TRIUMF

Canada's national laboratory for particle and nuclear physics
Laboratoire national canadien pour la recherche en physique nucleaire
et en physique des particules

The shell model as an ab initio tool: effective interactions and operators from IM-SRG

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Nuclear Physics from Lattice QCD
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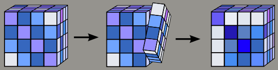
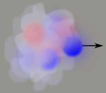
$$U = e^{\eta}$$



$$\frac{dH}{ds} = [\eta, H]$$



$$UOU^{\dagger} = \mathcal{O} + [\eta, \mathcal{O}] + \ldots$$

Relevance to this workshop

1. A nuclear model derived from QCD is only of use if we can solve the resulting equations.

2. Deficiencies of an interaction may be amplified in heavier nuclei.

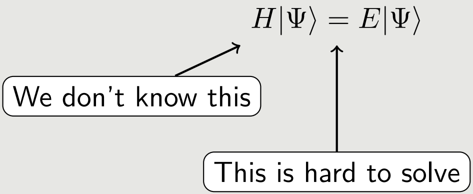
3. Valence-space IM-SRG is an ab-initio many-body method with a broad (and growing) range of applicability: $2 \lesssim A \lesssim 100$, open-shell/deformed systems, excited states, transitions . . .

Outline

- Conceptual introduction to valence space IM-SRG
- Targeted normal ordering
- Ensemble reference states
- Effective valence space operators

Introduction

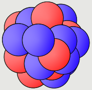
Starting point: non-relativistic Schrödinger equation with nucleons as our degrees of freedom.



$$H|\Psi\rangle = E|\Psi\rangle$$

We don't know this

This is hard to solve



- Effective theory → H is scheme and scale dependent.
- Strongly-interacting system → highly correlated → hard to solve.

> *The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.*
> *–Paul Dirac, 1929*

Many-body approaches

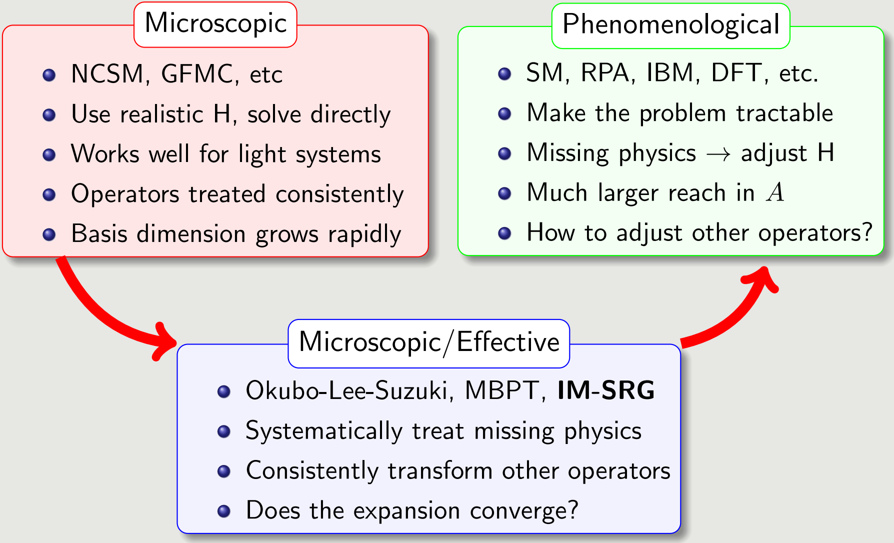
Microscopic

- NCSM, GFMC, etc
- Use realistic H, solve directly
- Works well for light systems
- Operators treated consistently
- Basis dimension grows rapidly

Phenomenological

- SM, RPA, IBM, DFT, etc.
- Make the problem tractable
- Missing physics → adjust H
- Much larger reach in A
- How to adjust other operators?

Many-body approaches



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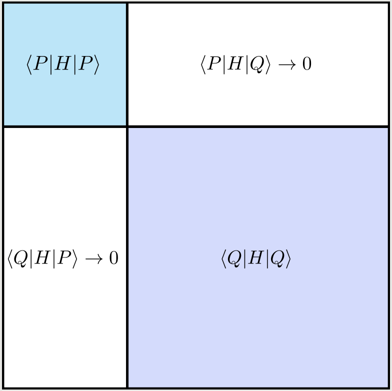
Microscopic/Effective

- Okubo-Lee-Suzuki, MBPT, **IM-SRG**
- Systematically treat missing physics
- Consistently transform other operators
- Does the expansion converge?

Microscopic/Effective approach

Effective Interaction



$\langle P\|H\|P\rangle$	$\langle P\|H\|Q\rangle \to 0$
$\langle Q\|H\|P\rangle \to 0$	$\langle Q\|H\|Q\rangle$

Goal: Find a unitary transformation U such that

- $\tilde{H} = UHU^\dagger$
- $\langle P|\tilde{H}|Q\rangle = \langle Q|\tilde{H}|P\rangle = 0$
- $\langle\tilde{\Psi}_i|\hat{P}\tilde{H}\hat{P}|\tilde{\Psi}_i\rangle = \langle\Psi_i|H|\Psi_i\rangle$

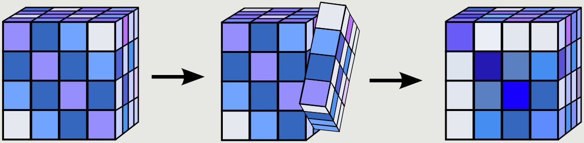
IM-SRG

In-Medium Similarity Renormalization Group

(IM-SRG)

IM-SRG

- U may always be written as $U = e^{\eta}$, for some generator η
- For two-level system, $\eta = \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}$
- For our Hamiltonian, take $\eta = \frac{1}{2}\mathrm{atan}\left(\frac{2H_{od}}{\Delta}\right) - h.c.$



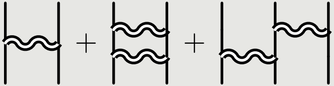
- Perform multiple rotations: $U_N = e^{\eta_N} \ldots e^{\eta_2} e^{\eta_1}$
- Iterate until $\eta_N = 0$
- Infinitessimal rotation of angle $ds \rightarrow \frac{dH(s)}{ds} = [\eta(s), H(s)]$

White 2002; Tsukiyama, Bogner, and Schwenk 2011; Morris, Parzuchowski, and Bogner 2015

IM-SRG

- Why “In-Medium”?
  ⇒ To deal with the problem of induced many-body forces

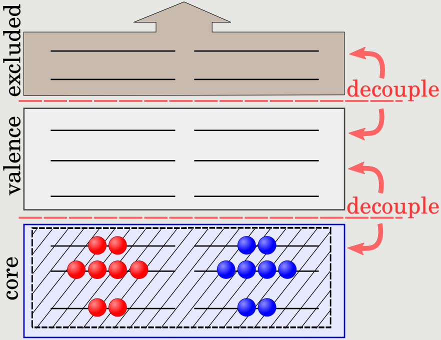
$$e^{\eta} = 1 + \eta + \frac{1}{2!}\eta^{2} + \ldots$$

$= 1 +$  $+ \ldots$

- All terms beyond two-body operators are too expensive to handle
- Define states with respect to a reference $|\Phi_0\rangle$ (Normal Ordering)
- If $|\Phi_0\rangle$ is a reasonable approximation of $|\Psi\rangle$, then many-body terms are less important

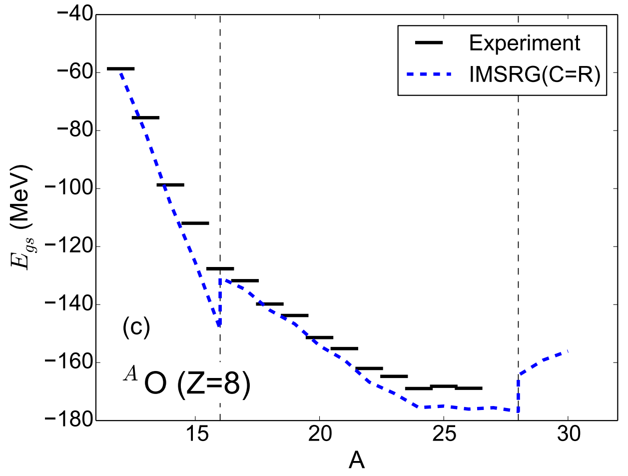
Valence space IM-SRG

- Excluded configurations treated with IM-SRG (definition of H_{od})
- Valence configurations treated explicitly with standard shell model diagonalization
- In following, all calculations use E&M N^{3}LO NN + local N^{2}LO 3N forces, SRG evolved to λ_{SRG}=1.88 fm (kindly provided by Angelo Calci)



Entem and Machleidt 2003; Navrátil 2007; Tsukiyama, Bogner, and Schwenk 2012

Valence space IM-SRG: Ground states



Bogner et al. 2014

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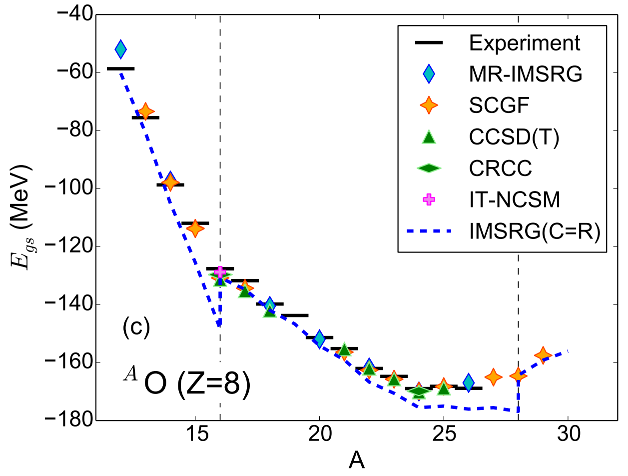
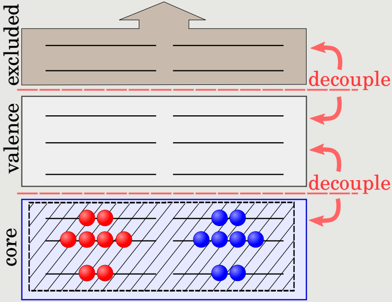


Bogner et al. 2014; Cipollone, Barbieri, and Navrátil 2013; Hergert et al. 2014

Valence space IM-SRG: Ground states

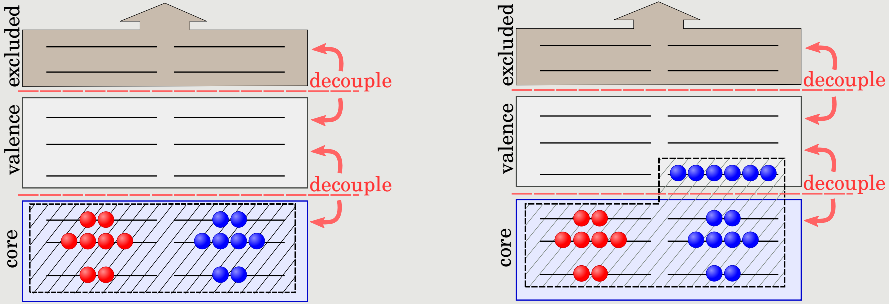
What are we missing?



- The other methods use the target nucleus as $|\Phi_0\rangle$, while we use the core
- Other methods better capture effect 3N forces between valence nucleons

Valence space IM-SRG: Ground states

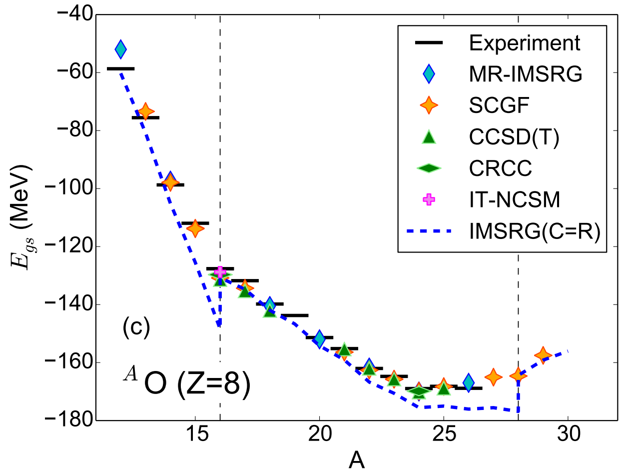
What are we missing?



Strategy:

- As valence neutrons are added, $|^{22}\mathrm{O}\rangle$ becomes a better reference than $|^{16}\mathrm{O}\rangle$, so use that
- But still decouple the full sd shell

Valence space IM-SRG: Ground states



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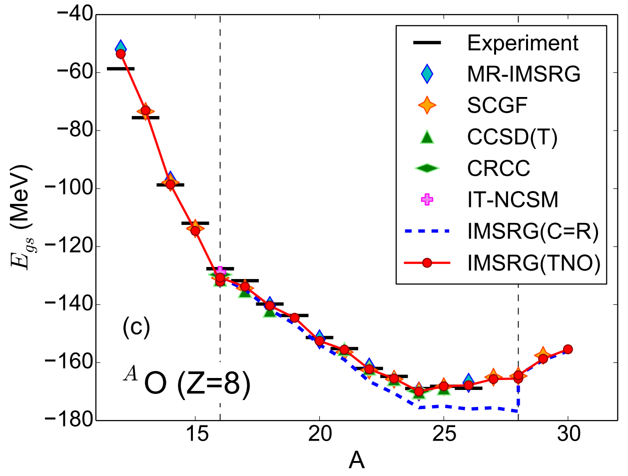
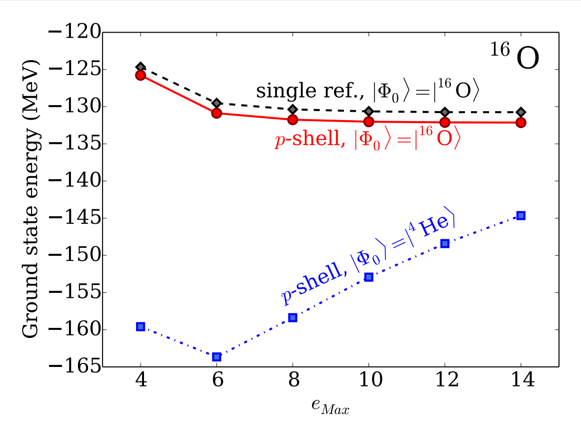
Valence space IM-SRG: Ground states



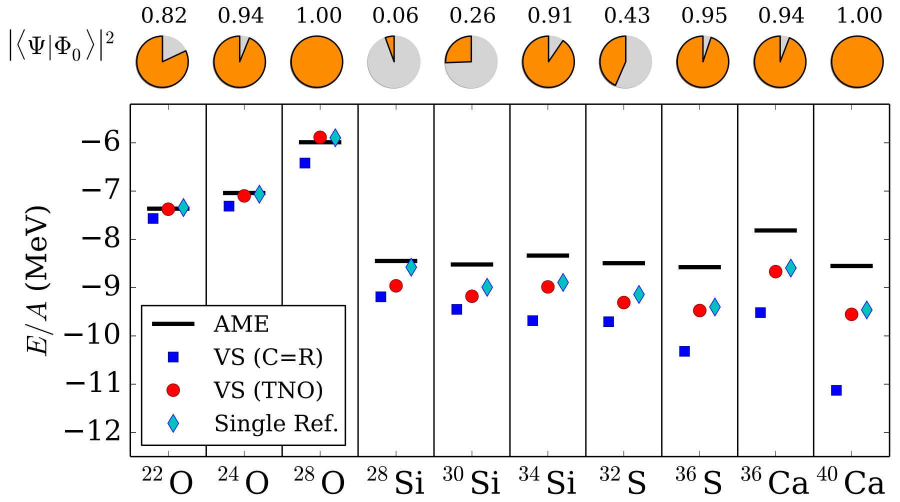
Bogner et al. 2014; Brown et al. 2006; Cipollone, Barbieri, and Navrátil 2013; Hergert et al. 2014

Convergence in the p-shell

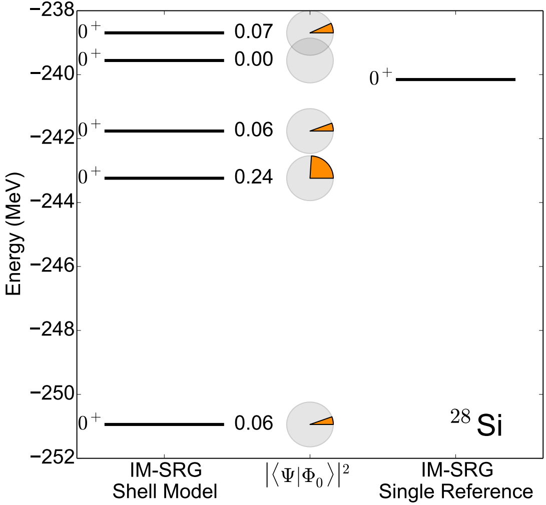


- TNO is required in upper p-shell to obtain convergence with model space size.
- Constant ∼1% offset w.r.t. single reference → price we pay for decouping the valence space.

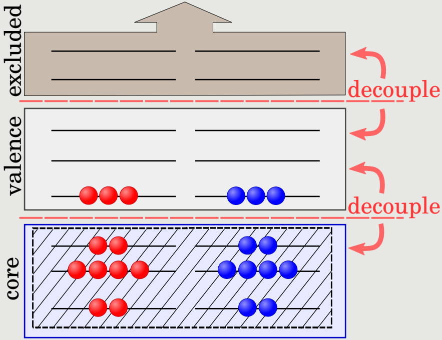
Valence space IM-SRG: Closed subshells



Valence space IM-SRG: Ground state of ^{28}Si

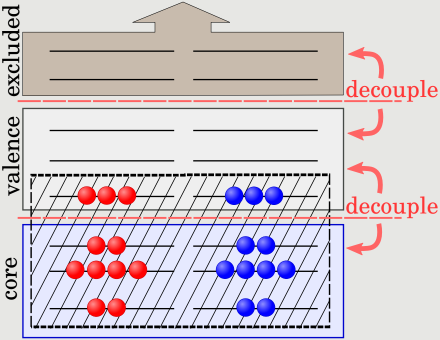


What to do about ^{22}Na?



$$|\Phi_0\rangle = |^{16}\text{O}\rangle$$

(Underestimate 3N)



$$|\Phi_0\rangle = |^{28}\text{Si}\rangle$$

(Overestimate 3N)

Ensemble reference state (Equal filling)

Replace $|\Phi_0\rangle$ with ensemble (mixed) state characterized by density matrix:

$$\rho = \sum_i \alpha_i |\Phi_i\rangle\langle\Phi_i|$$

Definition of normal ordering:

$$Tr(\rho\{a_1^\dagger \dots a_N\}) = \sum_i \alpha_i \langle\Phi_i|\{a_1^\dagger \dots a_N\}|\Phi_i\rangle = 0$$

Wick contraction:

$$\{\overbracket{a_p^\dagger a_q}\} = \sum_i \alpha_i \langle\Phi_i|a_p^\dagger a_q|\Phi_i\rangle \equiv n_p\delta_{pq}$$

$$\{\overbracket{a_p^\dagger a_q}\} = n_p\delta_{pq} \quad , \quad \{\overbracket{a_p a_q^\dagger}\} = (1 - n_p)\delta_{pq} \quad , \quad \{\overbracket{a_p a_q}\} = \{\overbracket{a_p^\dagger a_q^\dagger}\} = 0$$

Now n_p can be fractional, which is exactly what we want!

No N-representability problem.

Thouless 1957; Gaudin 1960; Perez-Martin and Robledo 2008

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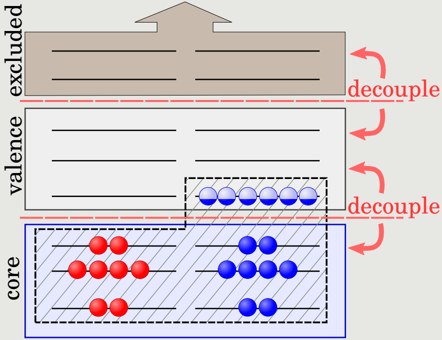
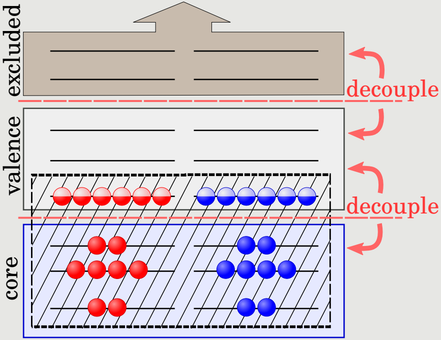


$$\rho = \frac{2}{3}|{}^{16}\mathrm{O}\rangle\langle{}^{16}\mathrm{O}| + \frac{1}{3}|{}^{22}\mathrm{O}\rangle\langle{}^{22}\mathrm{O}|$$

${}^{18}\mathrm{O}$

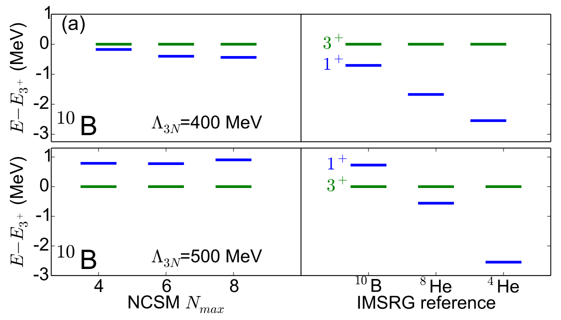


$$\rho = \frac{1}{2}|{}^{16}\mathrm{O}\rangle\langle{}^{16}\mathrm{O}| + \frac{1}{2}|{}^{28}\mathrm{Si}\rangle\langle{}^{28}\mathrm{Si}|$$

${}^{22}\mathrm{Na}$

Valence 3N forces: ^{10}B, ^{22}Na, ^{46}V

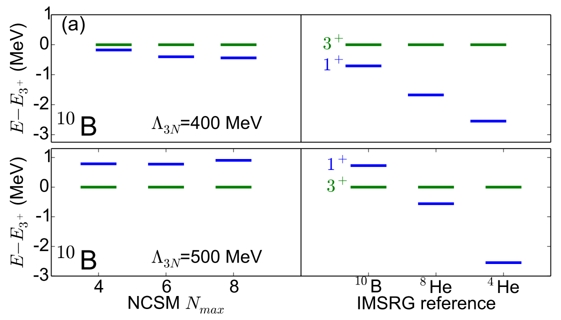
- Ground state of ^{10}B is 3^+
- 3N forces are required to reproduce this without fitting

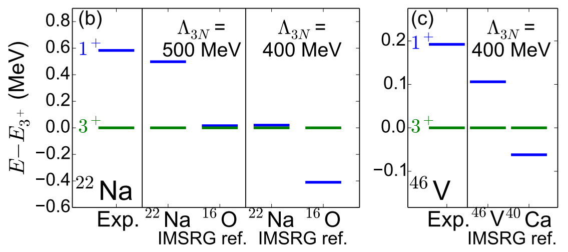


Navrátil and Ormand 2002; Pieper, Varga, and Wiringa 2002; Gebrerufael, Calci, and Roth 2015

Valence 3N forces: ^{10}B, ^{22}Na, ^{46}V

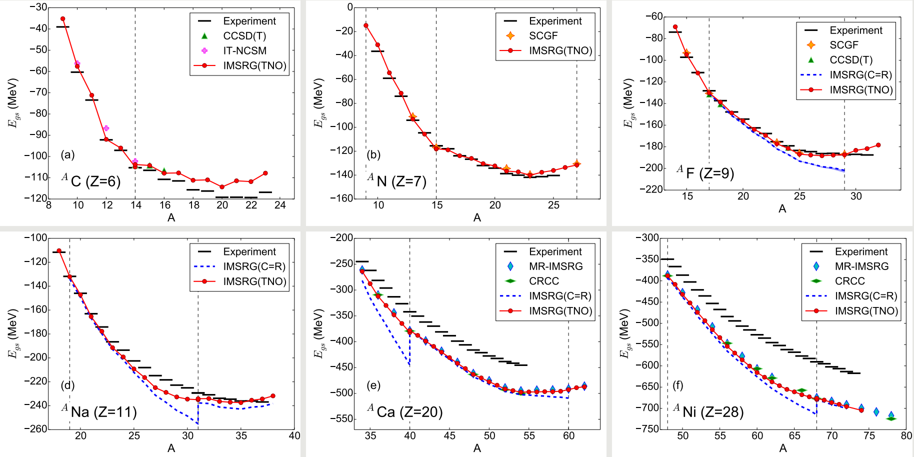
- Ground state of ^{10}B is 3^+
- 3N forces are required to reproduce this without fitting
- Similar situation for ^{22}Na and ^{46}V
- Normal ordering with ensemble reference captures this
- First ab initio calculations of ^{22}Na and ^{46}V to obtain correct ordering





Navrátil and Ormand 2002; Pieper, Varga, and V

Ground states with ensemble reference



Cipollone, Barbieri, and Navrátil 2013; Binder et al. 2014; Hergert et al. 2014; Jansen et al. 2015; Roth(priv. comm.)

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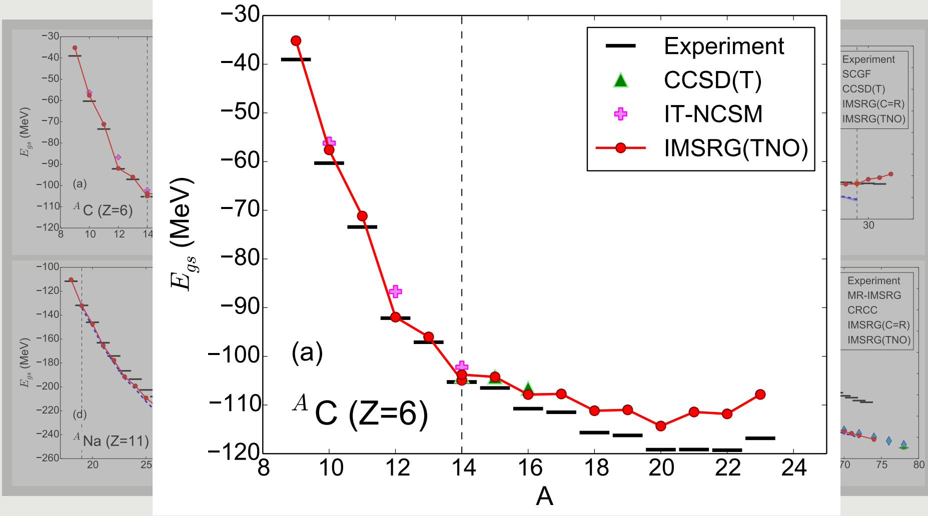

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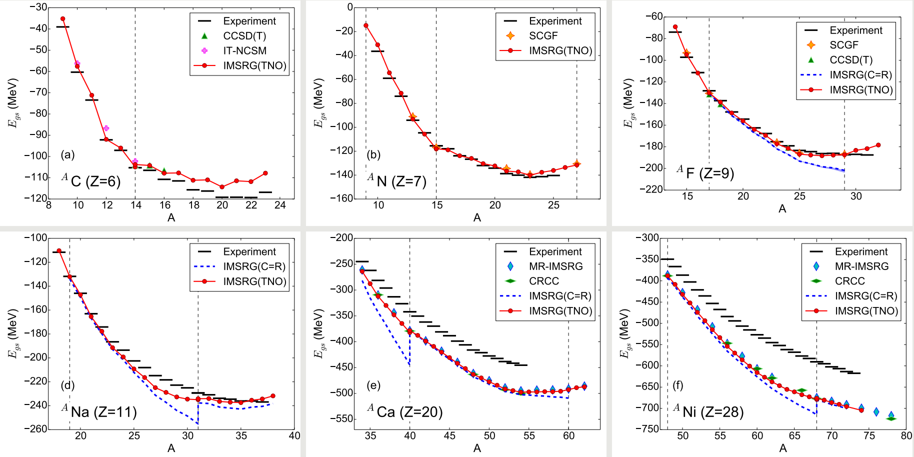

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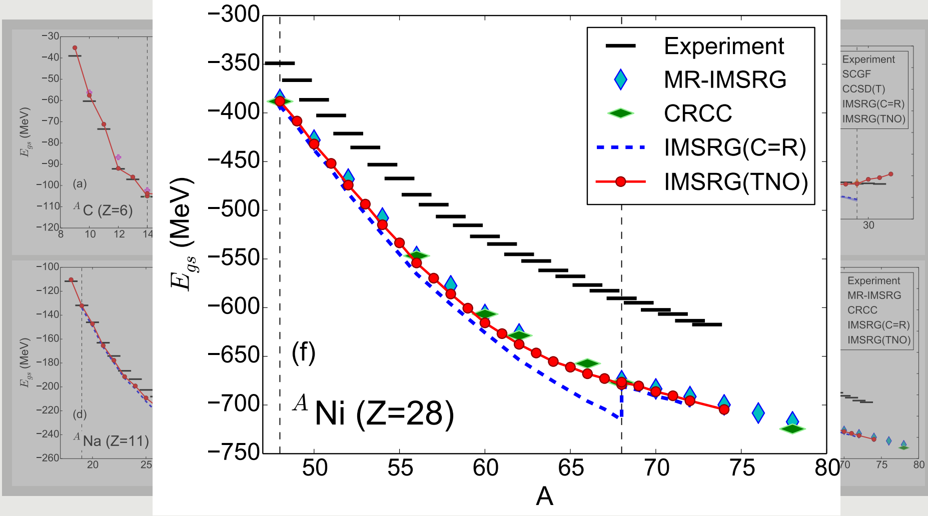
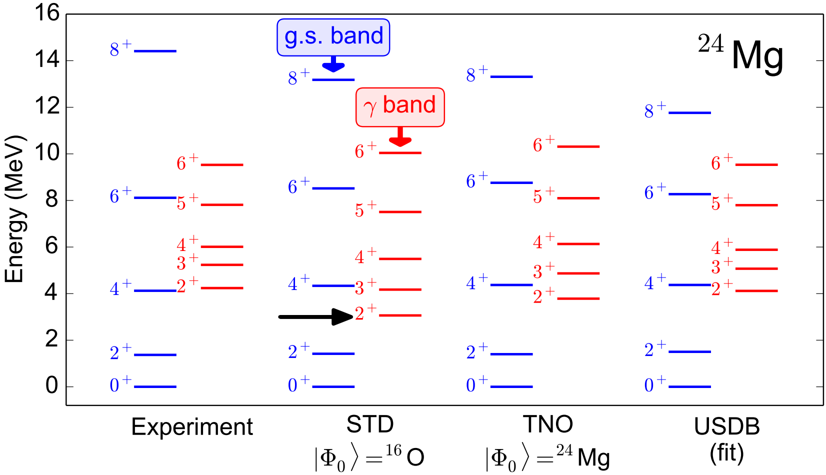


Cipollone, Barbieri, and Navrátil 2013; Binder et al. 2014; Hergert et al. 2014; Jansen et al. 2015; Roth(priv. comm.)

Rotational bands in ^{24}Mg



Effective operators

Some very preliminary results

Effective operators

- Operators transform just like H:

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

- Tensor operators require additional angular momentum coupling:

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

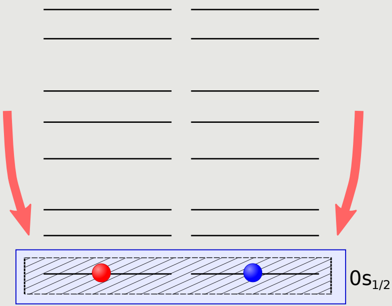
- Shell model expectation values then reflect full-space expectation values:

$$\langle\Psi|\mathcal{O}|\Psi\rangle = \langle\Psi_{SM}|\tilde{\mathcal{O}}|\Psi_{SM}\rangle$$

Effective operators

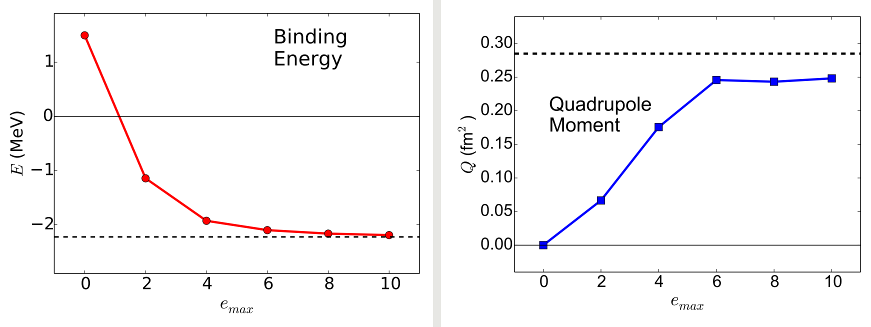
The deuteron

- Valence space: $0s$ shell
- No effects of induced many-body forces
- Bare quadrupole operator $(\lambda = 2)$ gives identically zero



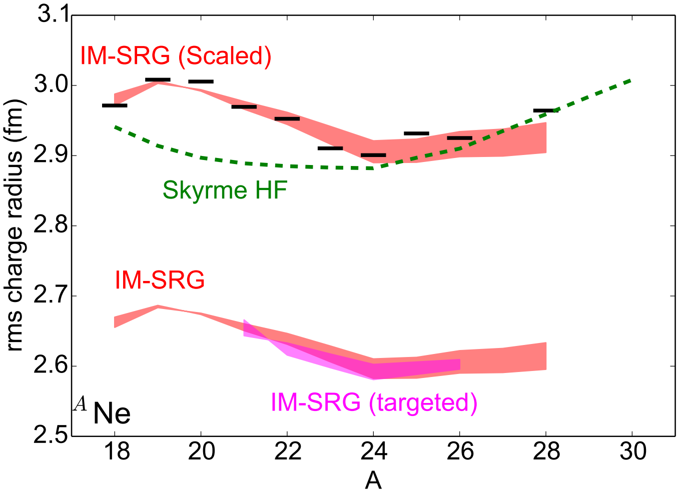
Effective operators

The deuteron



- Energy correctly reproduced
- $\langle 0s_{1/2}0s_{1/2}|\tilde{Q}|0s_{1/2}0s_{1/2}\rangle \neq 0$

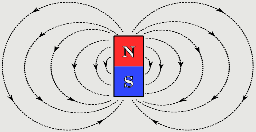
Into the sd shell: Neon Radii

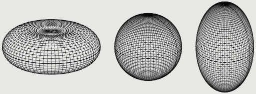


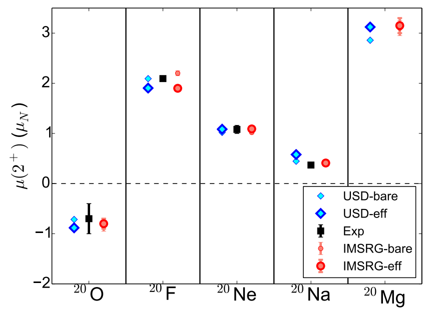
Marinova et al. 2011; Brown 1998

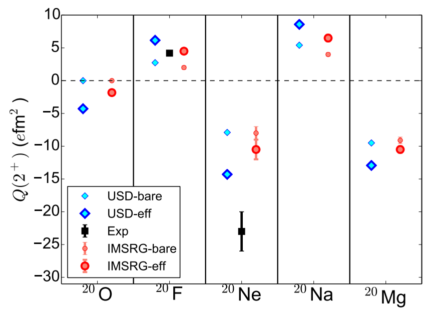
Tensor Operators

Moments



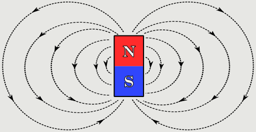


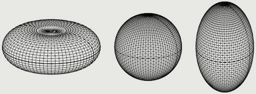


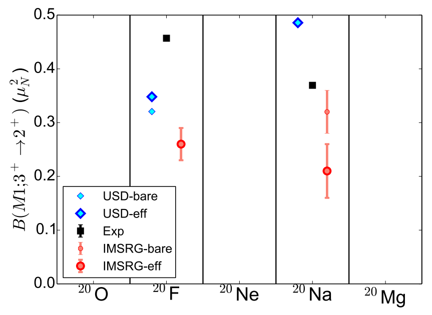


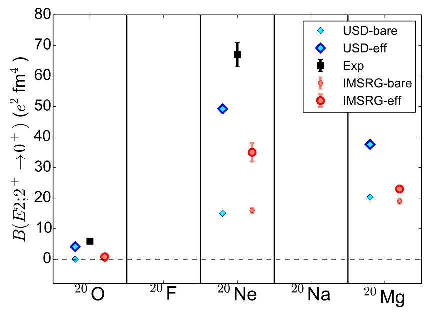
Tensor Operators

Transitions



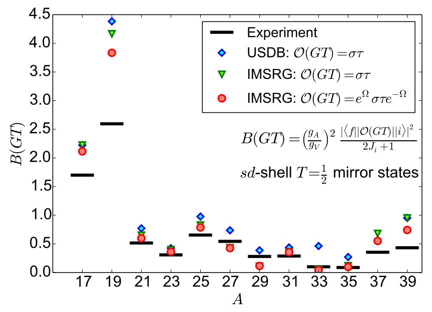


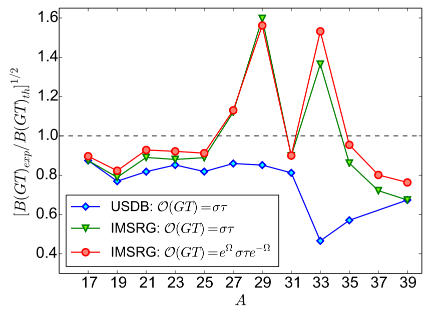




Tensor Operators

Gamow-Teller Transitions

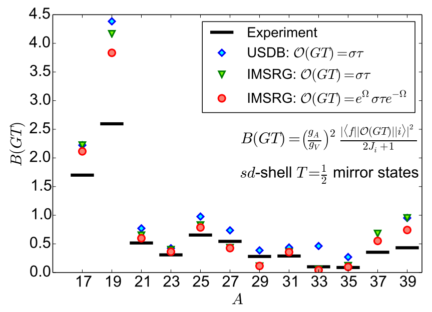


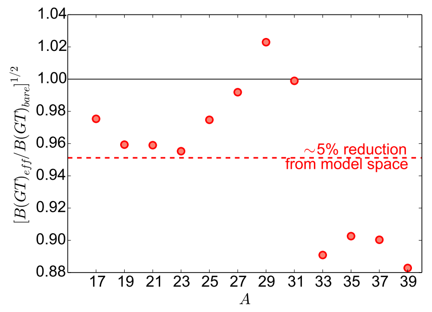


Brown et al. 2006; Brown, Chung, and Wildenthal 1978

Tensor Operators

Gamow-Teller Transitions





Brown et al. 2006; Brown, Chung, and Wildenthal 1978

Summary

- Ab initio methods provide a means to calculate nuclear structure properties where fitting to data is not possible
- Effective valence-space approach enables consistent treatment of excited states, transitions, open-shell/deformed systems
- Targeted normal ordering with an ensemble reference provides a reasonable approximation of valence 3N forces
- Evolved tensor operators produce some renormalization – more work to be done.
- MEC corrections to operators can be handled without additional trouble

Collaborators:

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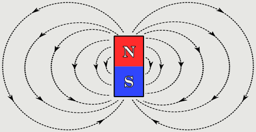
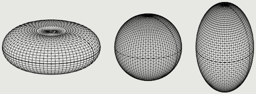
NSCL/MSU	S. Bogner, H. Hergert, T. Morris, N. Parzuchowski
TU Darmstadt	A. Schwenk, J. Simonis

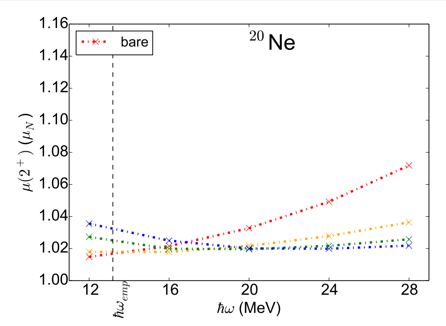
Appendix

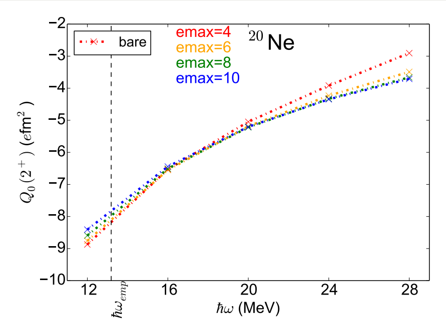
Tensor Operators

Moments



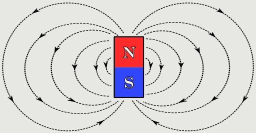


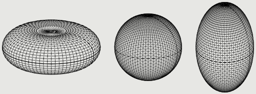


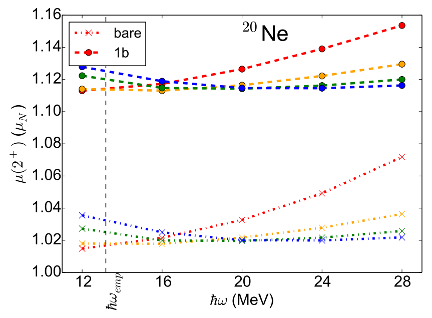


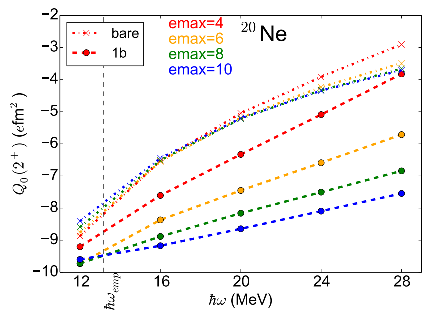
Tensor Operators

Moments



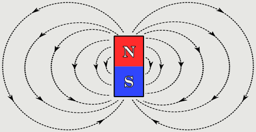


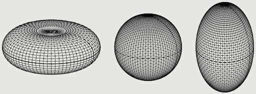


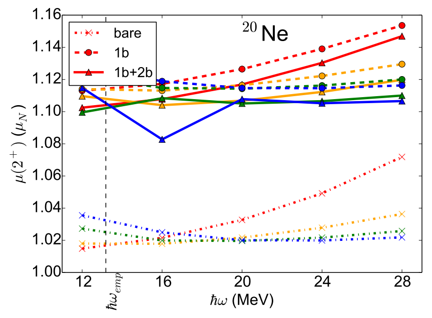


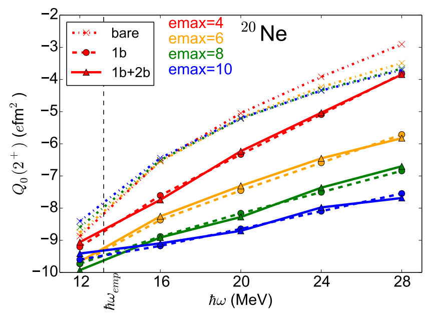
Tensor Operators

Moments



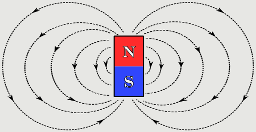


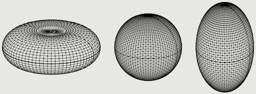


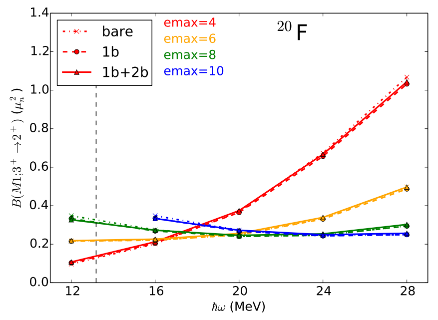


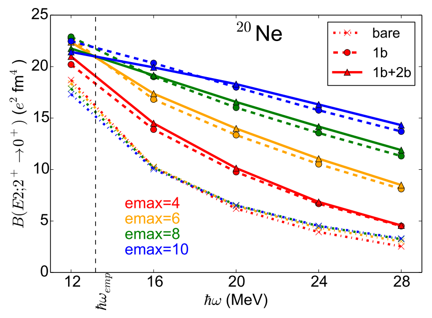
Tensor Operators

Transitions









How to choose $\hat{\Omega}$?

A toy problem:

$$\hat{H} = \begin{pmatrix} \epsilon_1 & h_{od} \\ h_{od} & \epsilon_2 \end{pmatrix}, \qquad \hat{\Omega} = \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}, \qquad e^{\hat{\Omega}} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$e^{\hat{\Omega}}\hat{H}e^{-\hat{\Omega}} = \begin{pmatrix} \epsilon_1 \cos^2\theta + \epsilon_2 \sin^2\theta + h \sin 2\theta & h_{od}\cos 2\theta + \frac{\epsilon_2 - \epsilon_1}{2}\sin 2\theta \\ h_{od}\cos 2\theta + \frac{\epsilon_2 - \epsilon_1}{2}\sin 2\theta & \epsilon_2 \cos^2\theta + \epsilon_1 \sin^2\theta - h\sin 2\theta \end{pmatrix}$$

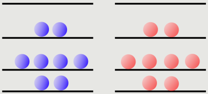
$$h'_{od} \to 0 \quad \Rightarrow \quad \theta = \frac{1}{2}\tan^{-1}\left(\frac{2h_{od}}{\epsilon_1 - \epsilon_2}\right)$$

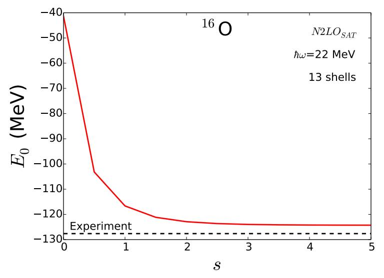
$$\theta \ll 1 \quad \Rightarrow \quad \theta \approx \frac{h_{od}}{\epsilon_1 - \epsilon_2}$$

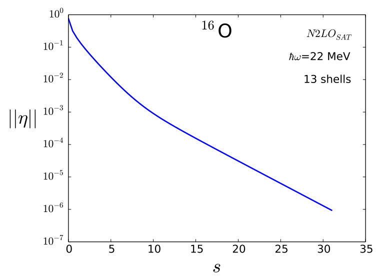
S. R. White, J. Chem. Phys. 117, 7472 (2002)

IM-SRG

Application to ^{16}O:

- $|\Phi_0\rangle =$ 
- $\eta \sim \frac{H_{od}}{\Delta} - h.c.$
- H_{od} is any term that connects $|\Phi_0\rangle$ to any other configuration
- s is the total "angle" rotated
- Ground state energy given by a single matrix element: $\langle\Phi_0|\tilde{H}|\Phi_0\rangle$





Tsukiyama, Bogner, and Schwenk 2011; Ekström et al. 2015

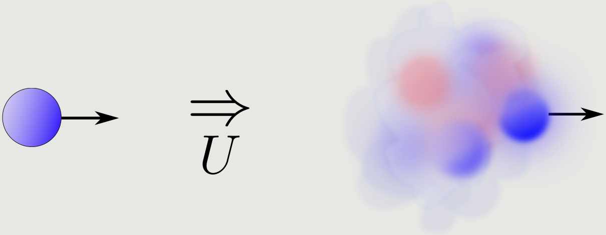
IM-SRG

Where did all the correlations go?

- Original single particle basis: $|\phi_i\rangle = a_i^\dagger|0\rangle$
- The transformed $\tilde{H}$ is implicitly in terms of $\tilde{a}_i^\dagger$

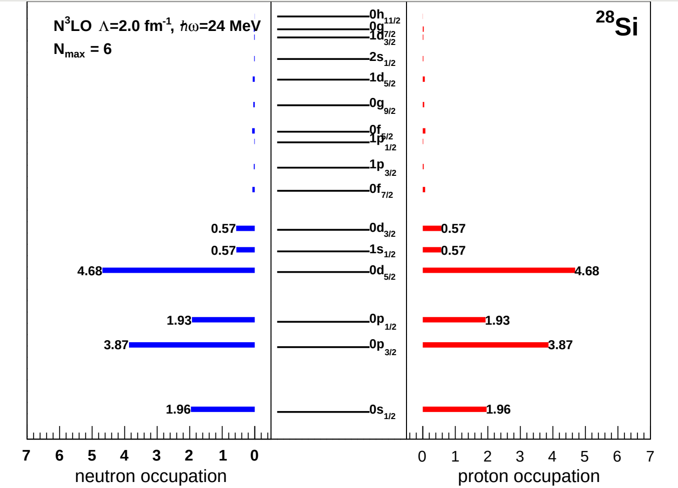
$$\begin{aligned}\tilde{a}_i^\dagger &= U^\dagger(a_i^\dagger)U \\ &= \mathcal{C}_i a_i^\dagger + \sum_{j\neq i}\mathcal{C}_j a_j^\dagger + \sum_{jk}\mathcal{C}_{jkl}a_j^\dagger a_k^\dagger a_l + \ldots\end{aligned}$$

- The single-particle orbits are now much more complicated!



Aside: Basis dependence of occupation numbers

$$a_i^\dagger a_i = U a_i'^\dagger a_i' U^\dagger$$



Occupations:
1) IM-SRG basis
2) Oscillator basis

	1	2
$0s_{1/2}$	2.0	1.96
$0p_{3/2}$	4.0	3.87
$0p_{1/2}$	2.0	1.93
$0d_{5/2}$	6.0	4.68
$1s_{1/2}$	0.0	0.57
$0d_{3/2}$	0.0	0.57
...	...	...

Same calculation, different occupations!

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