Valence space effective operators with In-Medium SRG

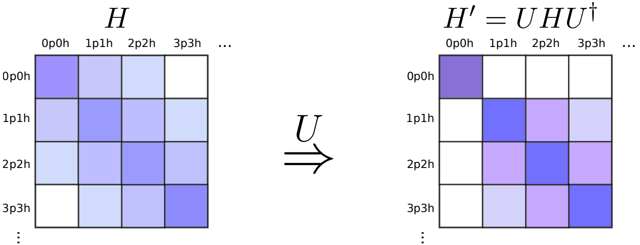
Ragnar Stroberg

TRIUMF

ICNT Workshop MSU

Outline

- In-Medium SRG with Magnus method
- Valence space effective interactions
- Scalar effective operators



In-Medium SRG

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

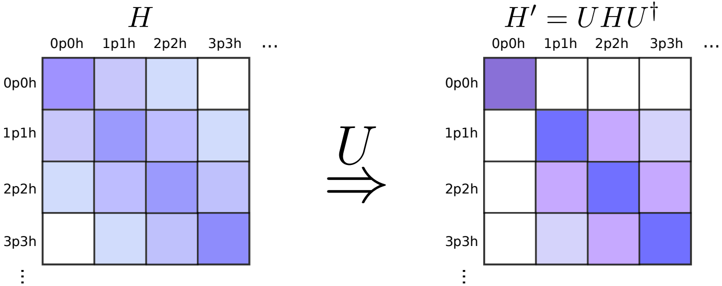
Perform unitary transformation to put H in a more convenient form:

$$\begin{aligned} H_{eff} &= UHU^{\dagger} \\ &= e^{\Omega}He^{-\Omega} \\ &= H + [\Omega, H] + \frac{1}{2}[\Omega,[\Omega,H]] + \dots \end{aligned}$$

Choice of Ω motivated by the desired form of H_{eff}.

T. Morris et. al (in prep)

$$H^{od} \equiv \langle p| H |h\rangle + \langle pp| H |hh\rangle$$
$$\to 0$$



$$E_0 = \langle \Phi_0| H' |\Phi_0\rangle = \langle \Psi_{gs}| H |\Psi_{gs}\rangle$$

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)

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

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

For a larger system, solution is iterative:

$$e^{\hat{\Omega}} = e^{\hat{\Omega}_N} e^{\hat{\Omega}_{N-1}} \dots e^{\hat{\Omega}_2} e^{\hat{\Omega}_1}$$

Update $\hat{\Omega}$ after each iteration using Baker-Campbell-Hausdorff expansion:

$$e^{\hat{\Omega}} = e^{\hat{\Omega}_2} e^{\hat{\Omega}_1}$$

$$\Downarrow$$

$$\hat{\Omega} = \hat{\Omega}_2 + \hat{\Omega}_1 + \tfrac{1}{2}\left[\hat{\Omega}_2, \hat{\Omega}_1\right] + \tfrac{1}{12}\left(\left[\hat{\Omega}_2, \left[\hat{\Omega}_2, \hat{\Omega}_1\right]\right] + \left[\hat{\Omega}_1, \left[\hat{\Omega}_1, \hat{\Omega}_2\right]\right]\right) + \dots$$

If you think you have a new idea...

$$U = e^{\hat{\Omega}}$$

$$\hat{\Omega} = \frac{1}{2}\tan^{-1}\left(\frac{h_{od}}{\epsilon_1 - \epsilon_2}\right)$$

$$\hat{H}' = \hat{H} + \left[\hat{\Omega}, \hat{H}\right] + \frac{1}{2}\left[\hat{\Omega}, \left[\hat{\Omega}, \hat{H}\right]\right] + \dots$$

Prog. Theor. Phys. Vol. 58 (1977), Sept.

Non-Perturbative Approach to Effective Interactions in Framework of Canonical Transformation Method

Kenji SUZUKI

$$U_n = \exp G_n$$

with

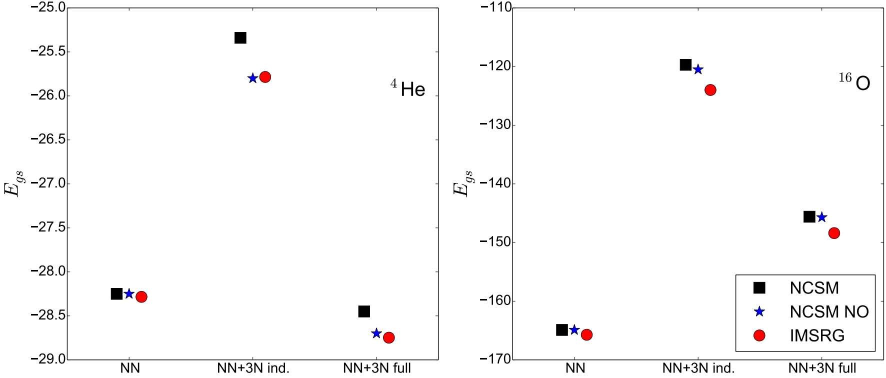
$$G_n = \sum_{p,q} g_{pq}^{(n)} (|p\rangle\langle q| - |q\rangle\langle p|),$$

$$g_{pq}^{(n)} = (1/2)\arctan\{2H_{pq}^{(n-1)}/(H_{qq}^{(n-1} - H_{pp}^{(n-1)} + \delta)\}$$

$$H^{(n)} = U_n{}^{-1} H^{(n-1)} U_n = H^{(n-1)} + [H^{(n-1)}, G_n] + (1/2) \times [[H^{(n-1)}, G_n], G_n] + \cdots .$$

Benchmark: ^{4}He and ^{16}O

Comparison with importance-truncated no-core shell model

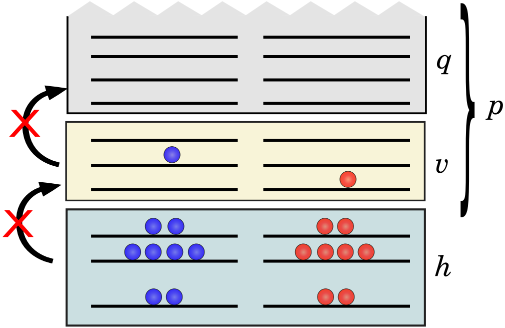


E&M N^{3}LO NN + N^{2}LO 3N (400,500 MeV cutoff)
$\hbar\omega$=20 MeV λ_{SRG}=1.88 fm^{-1}

IT-NCSM results from Roth et. al PRL 109 052501 (2012)

Decoupling a shell model valence space

$$H^{od} = \langle p|\, H\, |h\rangle + \langle pp|\, H\, |hh\rangle + \langle q|\, H\, |v\rangle + \langle pq|\, H\, |vv\rangle + \langle pp|\, H\, |hv\rangle$$



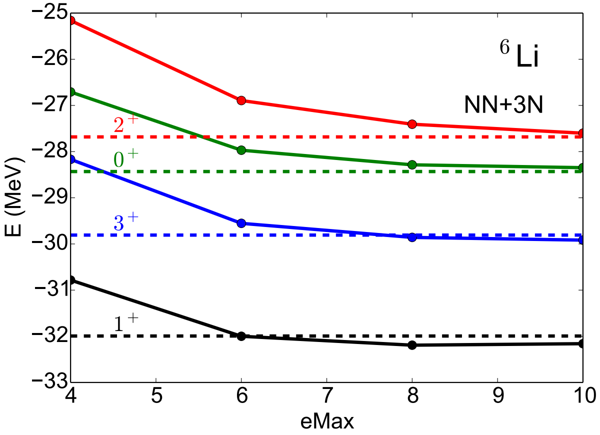
$$H_{SM}\, |\Psi_{SM}\rangle = E\, |\Psi_{SM}\rangle$$

and

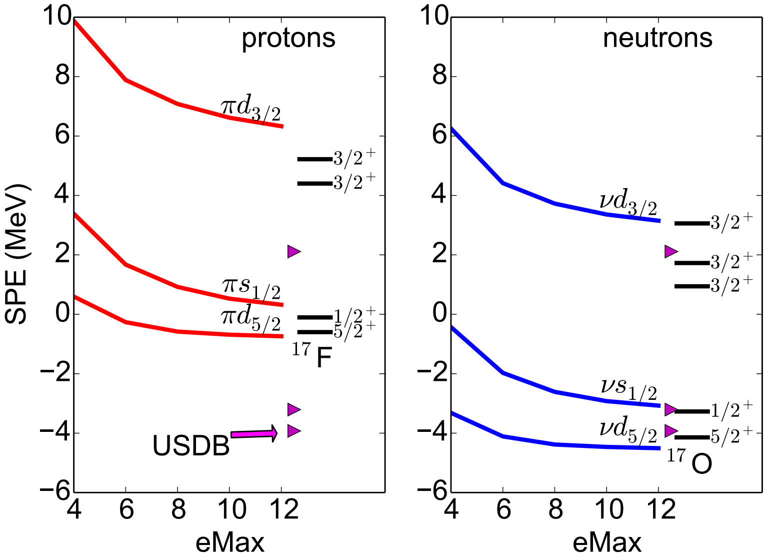
$$\langle \mathcal{O} \rangle = \langle \Psi_{SM}|\, \mathcal{O}_{SM}\, |\Psi_{SM}\rangle$$

Example: ^{6}Li

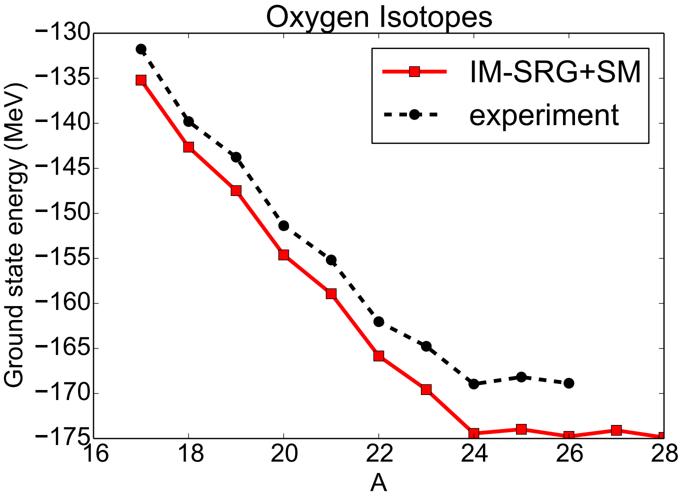
^{4}He core, diagonalization in p-shell



sd-shell single-particle energies



Oxygen Isotopes



Bogner et al. PRL 113 142501 (2014)

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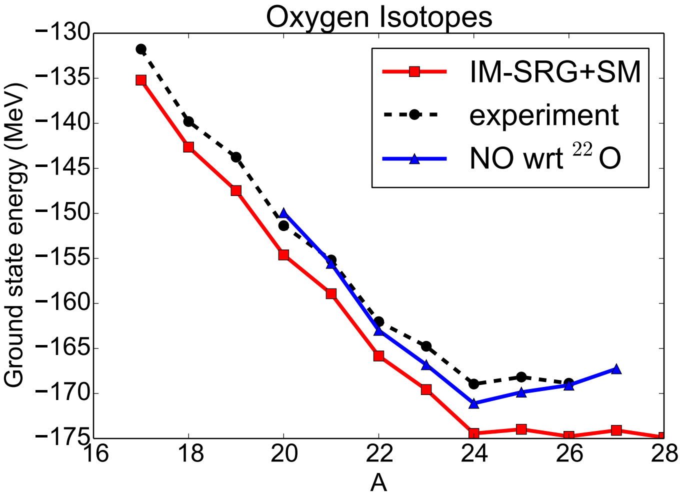
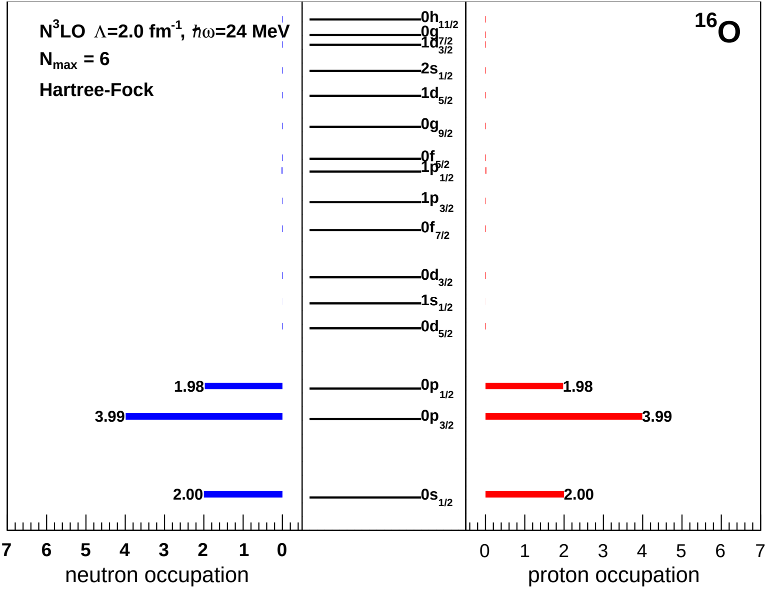


Bogner et al. PRL 113 142501 (2014)

"Observables" from evolved operators

$$\mathcal{O}' = U\mathcal{O}U^\dagger$$

“Observables”: occupation number



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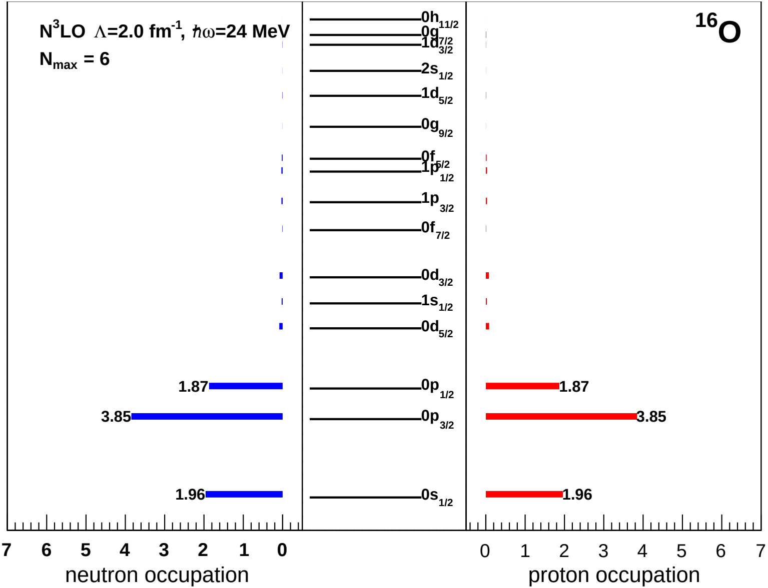

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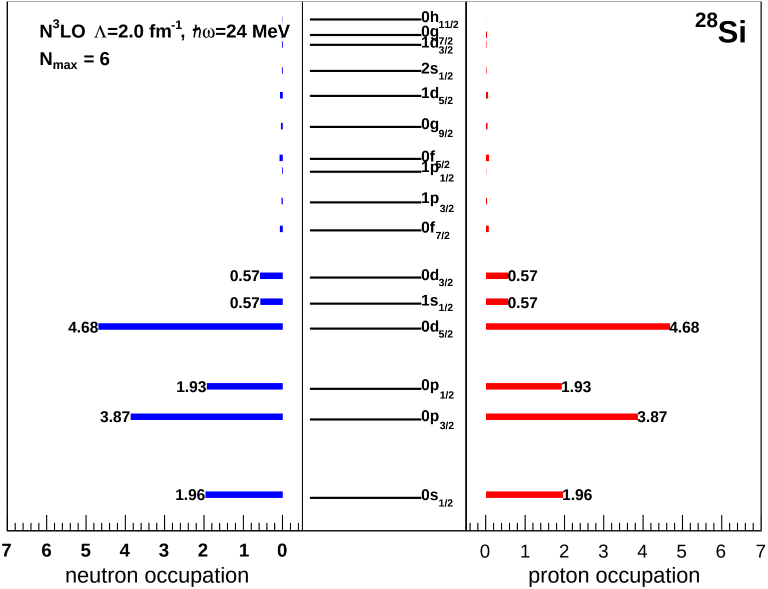

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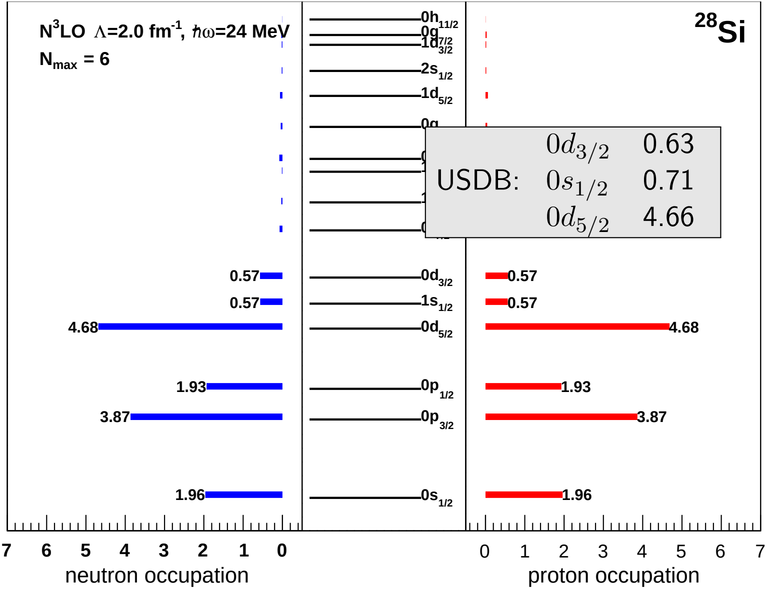
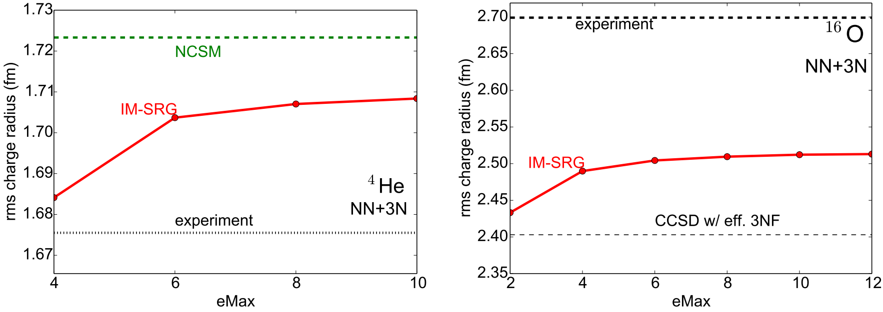


USDB:		
	$0d_{3/2}$	0.63
	$0s_{1/2}$	0.71
	$0d_{5/2}$	4.66

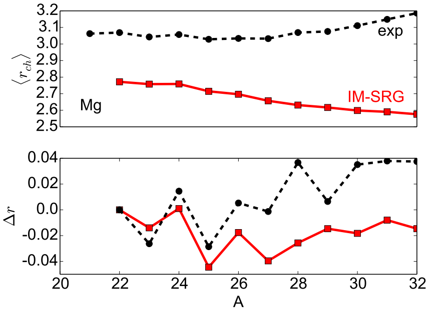
Charge radii

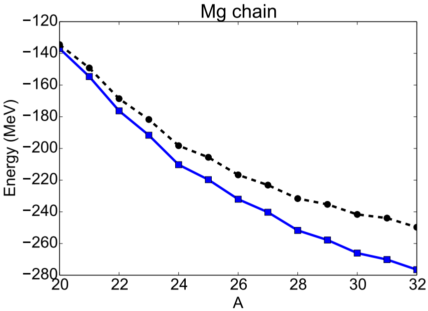


Good convergence for closed shells.

Angeli and Marinova Nucl. Dat. Tab. 99, 69 (2013)
Petr Navrátil, Priv. comm
Hagen et al. PRL 108 242501 (2012)

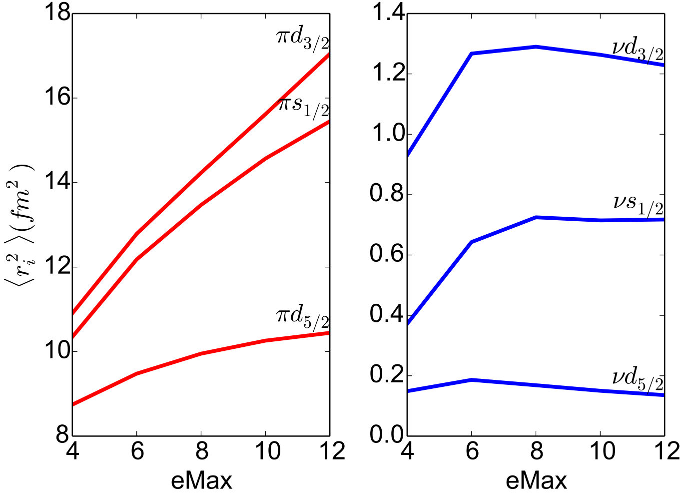
Mg Charge radii



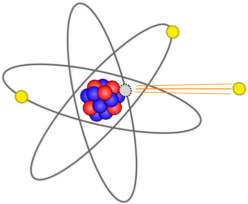


Radii for entire sd-shell are accessible.

One-body piece of proton r^2 operator



Electric monopole transitions



$$\frac{1}{\tau} = \underbrace{\kappa}_{electronic} \underbrace{\left|\langle \Psi_f \left| \hat{\rho}_{E0} \right| \Psi_i \rangle\right|^2}_{nuclear}$$

$$\hat{\rho}_{E0} \approx \frac{1}{eR^2} \sum_i e_i r_i^2$$

In a single major HO shell, $\left|\langle \Psi_f \left| \hat{\rho}_{E0} \right| \Psi_i \rangle\right|^2 \propto \delta_{fi}$

$$e^{\Omega} \left(\hat{\rho}_{E0}\right) e^{-\Omega} = \rho_{E0} + [\Omega, \rho_{E0}] + \ldots$$

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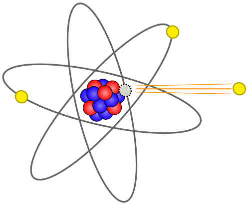

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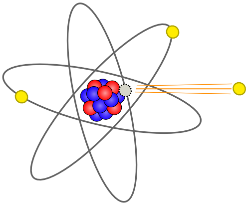

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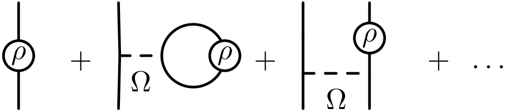

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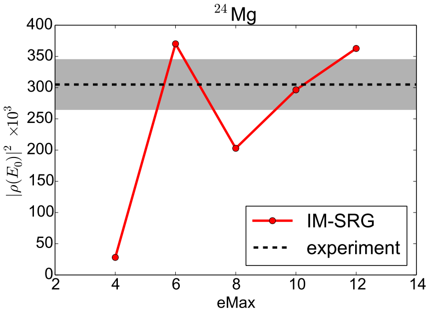
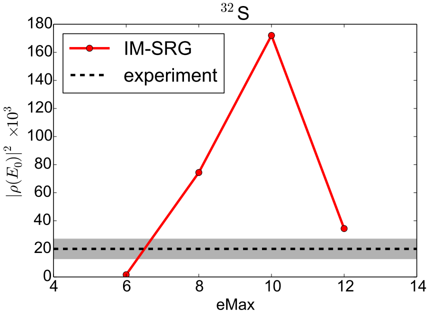




Convergence issues need to be understood.

Summary

- IM-SRG provides a formally straight-forward framework to calculate properties of medium-mass nuclei
- Effective valence-space interactions and operators open the door to excited states and open-shell systems
- The Magnus expansion method has several attractive features
- Radii appear to be slower to converge than energies
- We have the potential for obtaining $E0$ transition rates in the shell model
- Tensor operators coming soon

Collaborators:

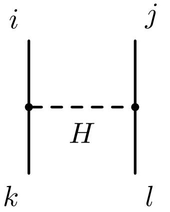
TRIUMF A Calci, **JD Holt**, P Navratil

NSCL/MSU **S Bogner**, **H Hergert**, T Morris, N Parzuchowski

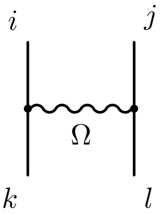
TU Darmstadt **A Schwenk**

Appendix

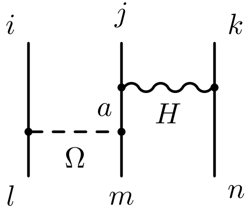
Induced forces and normal ordering (in-medium SRG)



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



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

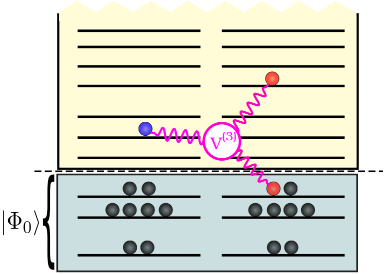


$$\left[\hat{\Omega}^{(2)}, \hat{H}^{(2)}\right] \sim \omega_{ialm} h_{jkan} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$$

Induced forces and normal ordering (in-medium SRG)

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

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



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

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

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

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

Commutator relations for tensor operators

Normal ordered operators in a J-coupled basis

$$e^{\Omega}\mathcal{O}^{\Lambda}e^{-\Omega} = \mathcal{O}^{\Lambda} + \left[\Omega, \mathcal{O}^{\Lambda}\right] + \frac{1}{2}\left[\Omega, \left[\Omega, \mathcal{O}^{\Lambda}\right]\right] + \dots$$

$$[X,Y]_0 = \sum_{ab}(n_a - n_b)\hat{j_a}^2 (X_{ab}Y_{ba}) + \frac{1}{2}\sum_{abcdJ} n_a n_b \bar{n}_c \bar{n}_d \hat{J}^2 X^J_{abcd} Y^J_{cdab}$$

$$\Downarrow$$

$$\left[X, Y^{\Lambda}\right]_0 = [X,Y]_0 \, \delta_{\Lambda 0}$$

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$$\Downarrow$$

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Commutator relations for tensor operators (one body)

$$
\begin{aligned}
[X,Y]_{ij} &= (1-P_{ij})\sum_a X_{ia}Y_{aj} \\
&+ \frac{1}{\hat{j}_i}\sum_{abJ}(n_a-n_b)\,\hat{J}^2\left(X_{ab}Y^J_{biaj} - Y_{ab}X^J_{biaj}\right) \\
&+ \frac{1}{2\hat{j}_i}\sum_{abcJ}(n_a n_b \bar{n}_c + \bar{n}_a\bar{n}_b n_c)\,\hat{J}^2\left(X^J_{ciab}Y^J_{abcj} - Y^J_{ciab}X^J_{abcj}\right)
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\left[X,Y^\Lambda\right]_{ij} &= (1-P_{ij})\sum_a X_{ia}Y^\Lambda_{aj} \\
&+ \frac{1}{\hat{j}_i}\sum_{\substack{ab\\JJ'}}(n_a-n_b)\,(-1)^{j_a+j_j+J}\,\hat{J}^2\,\hat{J}'\begin{Bmatrix} J' & J & \Lambda \\ j_i & j_j & j_a \end{Bmatrix} X_{ab}Y^{\Lambda JJ'}_{biaj} \\
&- \frac{1}{\hat{j}_i}\sum_{abJ}(n_a-n_b)\,(-1)^{j_b+j_i+J}\,\hat{J}^2\,\hat{j}_a\begin{Bmatrix} j_i & j_j & J \\ j_k & j_l & \Lambda \end{Bmatrix} Y^\Lambda_{ab}X^J_{biaj} \\
&+ \frac{1}{2\hat{j}_i}\sum_{\substack{abc\\JJ'}}(n_a n_b \bar{n}_c + \bar{n}_a\bar{n}_b n_c)\,\hat{J}^2\,\hat{J}'\begin{Bmatrix} J' & J & \Lambda \\ j_i & j_j & j_c \end{Bmatrix}\left(X^J_{ciab}Y^{\Lambda JJ'}_{abcj} - Y^{\Lambda JJ'}_{ciab}X^{J'}_{abcj}\right)
\end{aligned}
$$

Commutator relations for tensor operators (two body)

$$
\begin{aligned}
[X,Y]^J_{ijkl} &= P_{ij}P_{kl}\sum_a \left(X_{ia}Y^J_{ajkl} - Y_{ia}X^J_{ajkl}\right) \\
&+ \frac{1}{2}\sum_{ab}(\bar{n}_a - n_b)\left(X^J_{ijab}Y^J_{abkl} - Y^J_{ijab}X^J_{abkl}\right) \\
&+ P_{ij}P_{kl}\sum_{abJ'}(n_a - n_b)\,\hat{J'}^2 \begin{Bmatrix} j_i & j_j & J \\ j_k & j_l & J' \end{Bmatrix} \bar{X}^{J'}_{i\bar{l}a\bar{b}}\bar{Y}^{J'}_{a\bar{b}k\bar{j}}
\end{aligned}
$$

$$\Downarrow$$

$$
\begin{aligned}
\left[X,Y^{\Lambda}\right]^{\Lambda J J'}_{ijkl} &= P_{ij}P_{kl}\sum_a \left(X_{ia}Y^{\Lambda J J'}_{ajkl} - \hat{j}_i\hat{J}'(-1)^{j_i+j_j+J}\begin{Bmatrix} J' & J & \Lambda \\ j_i & j_a & j_j \end{Bmatrix} Y^{\Lambda}_{ia}X^{J'}_{ajkl}\right) \\
&+ \frac{1}{2}\sum_{ab}(\bar{n}_a - n_b)\left(X^J_{ijab}Y^{\Lambda J J'}_{abkl} - Y^{\Lambda J J'}_{ijab}X^{J'}_{abkl}\right) \\
&+ P_{ij}P_{kl}\sum_{abJ_1J_2}(n_a - n_b)\,\hat{J}'\hat{J_1}^2\hat{J}_2(-1)^{j_j+j_l+J'+J_2}\begin{Bmatrix} j_i & j_l & J_1 \\ j_j & j_k & J_2 \\ J & J' & \Lambda \end{Bmatrix} \bar{X}^{J_1}_{i\bar{l}a\bar{b}}\bar{Y}^{\Lambda J_1 J_2}_{a\bar{b}k\bar{j}}
\end{aligned}
$$

Commutator relations for tensor operators (two body)