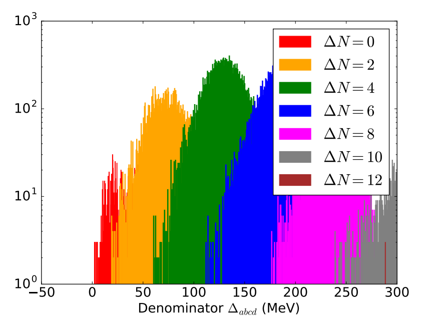


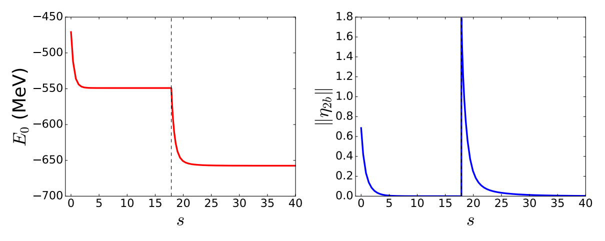


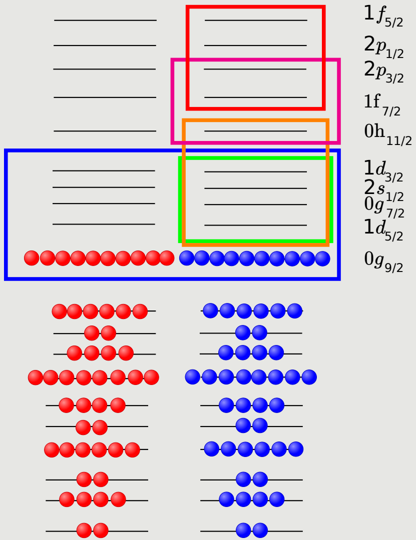


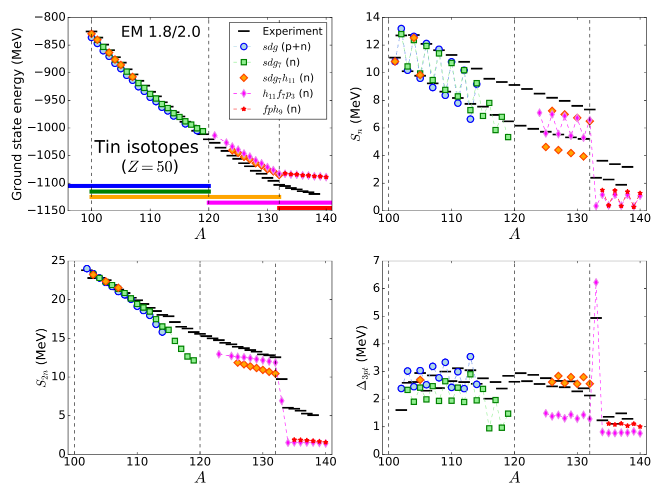
pf_5g_9 space, ^{76}Ge reference



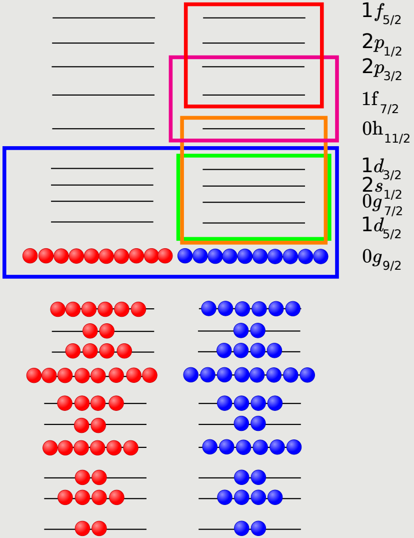


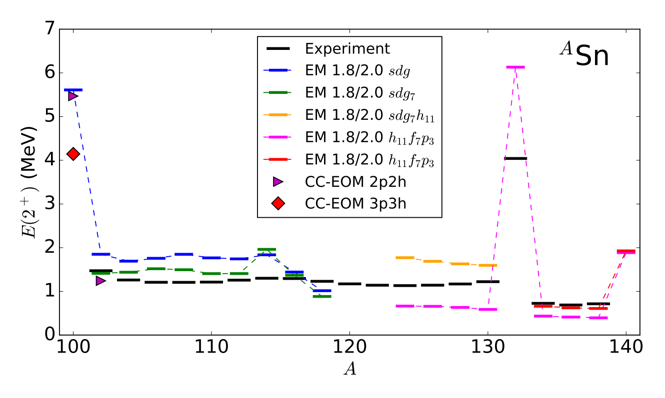



$1f_{5/2}$
$2p_{1/2}$
$2p_{3/2}$
$1f_{7/2}$
$0h_{11/2}$
$1d_{3/2}$
$2s_{1/2}$
$0g_{7/2}$
$1d_{5/2}$
$0g_{9/2}$


EM 1.8/2.0
Tin isotopes
($Z=50$)
Experiment
sdg (p+n)
sdg_7 (n)
sdg_7h_{11} (n)
$h_{11}f_7p_3$ (n)
fph_9 (n)
Ground state energy (MeV)
A
S_n (MeV)
S_{2n} (MeV)
Δ_{3pt} (MeV)

Non-standard valence spaces





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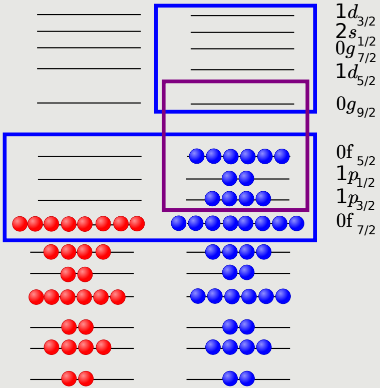
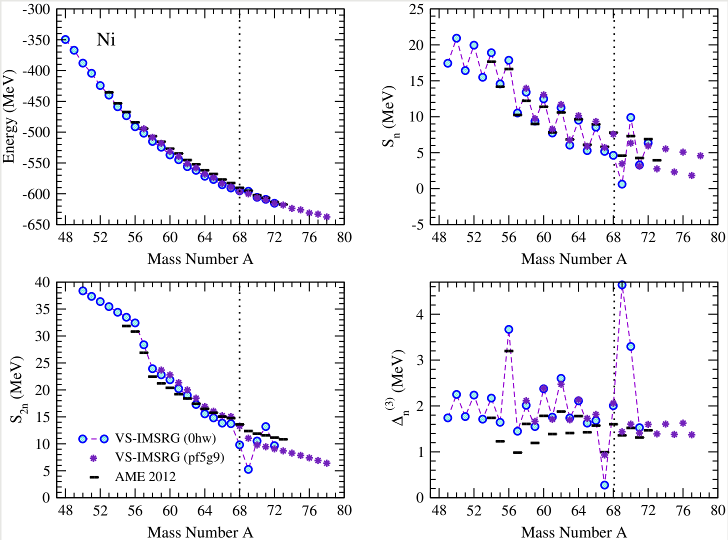
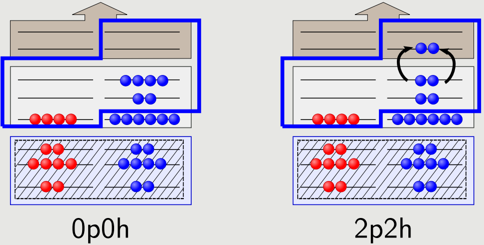
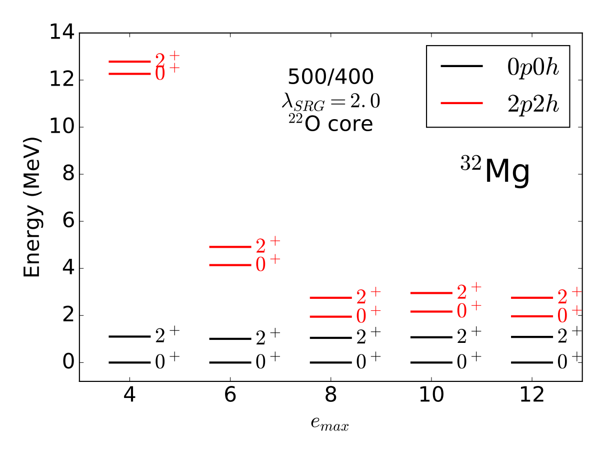


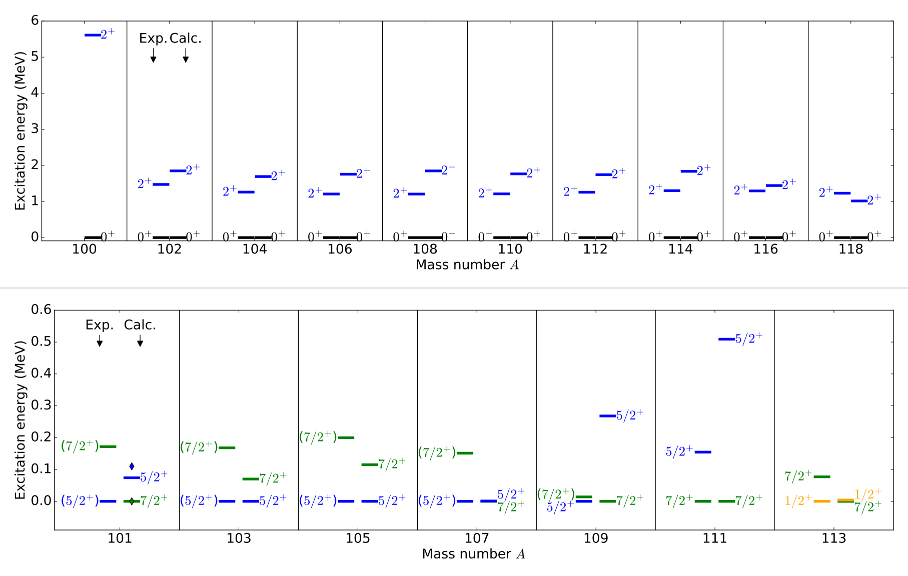




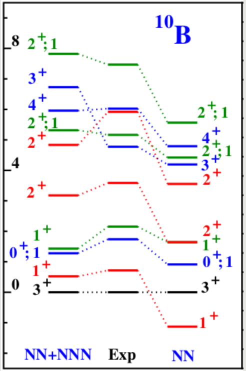


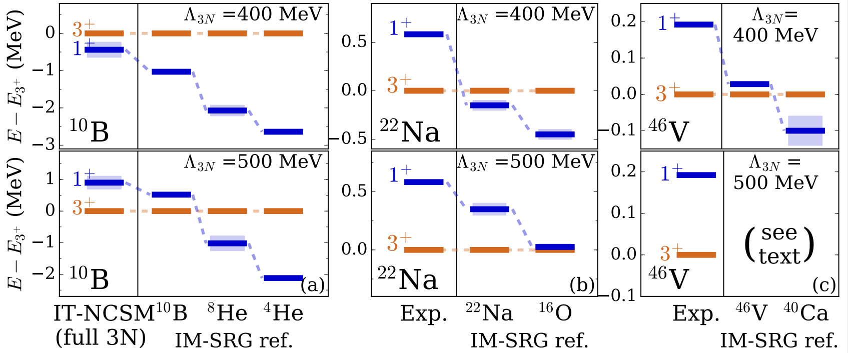
^{22}O core
$sd_3 f_7 p_3$ valence space for neutrons
sd valence space for protons

Spectroscopy of tin isotopes



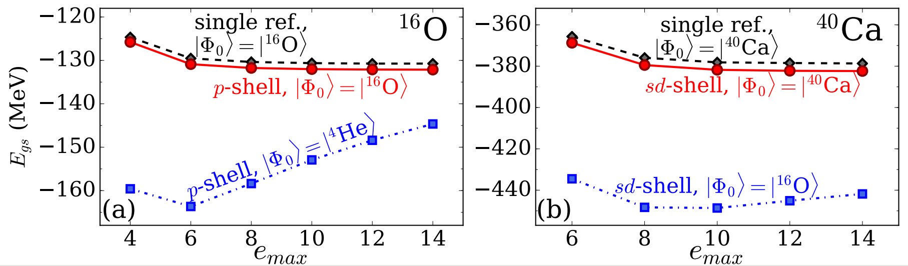
Capturing valence 3N effects w/ NN machinery:

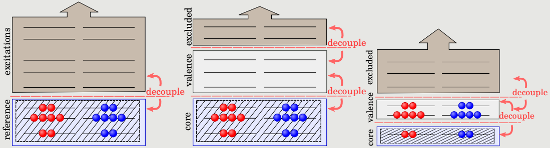




Navrátil et al. PRL (2007), SRS et al. PRL (2017)

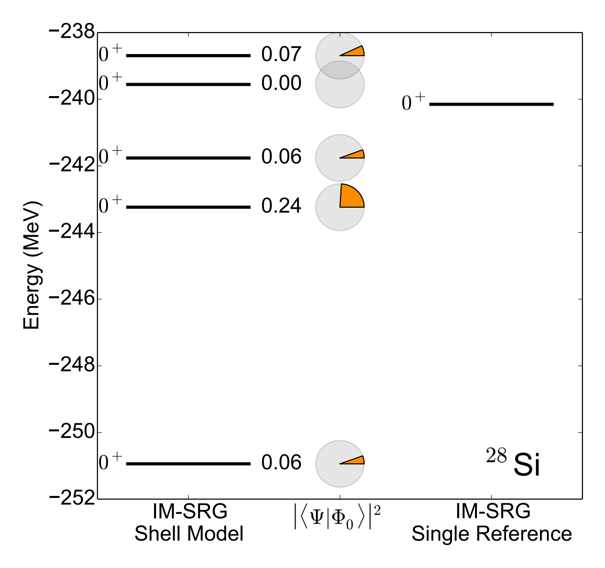
Convergence





- Convergence not possible without proper normal ordering reference
- Two competing effects
  - Missing 3N forces
  - Bad single particle basis
- $\sim$1% error due to additional decoupling

Picking out spherical excited states



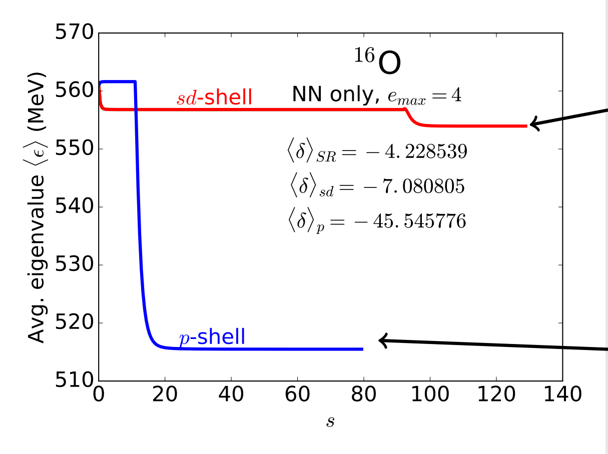
Invariant trace

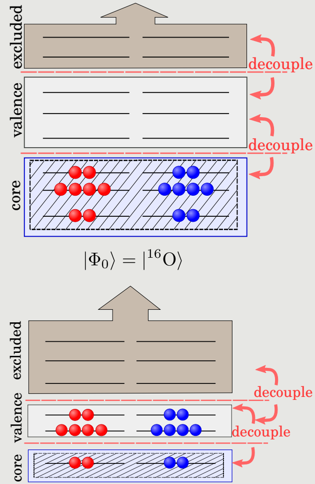
- Definition
  $Tr(H) = \sum_\alpha \langle \Phi_\alpha | H | \Phi_\alpha \rangle$
- Trace is invariant under unitary transformations:
  $$\begin{aligned} Tr(\tilde{H}) &= Tr(UHU^\dagger + X_{err}) \\ &= Tr(HU^\dagger U) + Tr(X_{err}) \\ &= Tr(H) + Tr(X_{err}) \end{aligned}$$
- Normalized trace gives average eigenvalue
  $Tr(H)/Tr(\mathbb{1}) = \langle \epsilon \rangle$
- Difference gives average error
  $\langle \tilde{\epsilon} \rangle - \langle \epsilon \rangle \equiv \langle \delta \rangle$

The many-body trace can be computed cheaply from the second-quantized Hamiltonian:

$$\begin{aligned} \langle \epsilon \rangle = E_0 &+ \frac{Z}{M}\sum_p h_{pp} + \frac{N}{M}\sum_n h_{nn} \\ &+ \frac{Z(Z-1)}{M(M-1)}\sum_{pp'} h_{pp'pp'} + \frac{N(N-1)}{M(M-1)}\sum_{nn'} h_{nn'nn'} \\ &+ \frac{NZ}{M^2}\sum_{pn} h_{pnpn} \end{aligned}$$

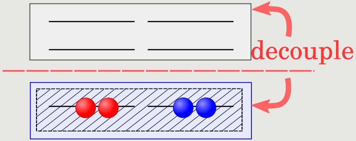
($M \equiv$ number of s.p. m-states in basis)

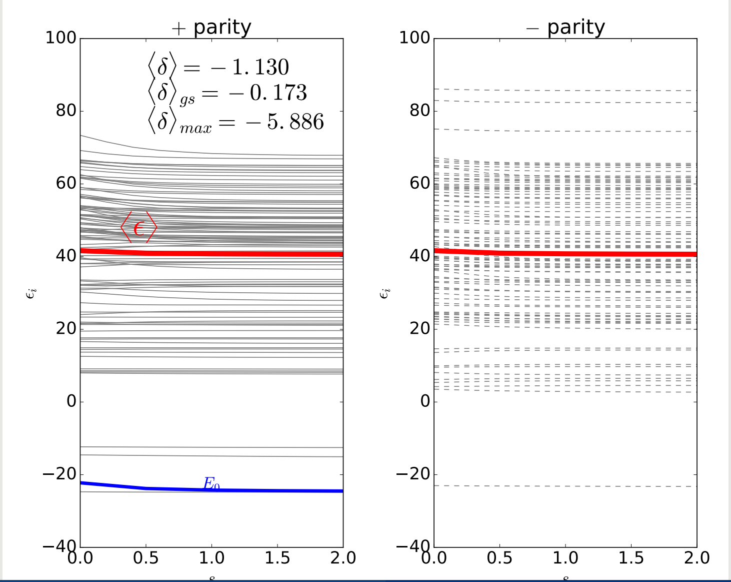

570
560
550
540
530
520
510
0
20
40
60
80
100
120
140
Avg. eigenvalue $\langle \epsilon \rangle$ (MeV)
s
^{16}O
sd-shell
NN only, $e_{max} = 4$
$\langle \delta \rangle_{SR} = -4.228539$
$\langle \delta \rangle_{sd} = -7.080805$
$\langle \delta \rangle_{p} = -45.545776$
p-shell

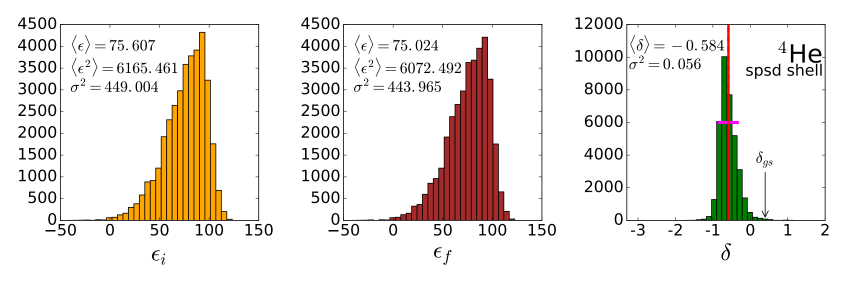

excluded
valence
core
decouple
decouple
$|\Phi_0\rangle = |^{16}\mathrm{O}\rangle$
excluded
valence
core
decouple
decouple

Invariant trace

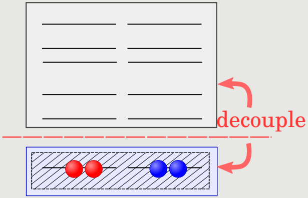
^{4}He in the $0s0p$ shell

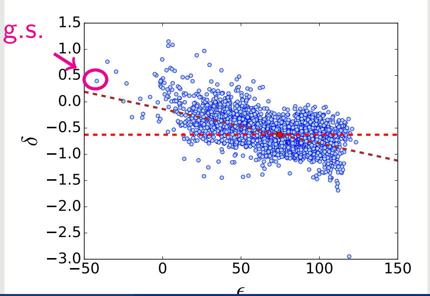






^{4}He in the $0s0p1s0d$ shell





References I

Bogner, S. K., R. J. Furnstahl, and R. J. Perry (2007). "Similarity renormalization group for nucleon-nucleon interactions". In: *Phys. Rev. C* 75.6, p. 061001. ISSN: 0556-2813. DOI: 10.1103/PhysRevC.75.061001. URL: http://link.aps.org/doi/10.1103/PhysRevC.75.061001.

Bogner, S. K. et al. (2014). "Nonperturbative shell-model interactions from the in-medium similarity renormalization group". In: *Phys. Rev. Lett.* 113.14, p. 142501. ISSN: 0031-9007. DOI: 10.1103/PhysRevLett.113.142501. URL: http://link.aps.org/doi/10.1103/PhysRevLett.113.142501.

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