Coupled Cluster Theory Applied to Spectroscopic Factors of Atomic Nuclei

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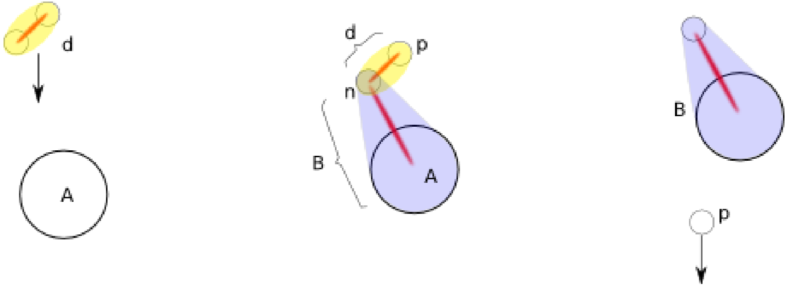
Aknowledgements

- Oak Ridge National Laboratory:
  - Gaute Hagen
  - Thomas Papenbrock
  - David Dean
- University of Oslo:
  - Morten Hjorth-Jensen
- University of Bergen:
  - Jan S. Vaagen

Outline

What are Spectroscopic Factors (SF) ?



- Direct reaction. Immediate stripping or pick-up of a particle.

$$T \sim \langle \Psi_B \Psi_p \chi^{(-)} | V | \Psi_A \Psi_d \chi^{(+)} \rangle \sim \langle O_A^B \chi^{(-)} | V | O_p^d \chi^{(+)} \rangle$$

- Modeled with single particle overlap function

$$O_A^B(\mathbf{x}) \equiv \sqrt{B} \int \mathrm{d}\xi \boldsymbol{\Psi}_A^*(\xi) \boldsymbol{\Psi}_B(\mathbf{x}, \xi) \sim \langle B | a^\dagger(\mathbf{x}) | A \rangle$$

- SF is experimentally determined as the norm of the overlap function that fits reaction model to measurement.

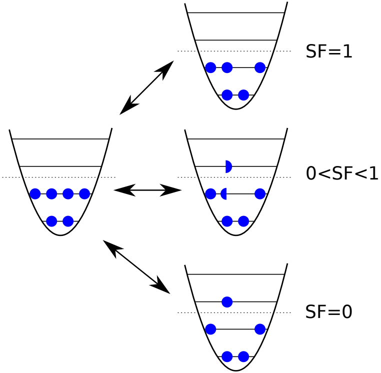
SF from perspective of structure theory

Definition

$$S_A^B(lj) = \int \mathrm{d}r r^2 O_A^{B*}(lj;r) O_A^B(lj;r)$$

SF is. . .

- the squared norm of the overlap function.
- determined from two independent many-body wavefunctions.
- a measure of correlations related to a given orbit in a given nucleus, i.e. validity of an independent particle description.



Coupled Cluster

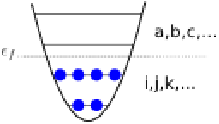
Wavefunction Ansatz

$$|\Psi_{\mathrm{CC}}\rangle = e^{T}\,|\Phi\rangle$$

$$T = T_1 + T_2 + \cdots$$

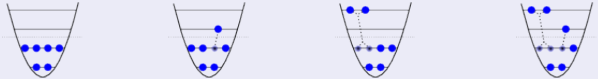
Correlated Hamiltonian

$$\overline{H} \equiv e^{-T} H e^{T} = (He^{T})_c$$



$$\begin{aligned} E &= \langle \Phi | \overline{H} | \Phi \rangle \\ 0 &= \langle \Phi_i^a | \overline{H} | \Phi \rangle \\ 0 &= \langle \Phi_{ij}^{ab} | \overline{H} | \Phi \rangle \end{aligned}$$

Wavefunction components



$$|\Psi_{\mathrm{CC}}\rangle = |\Phi\rangle + T_1\,|\Phi\rangle + T_2\,|\Phi\rangle + \underbrace{T_1 T_2}_{3p3h}\,|\Phi\rangle + \cdots$$

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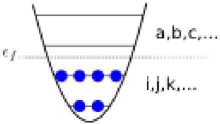

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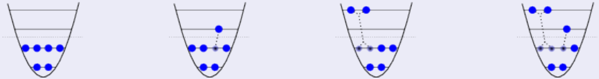

$$|\Psi_{\mathrm{CC}}\rangle = |\Phi\rangle + T_1\,|\Phi\rangle + T_2\,|\Phi\rangle + \underbrace{T_1 T_2}_{3p3h}|\Phi\rangle \; \boxed{+ \quad \cdots}$$

Recent of developments of Coupled Cluster

- Spherical Coupled Cluster
  1. Recognize that the cluster operator T is a *spherical tensor*
  2. Exploit spherical symmetry with the Wigner-Eckardt theorem.
  3. Enjoy a tremendous speedup.

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  3. Enjoy a tremendous speedup.
- Computational cost: $n_o^2 n_u^4 \longrightarrow n_o^{1.33} n_u^{2.66}$
  - 10 HO shells used to require $\sim 10^4$ processors, now requires a laptop!
  - In recent papers of the ORNL group, $N \sim 20$ HO shells. (arXiv:1003.1995, arXiv:0907.4167, arXiv:0905.3167)
  - Coupled Cluster can do medium-mass nuclei *ab-inito*.

Spectroscopic factors with EOM-Coupled-Cluster

- CC-solution defines a similarity transformed hamiltonian

$$\overline{H} = e^{-T} H e^{T} \tag{1}$$

Correlations in operator vs. in wavefunction

- EOMCC: Eigenstates of H written on the form

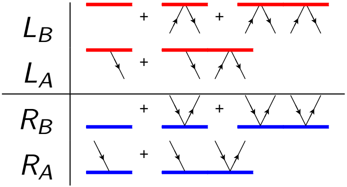
$$\langle\tilde{A}| = \langle\Phi_0| L_A e^{-T} \qquad |A\rangle = e^{T} R_A |\Phi_0\rangle$$
$$\langle\tilde{B}| = \langle\Phi_0| L_B e^{-T} \qquad |B\rangle = e^{T} R_B |\Phi_0\rangle$$

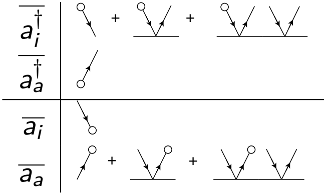
The operators L_A, L_B, R_A and R_B create eigenstates of $\overline{H}$.

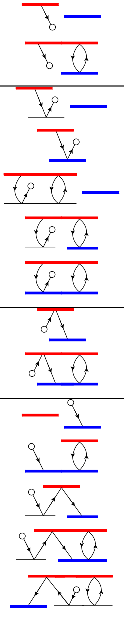
Hermitian expression for SF

$$S_A^B(lj) \propto \sum_n \frac{\langle\tilde{B}|a^\dagger_{nljm}|A\rangle \langle\tilde{A}|a_{nljm}|B\rangle}{\langle\tilde{A}|A\rangle \langle\tilde{B}|B\rangle}$$

$$S_A^B(lj) \propto \sum_n \frac{\langle L_B | \overline{a^\dagger_{nljm}} | R_A \rangle \, \langle L_A | \overline{a_{nljm}} | R_B \rangle}{\langle L_A | R_A \rangle \, \langle L_B | R_B \rangle}$$

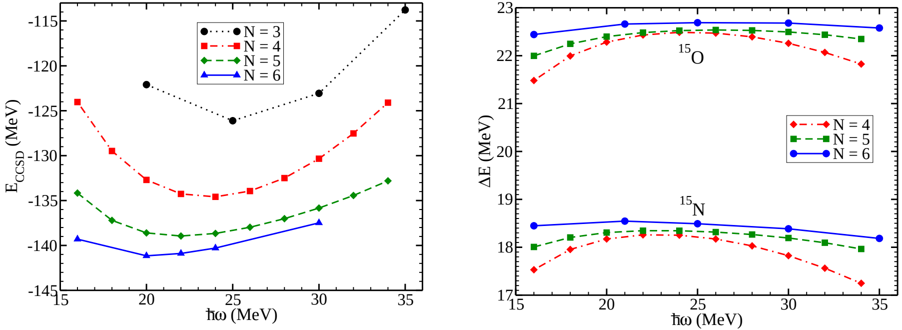






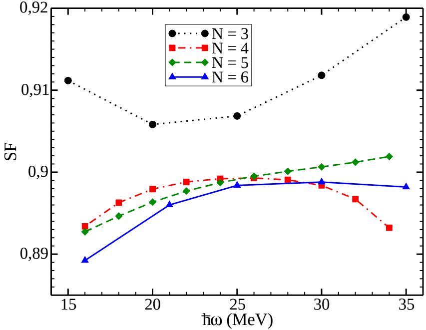
$\langle A \| a_i \| B \rangle$	$l^i r_0$
	$l^{ij}_a r^a_i$
$\langle A \| a_a \| B \rangle$	$l^i t^a_i r_0$
	$l^i r^a_i$
	$\frac{1}{2} l^{ij}_b t^{ab}_{ij} r_0$
	$l^{ij}_b t^a_i r^b_j$
	$\frac{1}{2} l^{ij}_b r^{ab}_{ij}$
$\langle B \| a^\dagger_a \| A \rangle$	$l^i_a r_i$
	$\frac{1}{2} l^{ij}_{ab} r^b_{ij}$
$\langle B \| a^\dagger_i \| A \rangle$	$l^0 r_i$
	$l^j_a r^a_{ij}$
	$-l^j_a t^a_i r_j$
	$-\frac{1}{2} l^{jk}_{ab} t^a_i r^b_{jk}$
	$-\frac{1}{2} l^{jk}_{ab} t^{ab}_{ik} r_j$

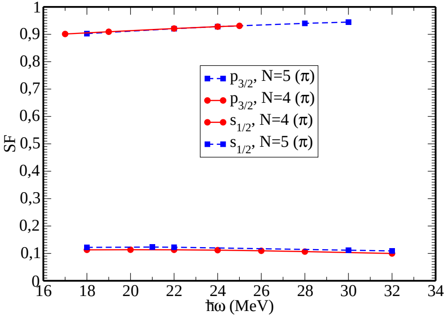
^{16}O and ^{15}N with EOMCC, model space convergence



- $V_{\mathrm{low-k}}(N3LO)$, at $\lambda = 2.0 fm^{-1}$.
- Up to 7 oscillator shells
- O16 and energy difference converged up to a few MeV

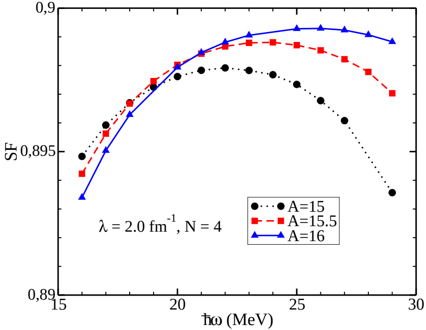
^{16}O and ^{15}N Spectroscopic Factors

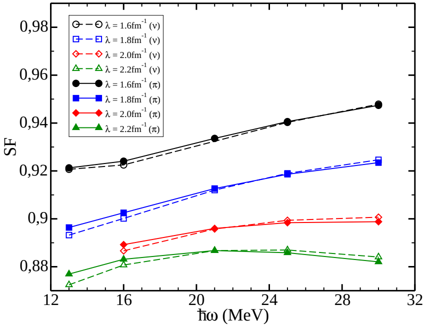




- Very good convergence w.r.t. model space
- $p_{3/2}$ and $p_{1/2}$ almost identical
- $s_{1/2}$ much smaller

A-dependence, λ dependence





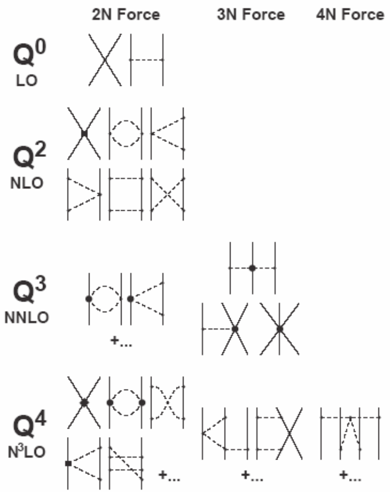
- Very weak *A*-dependence
- Short-range correlations important for the SF (λ dependence)
- Very weak isospin dependence

Conclusion and Outlook

- We can do *ab-initio* spectroscopic factors with CC.
- Implementation for Spherical Coupled Cluster (in progress)
- Physically motivated calulations.
- Application to $^{40}\mathrm{Ca},^{48}\mathrm{Ca},^{56}\mathrm{Ni}$

Thanks for your time!

A nuclear hamiltonian from QCD



- QCD is non-perturbative at nuclear energy scales.
  $\Longrightarrow$ Effective Field Theory:
  - Organize the QCD Lagrangian in powers of $\frac{Q}{\Lambda}$
  - Λ defines a radius of convergence.
  - Regularization for $Q > \Lambda$.
- Infinite number of "correct" Λ.

Dependence on momentum cut-off Λ

- Nuclear dynamics involve a wide range of energies
  - $E_B \approx 1 - 8 MeV$
  - $M_\pi \approx 140 MeV$
  - $E_{kin} \approx 80 MeV$
  - $E_\Delta \approx 300 MeV$
- Λ too low: you may exclude important physics.
- Λ too high: interaction must account for more QCD
  - numerically tougher
  - eventually: more diagrams, more parameters.
- Λ-dependence estimates importance of the high momentum physics.
- Quantities that are very sensitive to Λ are not physical properties(!)

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- Λ-dependence estimates importance of the high momentum physics.
- Quantities that are very sensitive to Λ are not physical properties(!)
- "Bare" interaction is strongly repulsive and needs huge model spaces.
- The cut-off can be lowered further, e.g. by similarity transformations. (V_{low-k})