Valence space effective operators with In-Medium SRG

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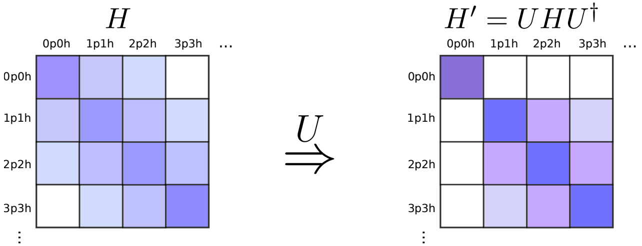
TRIUMF

TRIUMF Nuclear Theory Workshop

Outline

- In-Medium SRG with generator flow (Magnus method)
- Effective operators
- Scalar operators in a valence space
- Tensor operators



IM-SRG

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

$$\hat{H} = \underbrace{\hat{H}^{d}}_{Easy} + \underbrace{\hat{H}^{od}}_{Hard}$$

$$\left(U\hat{H}U^{\dagger}\right)^{od} \rightarrow 0$$

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SRG flow equation (solve for U *implicitly*):

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

U may be found explicitly:

$$\frac{dU}{ds} = \eta(s)U(s)$$

In-Medium SRG $\rightarrow$ write H relative to $|\Phi_0\rangle$

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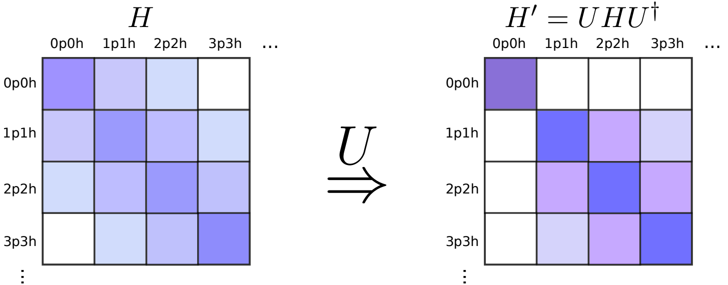
Decoupling the ground state of a closed-shell nucleus

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



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

IM-SRG

Alternative strategy (Magnus expansion):

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

U is solved for *explicitly*:

$$\frac{dU}{ds} = \eta(s)U(s) \quad \Rightarrow \quad U = e^{\Omega} = \mathcal{T}e^{\int \eta(s)ds}$$

Numerically,

$$e^{\Omega_{n+1}} = e^{\eta\delta s}e^{\Omega_n}$$

$$\Omega_{n+1} = \Omega_n + \eta\delta s + \frac{1}{2}\delta s\,[\eta, \Omega_n] + \ldots$$

T. Morris et al. (in preparation)

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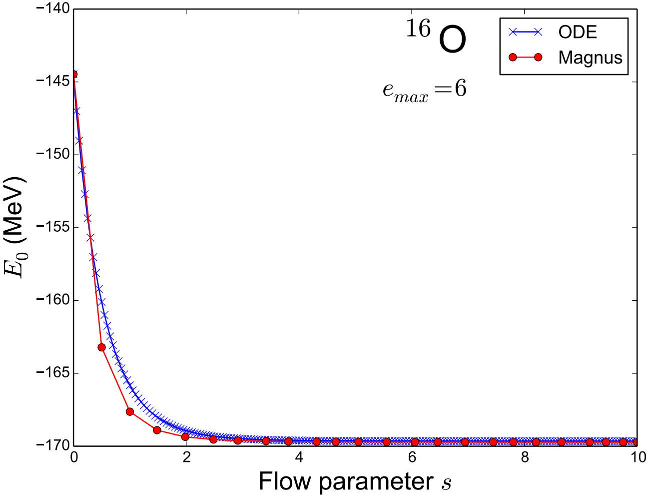
T. Morris et al. (in preparation)

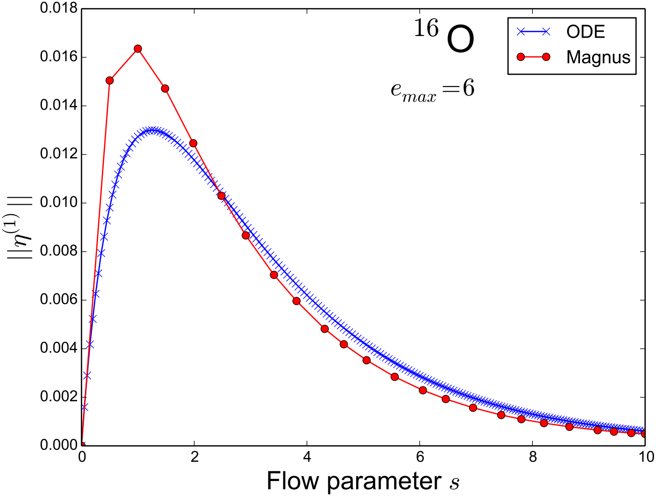
Advantages of explicit construction of $\hat{U}$

Implicit:	Explicit:
$\frac{d\hat{H}(s)}{ds} = \left[\hat{\eta}(s), \hat{H}(s)\right]$	$\hat{U}_N = e^{\hat{\Omega}_N} = e^{\hat{\eta}_N \delta s} e^{\hat{\Omega}_{N-1}}$ $\hat{H}_N = e^{\hat{\Omega}_N} \hat{H}_0 e^{-\hat{\Omega}_N}$
Truncation error accumulates $\rightarrow$ loss of unitarity	Unitary as long as $\hat{\Omega} = -\hat{\Omega}^\dagger$. Error only in final application of $\hat{U}$
Operators must be co-evolved, or need separate routines to calculate $U\mathcal{O}U^\dagger$	Fast transformation of operators. Write $\hat{\Omega}$ to file, transform operators later. Everything uses same commutator expressions.

Ground state energy

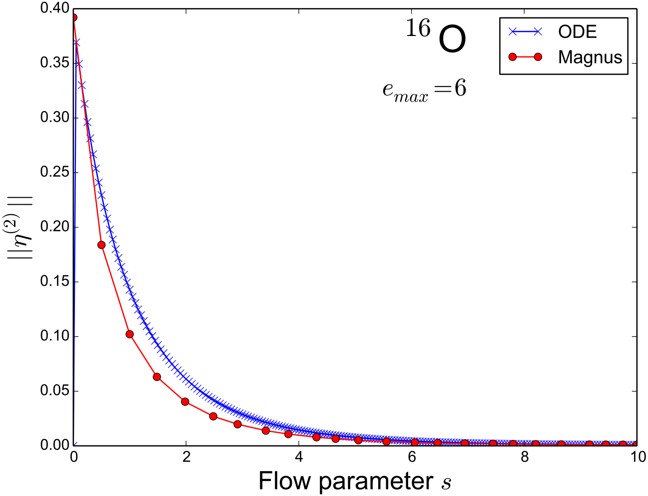


Two-body piece of generator $\eta^{(1)}$



Comparison of solution methdods

Two-body piece of generator $\eta^{(2)}$



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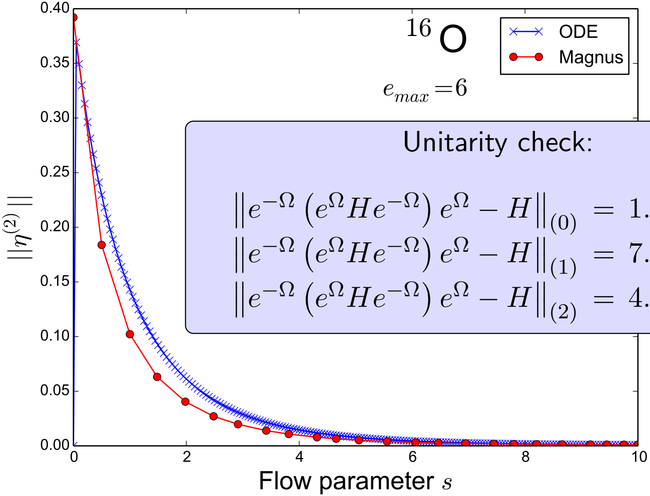
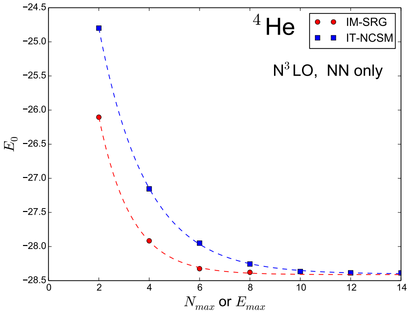


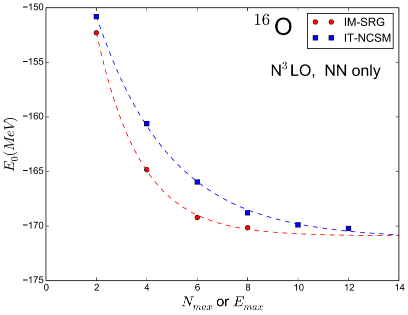
Unitarity check:

$$\left\| e^{-\Omega} \left(e^{\Omega} H e^{-\Omega} \right) e^{\Omega} - H \right\|_{(0)} = 1.9 \times 10^{-5}$$
$$\left\| e^{-\Omega} \left(e^{\Omega} H e^{-\Omega} \right) e^{\Omega} - H \right\|_{(1)} = 7.5 \times 10^{-6}$$
$$\left\| e^{-\Omega} \left(e^{\Omega} H e^{-\Omega} \right) e^{\Omega} - H \right\|_{(2)} = 4.7 \times 10^{-6}$$

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

Comparison with importance-truncated no-core shell model

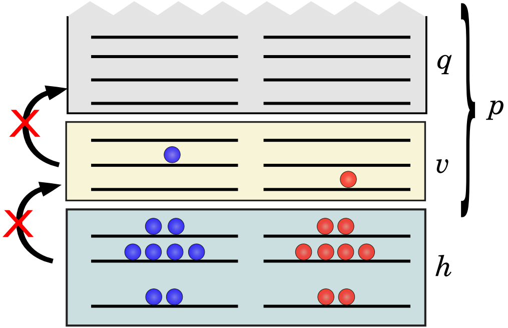




IT-NCSM results courtesy A. Calci

Decoupling a shell model valence space

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



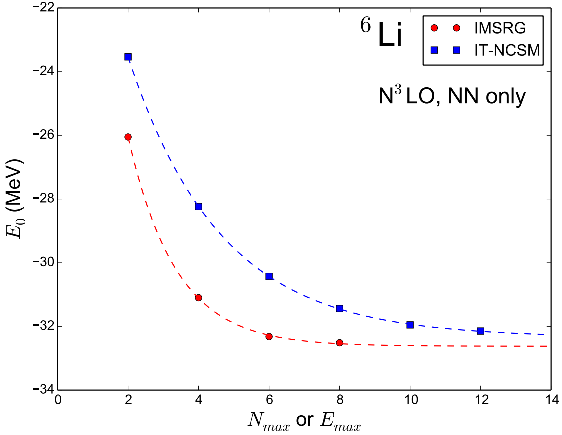
$$H_{SM} |\Psi_{SM}\rangle = E |\Psi_{SM}\rangle$$

and

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

Example: ^{6}Li

Comparison with importance-truncated no-core shell model



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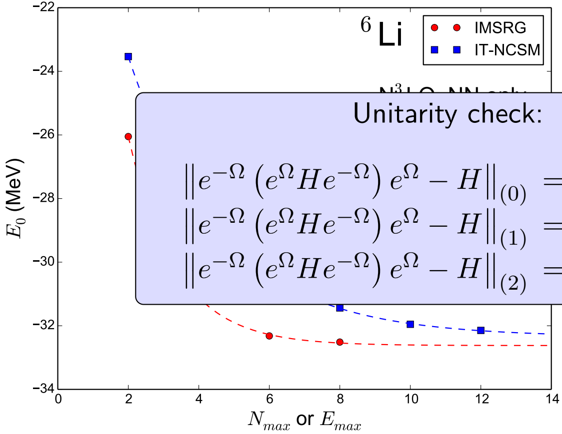


Unitarity check:

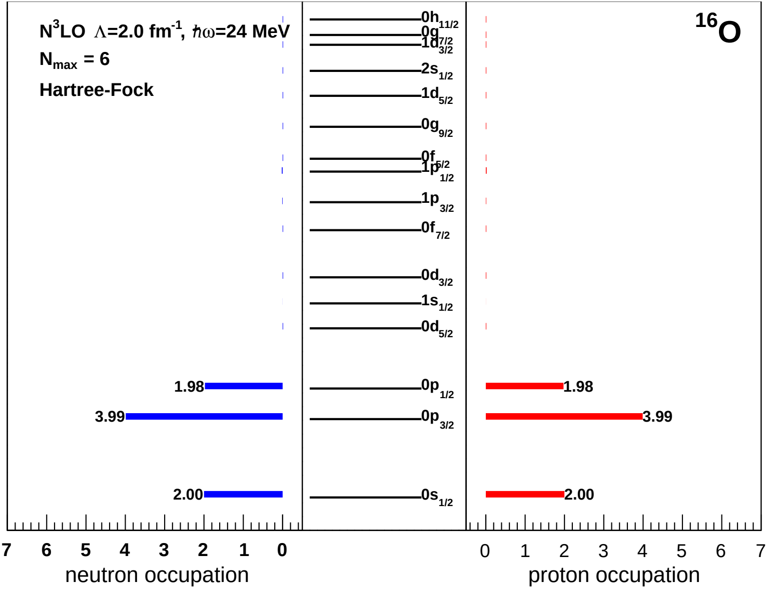
$$\left\| e^{-\Omega}\left(e^{\Omega} H e^{-\Omega}\right) e^{\Omega} - H \right\|_{(0)} = 2.7 \times 10^{-5}$$
$$\left\| e^{-\Omega}\left(e^{\Omega} H e^{-\Omega}\right) e^{\Omega} - H \right\|_{(1)} = 2.2 \times 10^{-5}$$
$$\left\| e^{-\Omega}\left(e^{\Omega} H e^{-\Omega}\right) e^{\Omega} - H \right\|_{(2)} = 1.5 \times 10^{-4}$$

IT-NCSM results courtesy A. Calci

“Observables” from evolved operators

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

"Observables": occupation number



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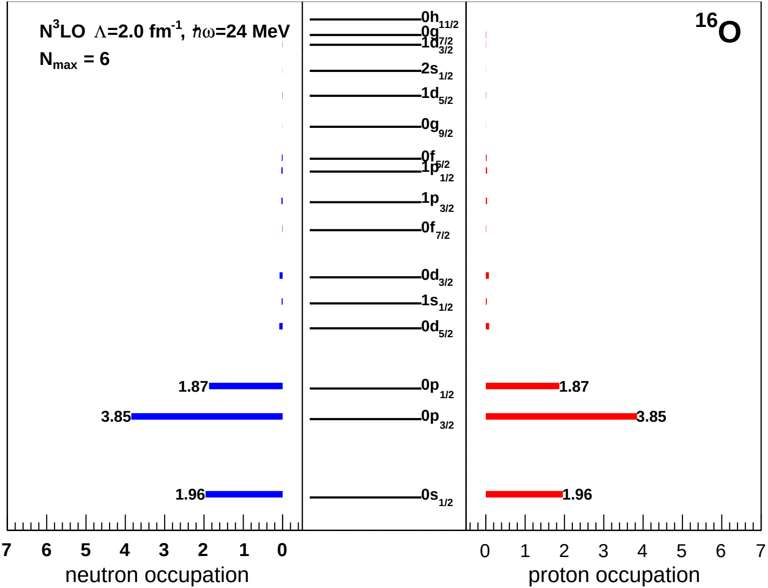

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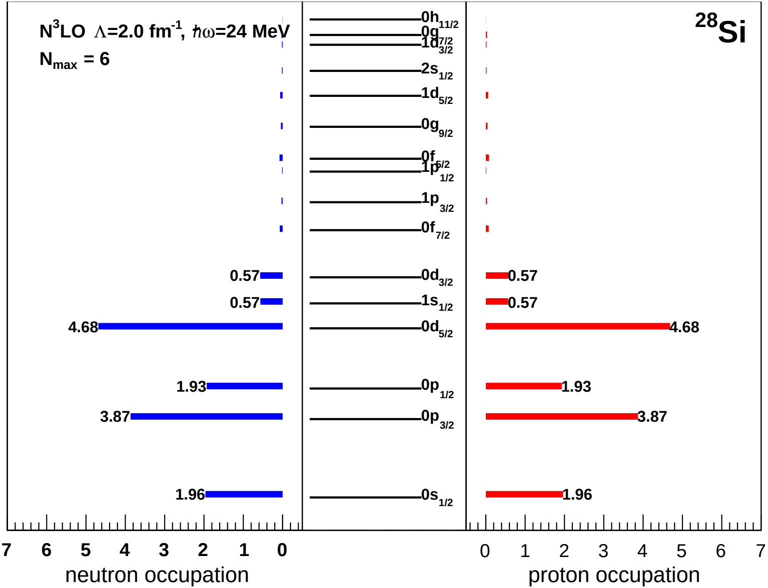

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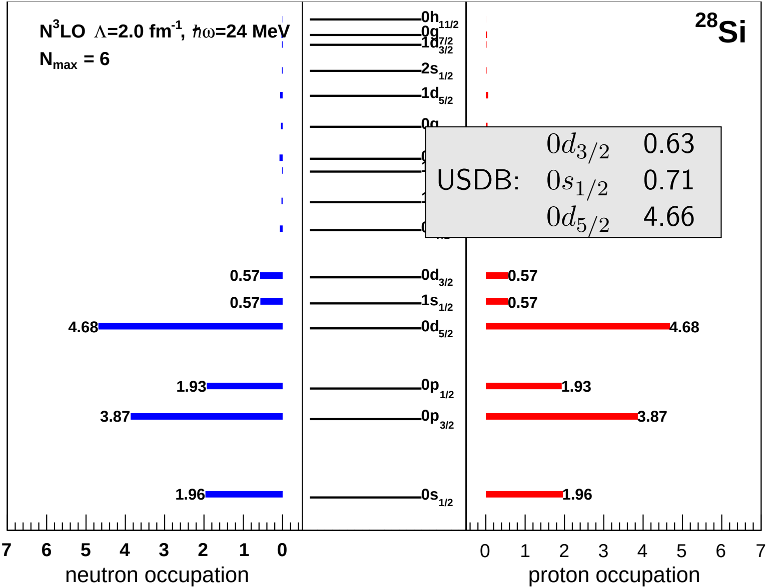
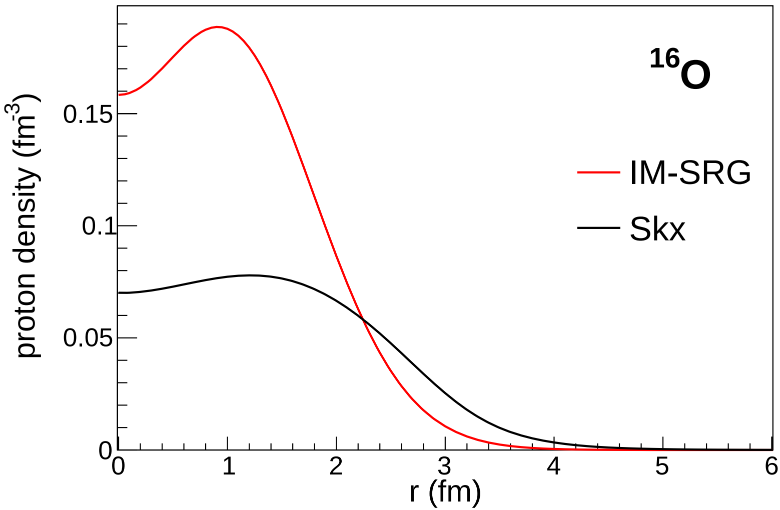


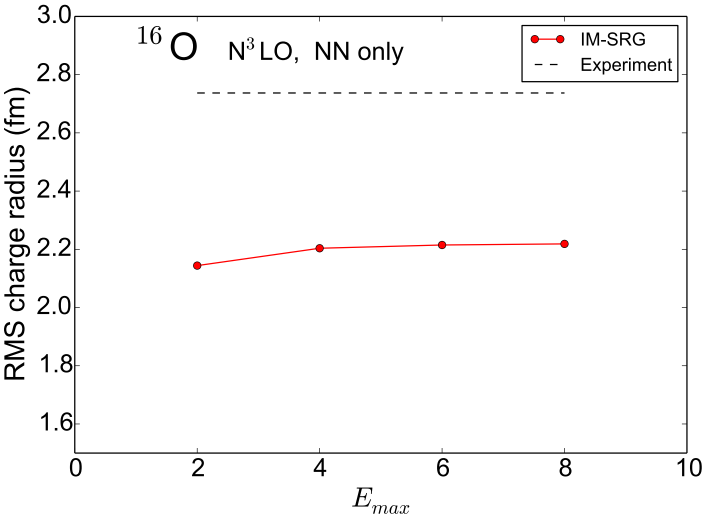
USDB: $0d_{3/2}$ 0.63, $0s_{1/2}$ 0.71, $0d_{5/2}$ 4.66

"Observables": proton density

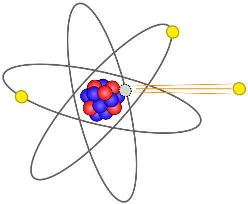
$$\hat{\rho}(r) = \sum_i \hat{n}_i e_i \left|\phi_i(r)\right|^2$$



Charge radii



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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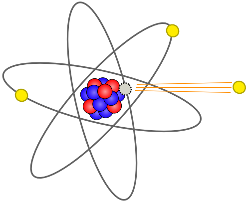

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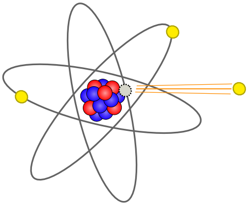

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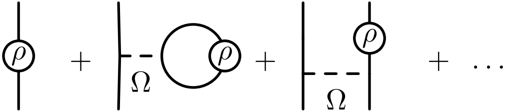
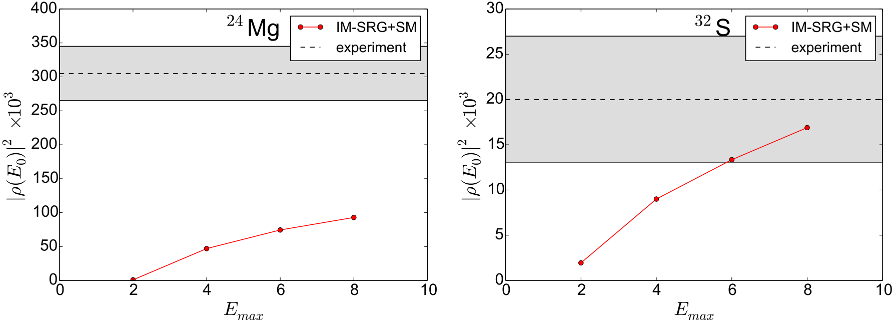


Electric monopole transitions

NN only, and not converged.



Commutator relations for tensor operators

Normal ordered operators in a J-coupled basis

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

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

$$\Downarrow$$

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

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$$\Downarrow$$

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

Commutator relations for tensor operators (one body)

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

$$\Downarrow$$

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

Commutator relations for tensor operators (two body)

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

$$\Downarrow$$

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

Commutator relations for tensor operators

Results?

Coming soon. . .

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
- $E0$ transition rates can be handled in the shell model
- Tensor operators coming soon

Collaborators:

TRIUMF A Calci, J Holt, P Navratil

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

TU Darmstadt A Schwenk

Appendix

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

A toy problem:

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

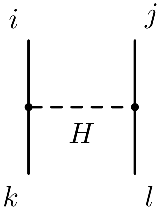
$$e^{\hat{\Omega}}\hat{H}e^{-\hat{\Omega}} = \begin{pmatrix} \epsilon_1 \cos^2\theta + \epsilon_2 \sin^2\theta + h \sin 2\theta & h_{od}\cos 2\theta + \frac{\epsilon_2 - \epsilon_1}{2}\sin 2\theta \\ h_{od}\cos 2\theta + \frac{\epsilon_2 - \epsilon_1}{2}\sin 2\theta & \epsilon_2 \cos^2\theta + \epsilon_1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

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

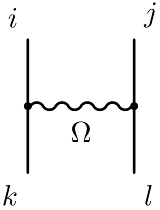
$$\theta \ll 1 \quad \Rightarrow \quad \theta \approx \frac{h_{od}}{\epsilon_1 - \epsilon_2}$$

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

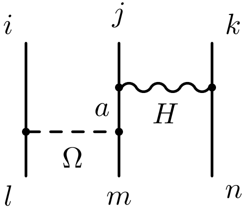
Induced forces and normal ordering (in-medium SRG)



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



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

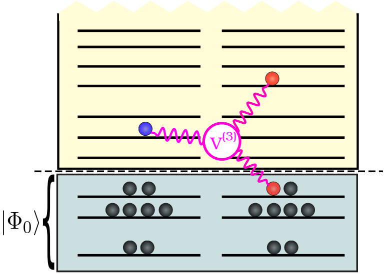


$$\left[\hat{\Omega}^{(2)}, \hat{H}^{(2)}\right] \sim \omega_{ialm} h_{jkan} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$$

Induced forces and normal ordering (in-medium SRG)

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

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



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

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

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

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