The shell model as an ab-initio tool

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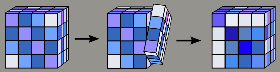
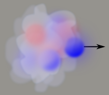
TRIUMF

Progress in Ab Initio Techniques in Nuclear Physics

$$U = e^{\eta}$$



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



$$U\mathcal{O}U^{\dagger} = \mathcal{O} + [\eta, \mathcal{O}] + \dots$$

Outline

- Conceptual introduction to IM-SRG with shell model
- Applications to ground state eneriges
- Excited states, radii, deformation
- Evolved tensor operators (transitions, moments)

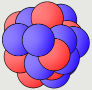
Introduction

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



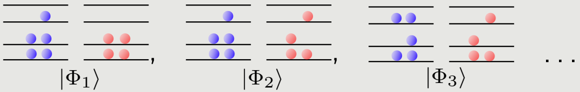
- Effective theory $\rightarrow$ H is scheme and scale dependent.
- Strongly-interacting system $\rightarrow$ highly correlated $\rightarrow$ hard to solve.

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

Introduction

Straightforward approach: Expand H in a convenient basis $|\Phi_i\rangle$,

e.g.



$$\begin{pmatrix} \langle\Phi_1|H|\Phi_1\rangle & \cdots & \cdots \\ \vdots & \langle\Phi_i|H|\Phi_j\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \underset{\text{diagonalize}}{\Rightarrow} \quad |\Psi\rangle = \sum_i c_i|\Phi_i\rangle$$

- Correlation manifested as superposition of configurations.
- Works well for light systems.
- Basis dimension $\sim \frac{N!}{A!(N-A)!}$, current limit on dimension $\sim 10^{10}$.
- $A \lesssim 12 \quad (A \lesssim 16$ with importance truncation).

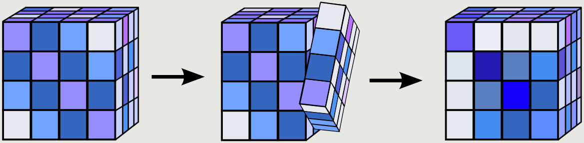
In-Medium Similarity Renormalization Group

$$\tilde{H} = UHU^\dagger$$

$$\tilde{H}|\Phi_0\rangle = E|\Phi_0\rangle$$

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 $\eta = \frac{1}{2}\text{atan}\left(\frac{2H_{od}}{\Delta}\right) - h.c.$



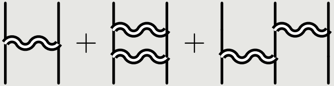
- Perform multiple rotations: $U_N = e^{\eta_N} \ldots e^{\eta_2} e^{\eta_1}$
- Iterate until $\eta_N = 0$
- Infinitessimal rotation of angle $ds \rightarrow \frac{dH(s)}{ds} = [\eta(s), H(s)]$

White (2002), Tsukiyama (2011), Morris (2015)

IM-SRG

- Why "In-Medium"?
  $\Rightarrow$ To deal with the problem of induced many-body forces

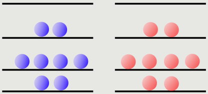
$$e^{\eta} = 1 + \eta + \frac{1}{2!}\eta^2 + \dots$$

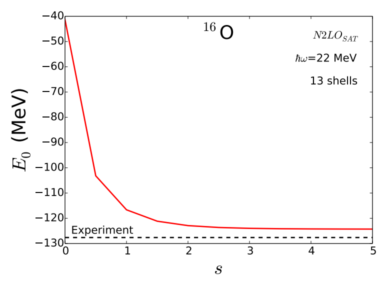
$= 1 +$  $+ \dots$

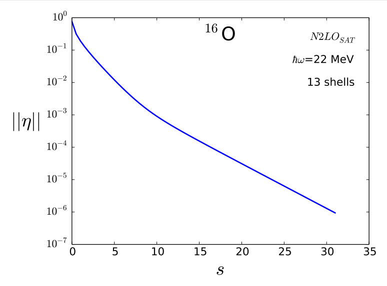
- All terms beyond two-body operators are too expensive to handle
- Define states with respect to a reference $|\Phi_0\rangle$ (Normal Ordering)
- If $|\Phi_0\rangle$ is a reasonable approximation of $|\Psi\rangle$, then many-body terms are less important

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 (2011), Ekström (2015)

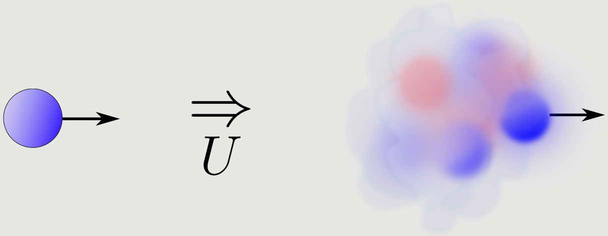
IM-SRG

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 $\tilde{a}_i^\dagger$

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

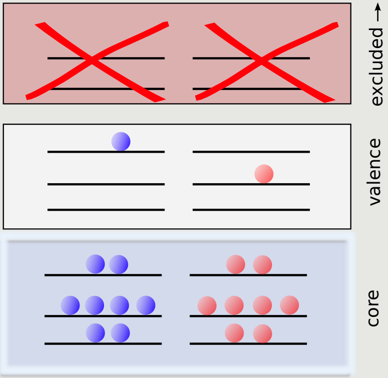
- The single-particle orbits are now much more complicated!



IM-SRG + shell model: The middle ground

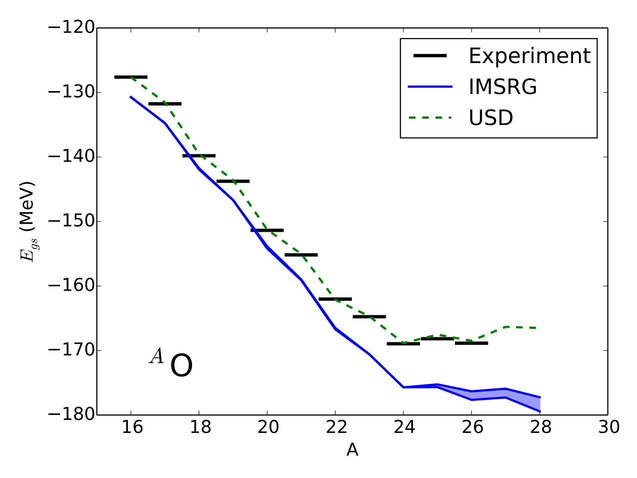
IM-SRG + Shell model

- Excluded configurations treated with IM-SRG (redefinition of H_{od})
- Valence configurations treated explicitly with standard shell model code
- In following, all calculations use E&M N^{3}LO NN + local N^{2}LO 3N (kindly provided by Angelo Calci)



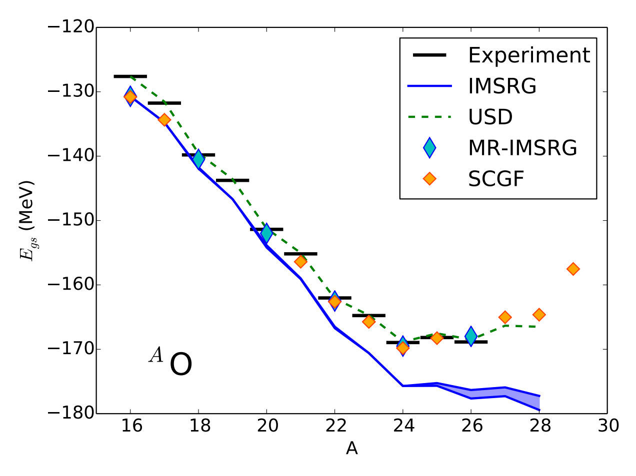
Emtem and Machleidt (2003), Navrátil (2007), Tsukiyama (2012)

IM-SRG + Shell model: Ground states



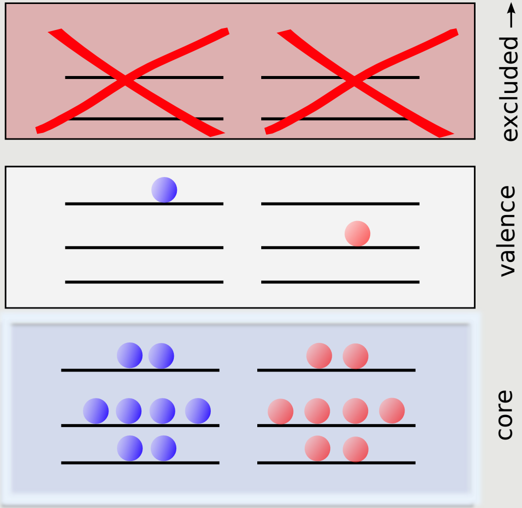
Bogner (2014), Brown (2006)

IM-SRG + Shell model: Ground states



Bogner (2014), Brown (2006), Cipollone (2013), Hergert (2014)

IM-SRG + Shell model: Ground states



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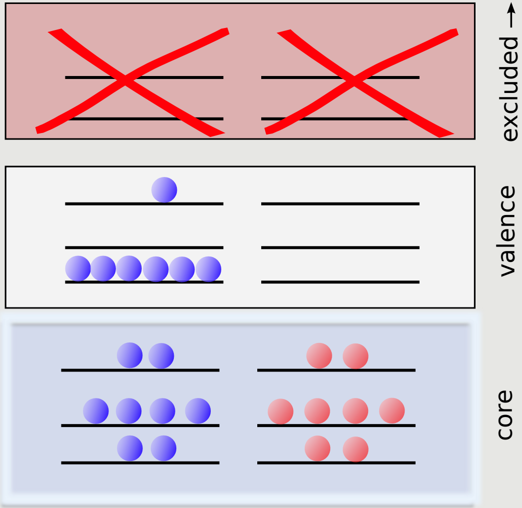
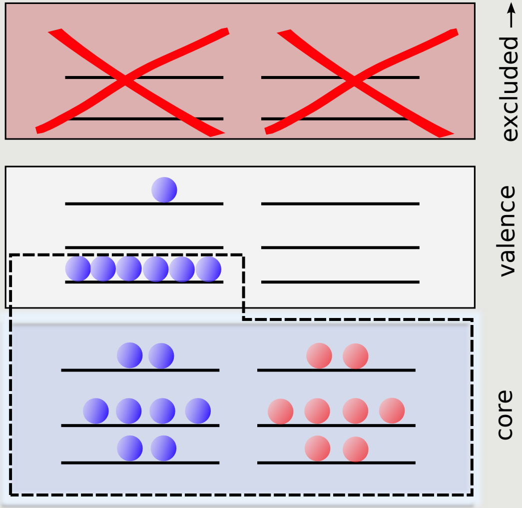
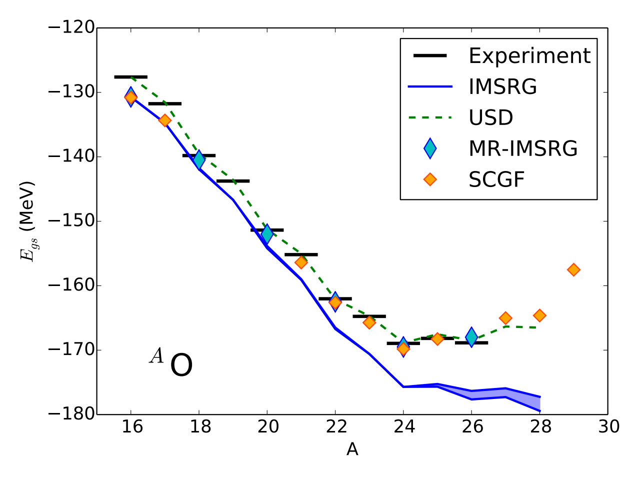


IM-SRG + Shell model: Ground states

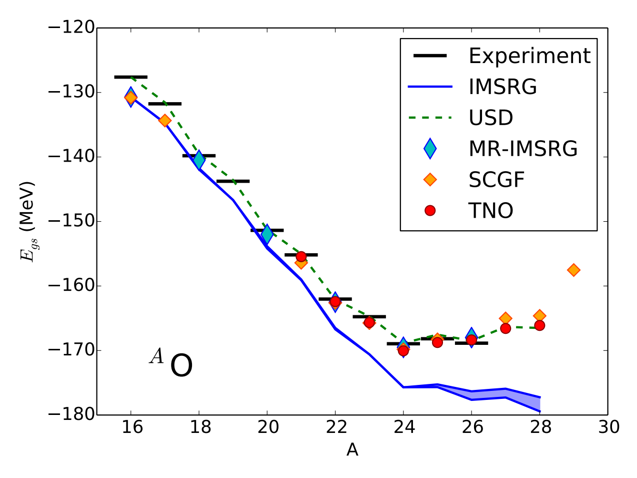


IM-SRG + Shell model: Ground states



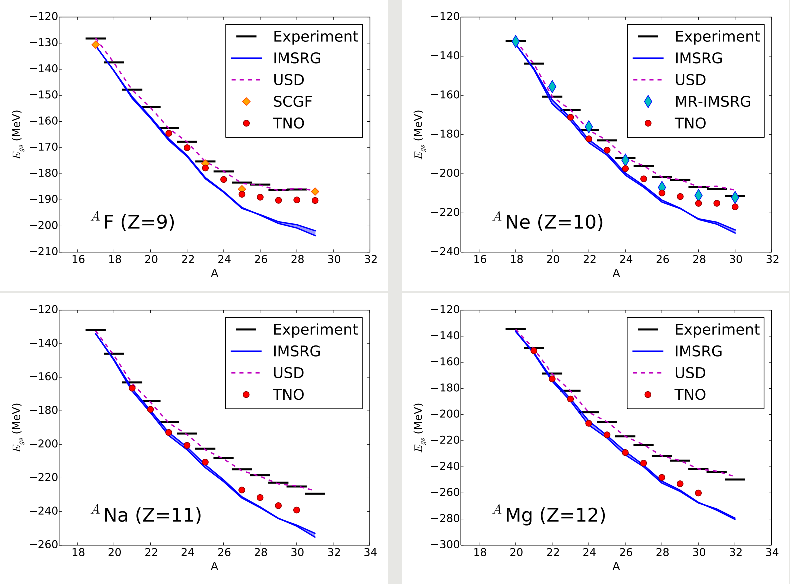
Bogner (2014), Brown (2006), Cipollone (2013), Hergert (2014)

IM-SRG + Shell model: Ground states

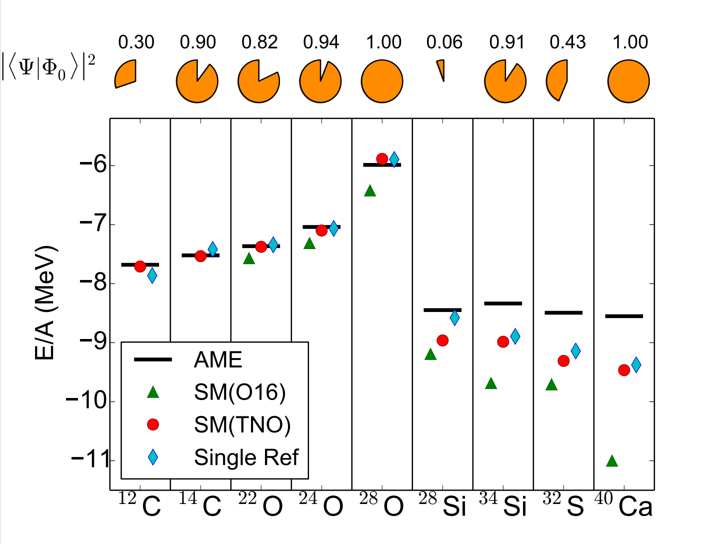


Bogner (2014), Brown (2006), Cipollone (2013), Hergert (2014)

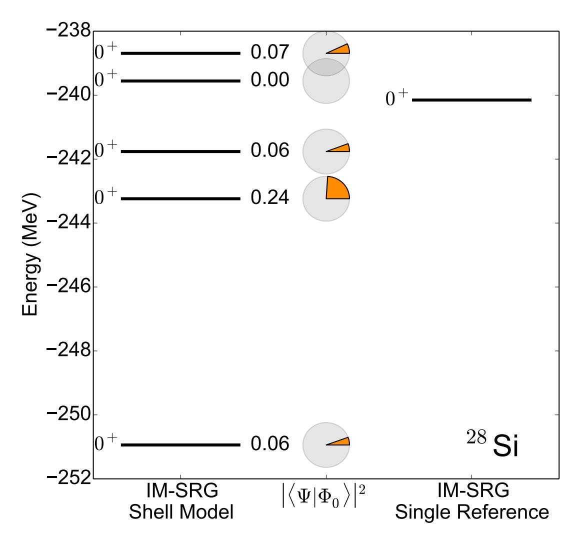
IM-SRG + Shell model: Ground states



IM-SRG + Shell model: Closed subshells

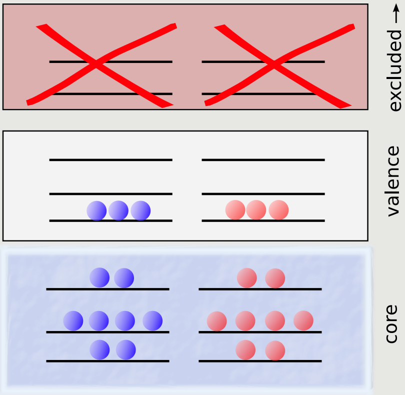


IM-SRG + Shell model: Ground state of ^{28}Si



IM-SRG + Shell model: ^{22}Na ground state

- Ground state spin of ^{22}Na is difficult for microscopic calculations
- Likely due to 3N forces, analogous to ^{10}B in p-shell



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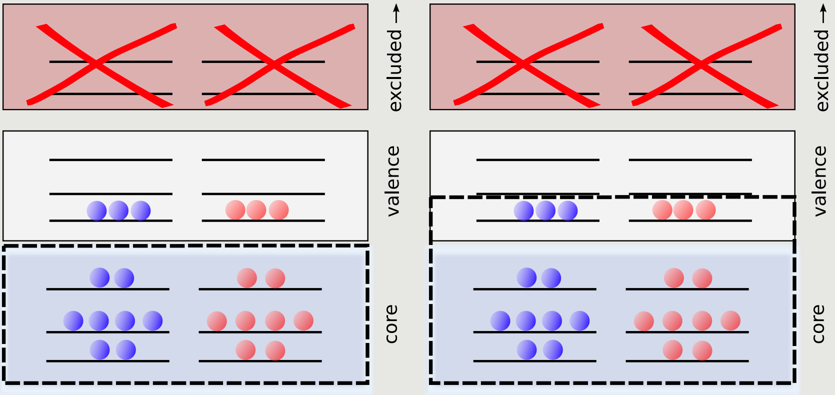
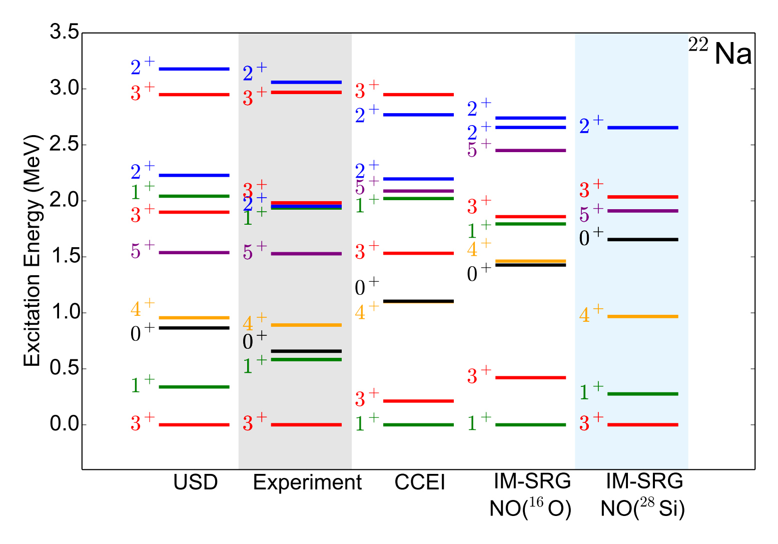
IM-SRG + Shell model: ^{22}Na ground state



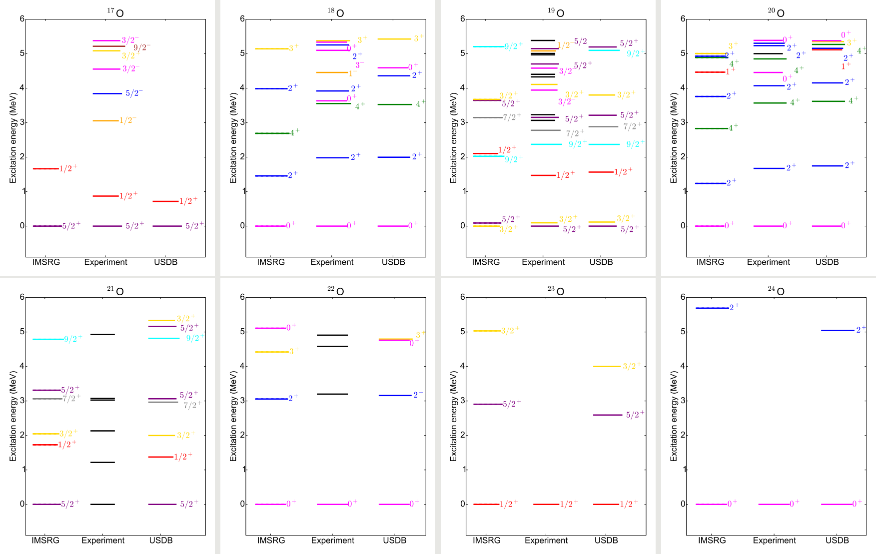
$|\Phi_0\rangle = {}^{16}\mathrm{O}$ $|\Phi_0\rangle = {}^{28}\mathrm{Si}$

IM-SRG + Shell model: ^{22}Na ground state

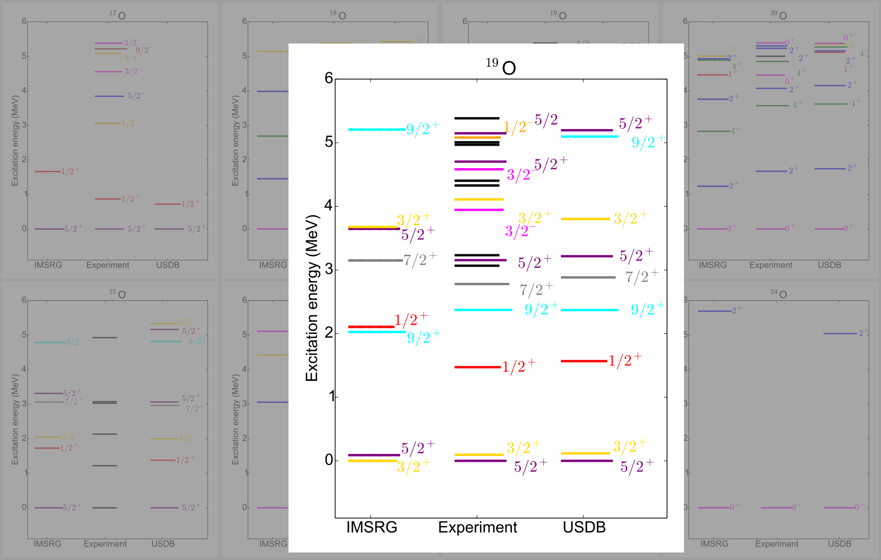


Excited States

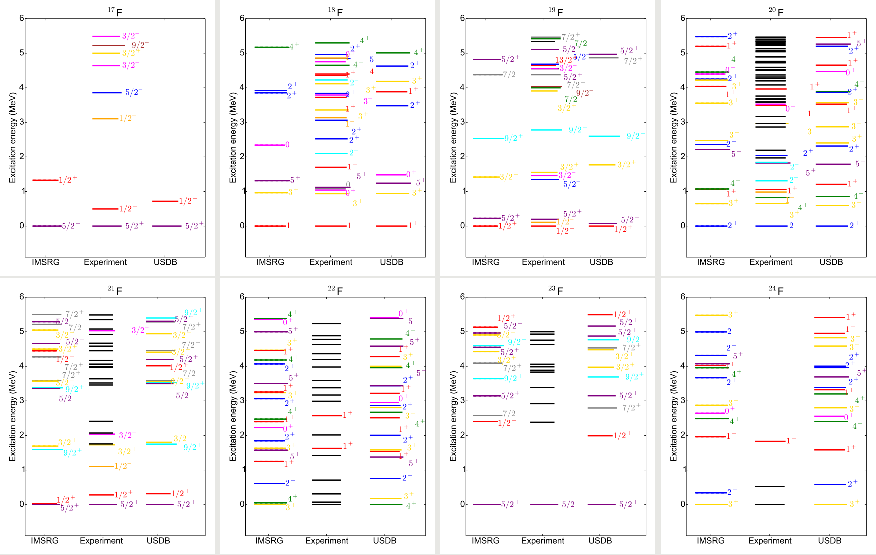
IM-SRG + Shell model: Excited states



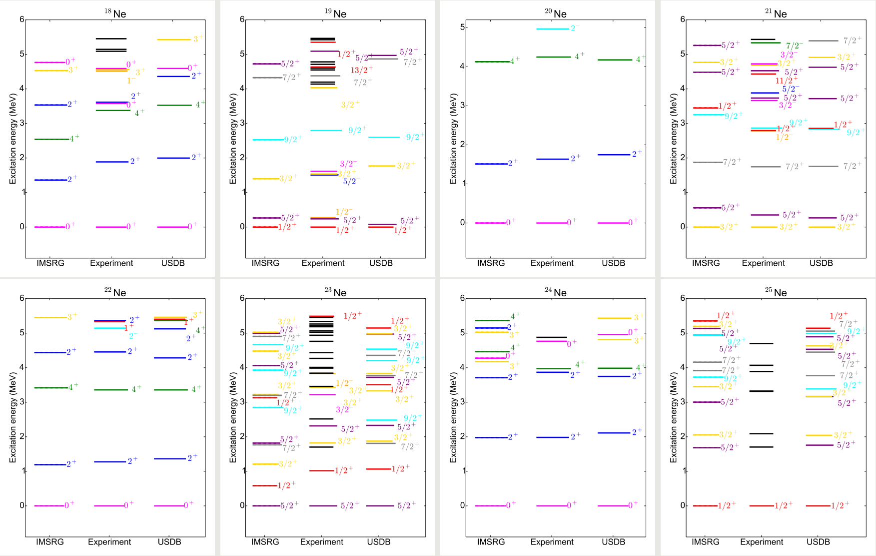
IM-SRG + Shell model: Excited states



IM-SRG + Shell model: Excited states



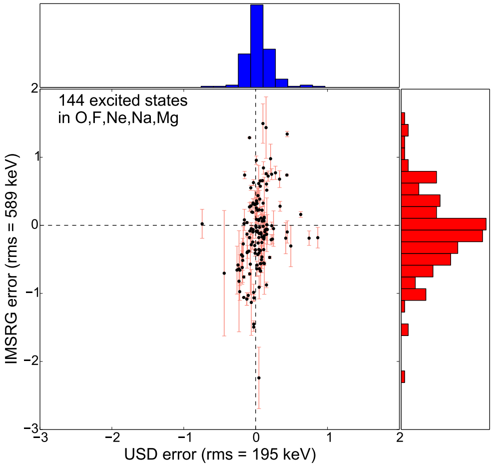
IM-SRG + Shell model: Excited states



IM-SRG + Shell model: Excited states

Deviation from experiment:

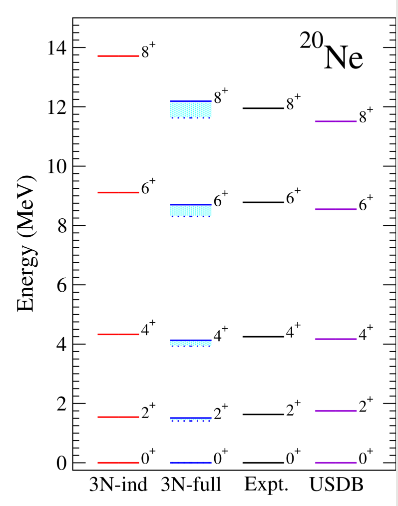
Interaction	RMS
USD	195
IM-SRG	589
CCEI	582
Kuo	817
Bonn A	832



Brown (2006), Jansen (2015), Hjorth-Jensen (2000), Kuo (1967)

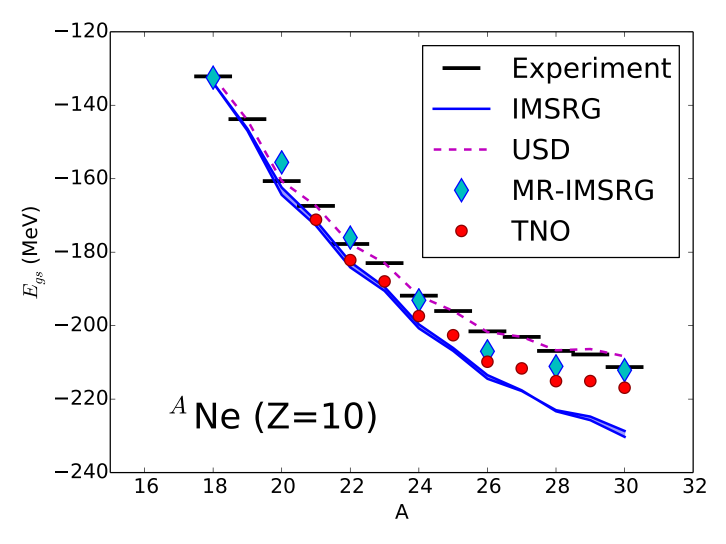
Deformation

IM-SRG + Shell model: Deformation

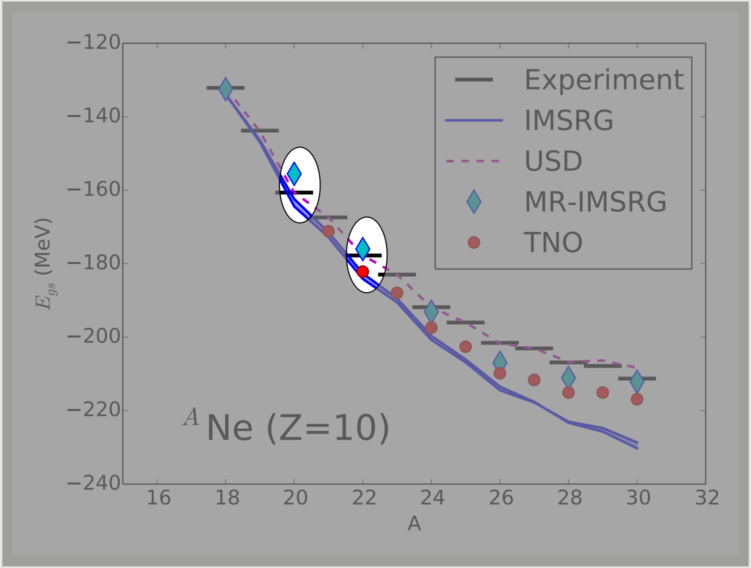


See also, Jansen et al (2015)

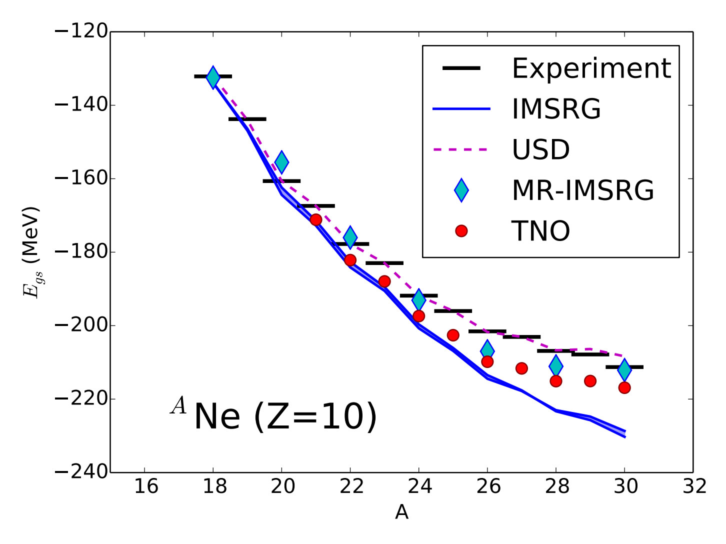
IM-SRG + Shell model: Deformation



IM-SRG + Shell model: Deformation



IM-SRG + Shell model: Deformation



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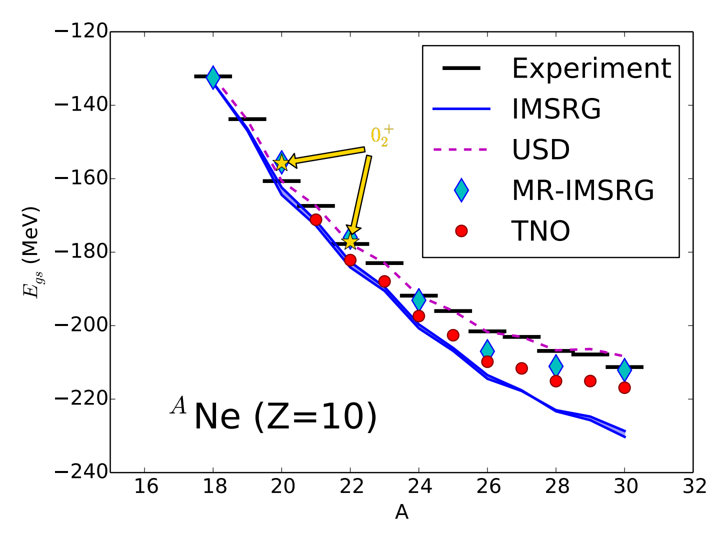
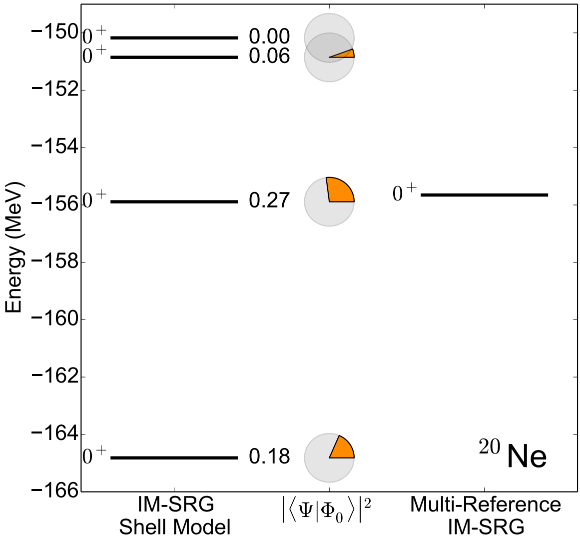


IM-SRG + Shell model: Deformation

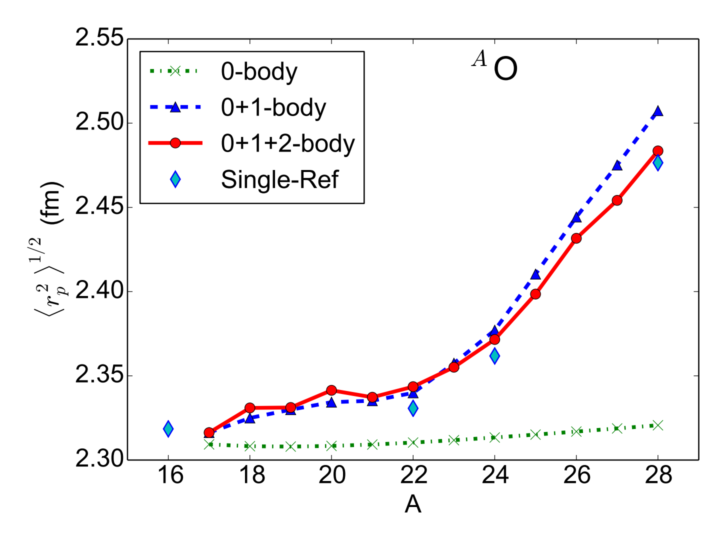


Radii

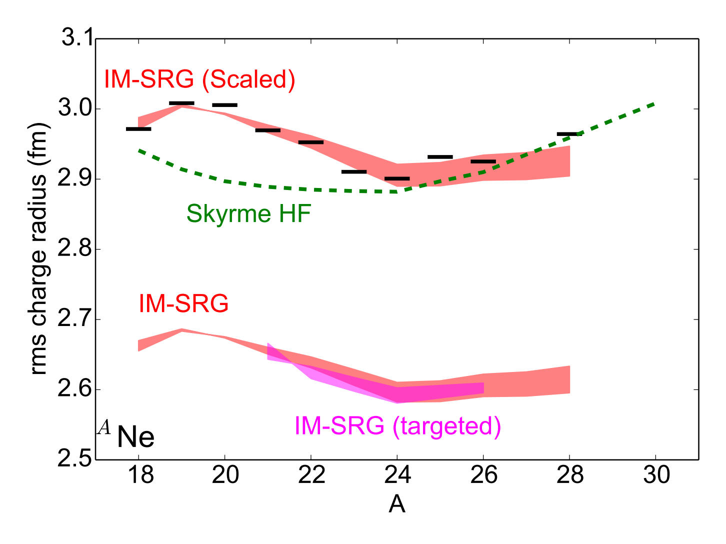
$$\tilde{R}^2 = U R^2 U^\dagger$$

$$\langle R^2 \rangle = \langle \Phi_0 | \tilde{R}^2 | \Phi_0 \rangle + \langle \Psi_{SM} | \tilde{R}^2 | \Psi_{SM} \rangle$$

IM-SRG + Shell model: Oxygen Radii



IM-SRG + Shell model: Neon Radii



Marinova (2011), Brown (1998)

Evolution of Tensor Operators*

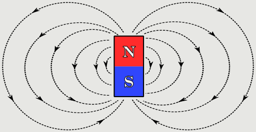
$$\langle \Psi^f \| \mathcal{O}^\Lambda \| \Psi^i \rangle = \langle \Psi^f_{SM} \| \tilde{\mathcal{O}}^\Lambda \| \Psi^i_{SM} \rangle$$

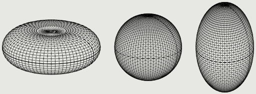
$$\tilde{\mathcal{O}}^\Lambda = e^\Omega \mathcal{O}^\Lambda e^{-\Omega} = \mathcal{O}^\Lambda + [\Omega, \mathcal{O}^\Lambda] + [\Omega, [\Omega, \mathcal{O}^\Lambda]] + \dots$$

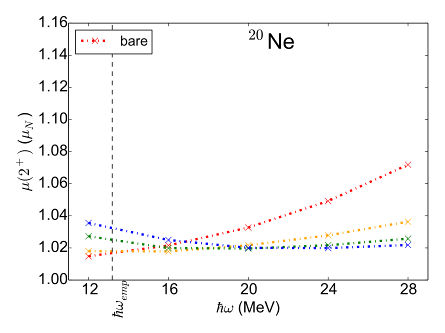
* More benchmarking remains to be done

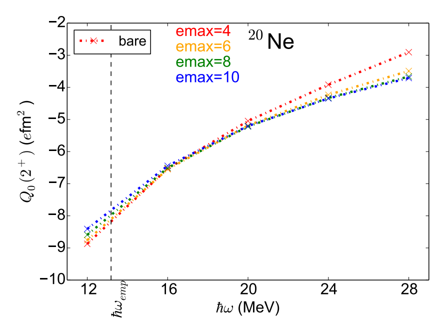
IM-SRG + Shell model: Tensor Operators

Moments



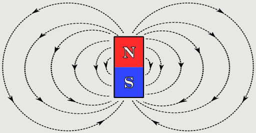


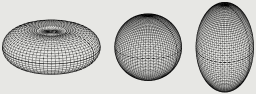


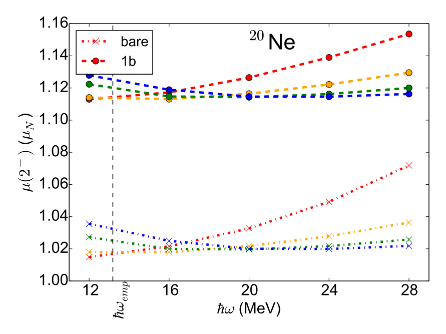


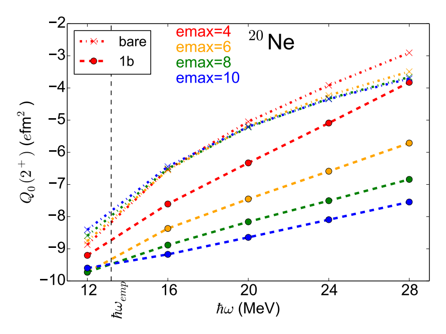
IM-SRG + Shell model: Tensor Operators

Moments



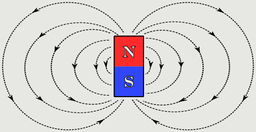


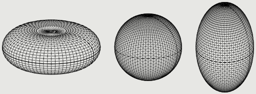


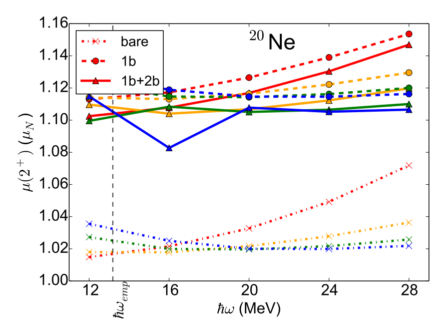


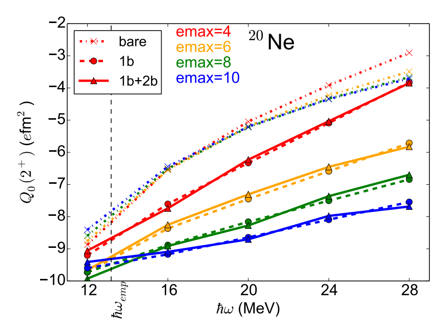
IM-SRG + Shell model: Tensor Operators

Moments



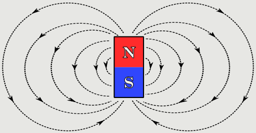


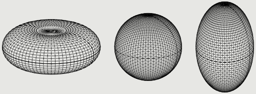


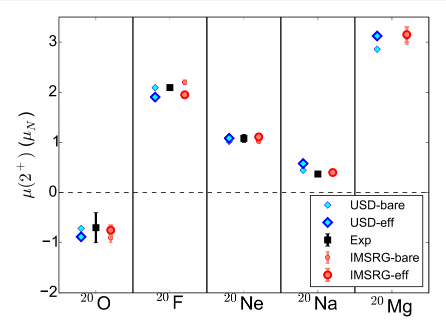


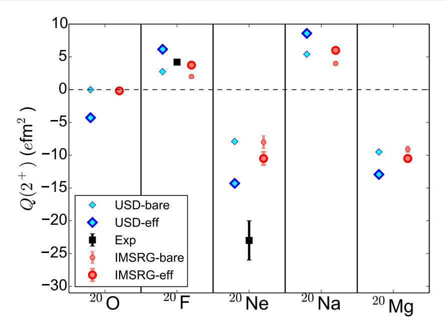
IM-SRG + Shell model: Tensor Operators

Moments



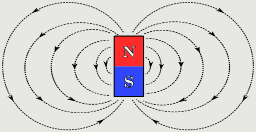


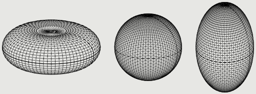


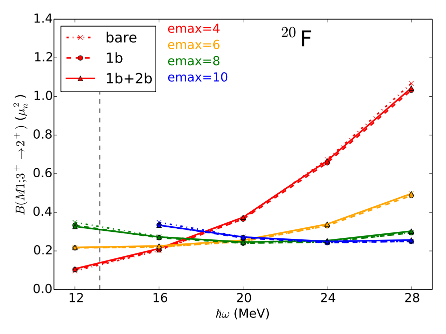


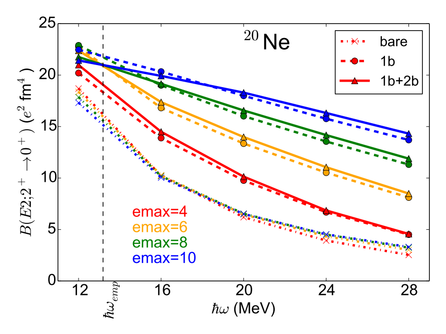
IM-SRG + Shell model: Tensor Operators

Transitions



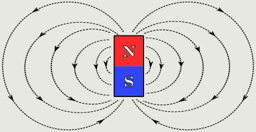


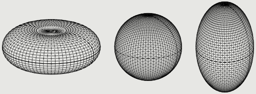


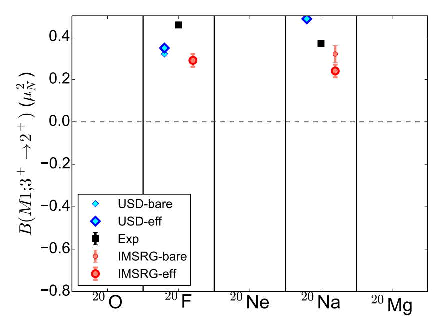


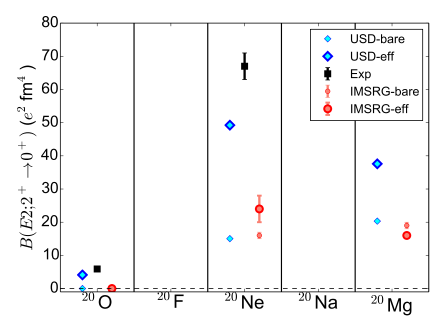
IM-SRG + Shell model: Tensor Operators

Transitions









Summary

- IM-SRG provides an appealing ab initio framework to address medium-mass nuclei and test microscopic interactions
- Effective valence-space interactions and operators open the door to excited states, transitions, open-shell/deformed systems
- Targeted normal ordering provides a reasonable first approximation of valence 3N forces, with more improvements still possible
- A first look at tensor operators yields relatively small renormalization – more work to be done.

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Appendix

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

A toy problem:

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

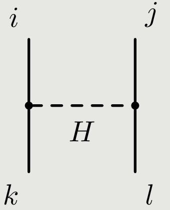
$$e^{\hat{\Omega}}\hat{H}e^{-\hat{\Omega}} = \begin{pmatrix} \epsilon_1\cos^2\theta + \epsilon_2\sin^2\theta + h\sin 2\theta & h_{od}\cos 2\theta + \frac{\epsilon_2-\epsilon_1}{2}\sin 2\theta \\ h_{od}\cos 2\theta + \frac{\epsilon_2-\epsilon_1}{2}\sin 2\theta & \epsilon_2\cos^2\theta + \epsilon_1\sin^2\theta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

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

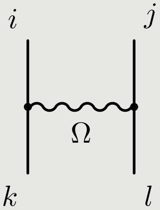
$$\theta \ll 1 \quad \Rightarrow \quad \theta \approx \frac{h_{od}}{\epsilon_1-\epsilon_2}$$

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

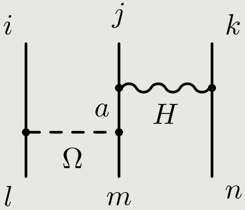
Induced forces and normal ordering



$$\hat{H}^{(2)} \sim h_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$



$$\hat{\Omega}^{(2)} \sim \omega_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

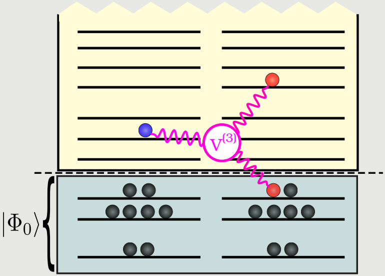


$$\left[\hat{\Omega}^{(2)}, \hat{H}^{(2)}\right] \sim \omega_{ialm} h_{jkan} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$$

Induced forces and normal ordering

$$\hat{H}_{\text{free}} = \overbrace{\sum_{ij} t_{ij} a_i^\dagger a_j}^{\text{1-body}} + \overbrace{\frac{1}{(2!)^2}\sum_{ijkl} V^{(2)}_{ijkl} a_i^\dagger a_j^\dagger a_k a_l}^{\text{2-body}} + \overbrace{\frac{1}{(3!)^2}\sum_{ijklmn} V^{(3)}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l}^{\text{3-body}}$$

$$\hat{H}_{\text{NO}} = \overbrace{E_0}^{\text{0-body}} + \overbrace{\sum_{ij} f_{ij}\left\{a_i^\dagger a_j\right\}}^{\text{1-body}} + \overbrace{\frac{1}{(2!)^2}\sum_{ijkl} \Gamma_{ijkl}\left\{a_i^\dagger a_j^\dagger a_k a_l\right\}}^{\text{2-body}} + \overbrace{\frac{1}{(3!)^2}\sum_{ijklmn} W_{ijklmn}\left\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\right\}}^{\text{3-body}}$$



$$E_0 = \sum_{\substack{i \\ \in|\Phi_0\rangle}} t_{ii} + \frac{1}{2}\sum_{\substack{ij \\ \in|\Phi_0\rangle}} V^{(2)}_{ijij} + \frac{1}{6}\sum_{\substack{ijk \\ \in|\Phi_0\rangle}} V^{(3)}{}_{ijkijk}$$

$$f_{ij} = t_{ij} + \sum_{\substack{k \\ \in|\Phi_0\rangle}} V^{(2)}_{ikjk} + \frac{1}{2}\sum_{\substack{kl \\ \in|\Phi_0\rangle}} V^{(3)}{}_{ikljkl}$$

$$\Gamma_{ijkl} = V_{ijkl} + \sum_{\substack{m \\ \in|\Phi_0\rangle}} V^{(3)}{}_{ijmklm}$$

$$W_{ijklmn} = V^{(3)}{}_{ijklmn}$$