Computing nuclear responses for open-shell nuclei in coupled-cluster theory

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MPA MAINZ PHYSICS ACADEMY

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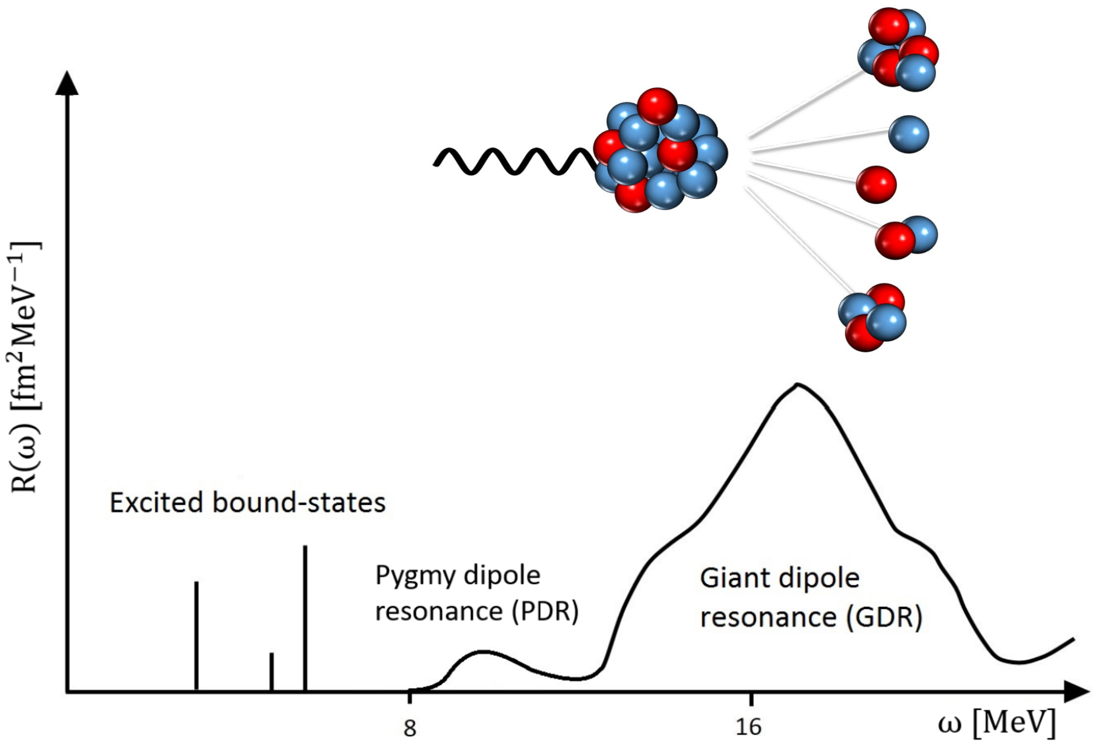
Motivation

$$R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle \Psi_f|\Theta|\Psi_0\rangle|^2 \delta(E_f - E_0 - \omega)$$



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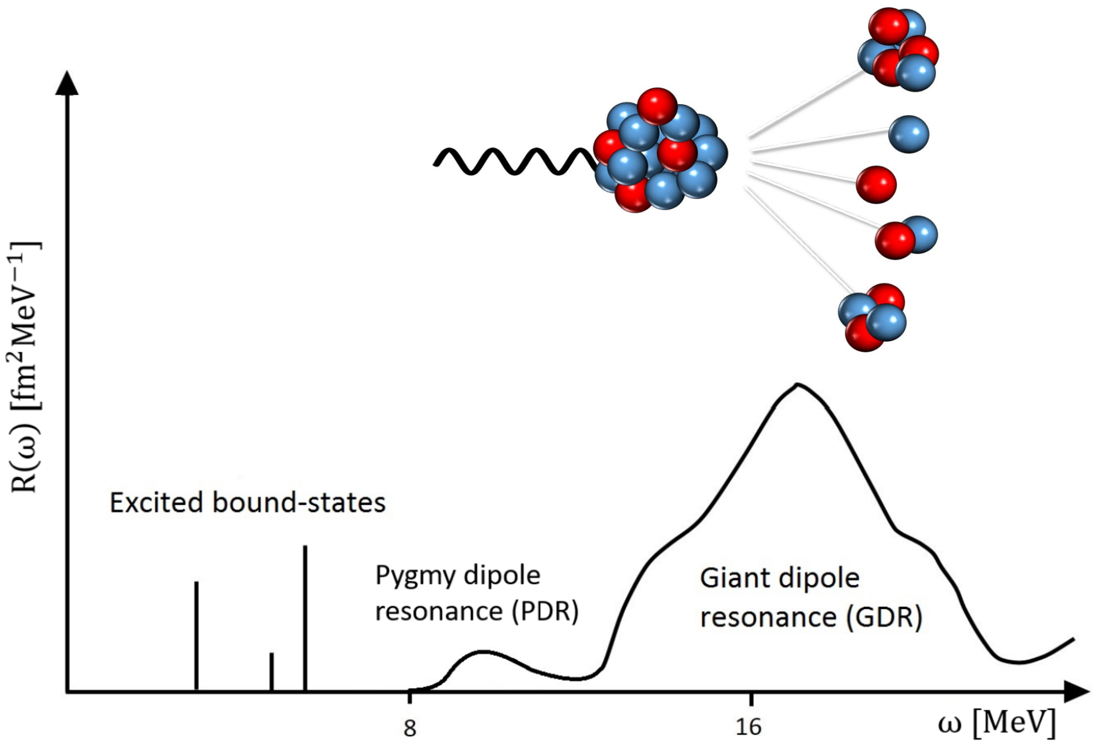
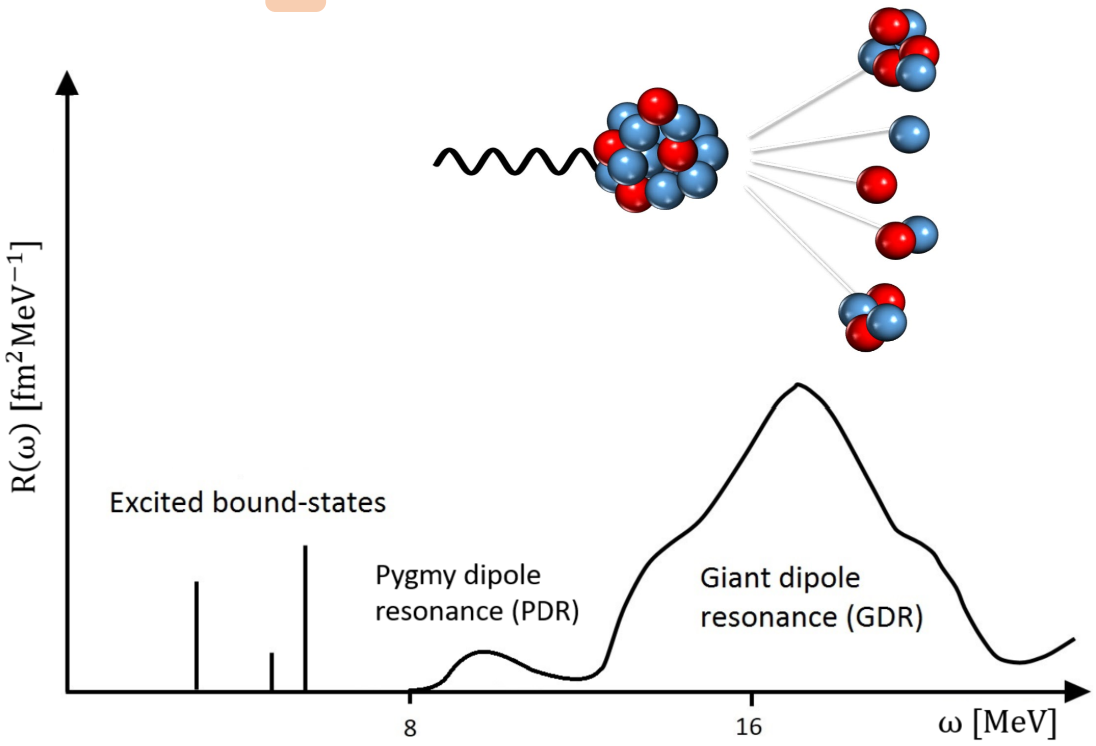
Coupled-Cluster theory (CC)



Motivation

$$R(\omega) = \sum\!\!\!\!\!\!\int_f \left| \langle \Psi_f | \Theta | \Psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Lorentz Integral Transform (LIT)



LIT-CC developed just for closed-shell nuclei → extension to open-shell

Coupled-cluster theory

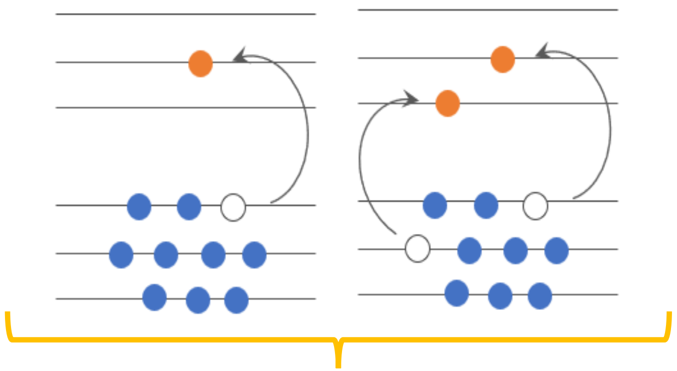
- Start from **Hartree-Fock** reference state $|\Phi_0\rangle$.
- Add correlations via:

$$e^{-T}He^{T}|\Phi_0\rangle = \overline{H}|\Phi_0\rangle = E_0|\Phi_0\rangle$$

Similarity-transformed Hamiltonian (non-Hermitian)

with

$$T = \sum t_i^a a_a^\dagger a_i + \sum t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \dots$$



CCSD

LIT-CC for closed-shell nuclei

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Integral Transform

$$L(\sigma,\Gamma) = \frac{\Gamma}{\pi}\int d\omega \, \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2} = \frac{\Gamma}{\pi}\langle\Psi_L|\Psi_R\rangle$$

where

$$(\overline{H} - E_0 - \sigma - i\Gamma)\,|\Psi_R\rangle = \overline{\Theta}\,|\Phi_0\rangle$$

CC equation of motion
with a source

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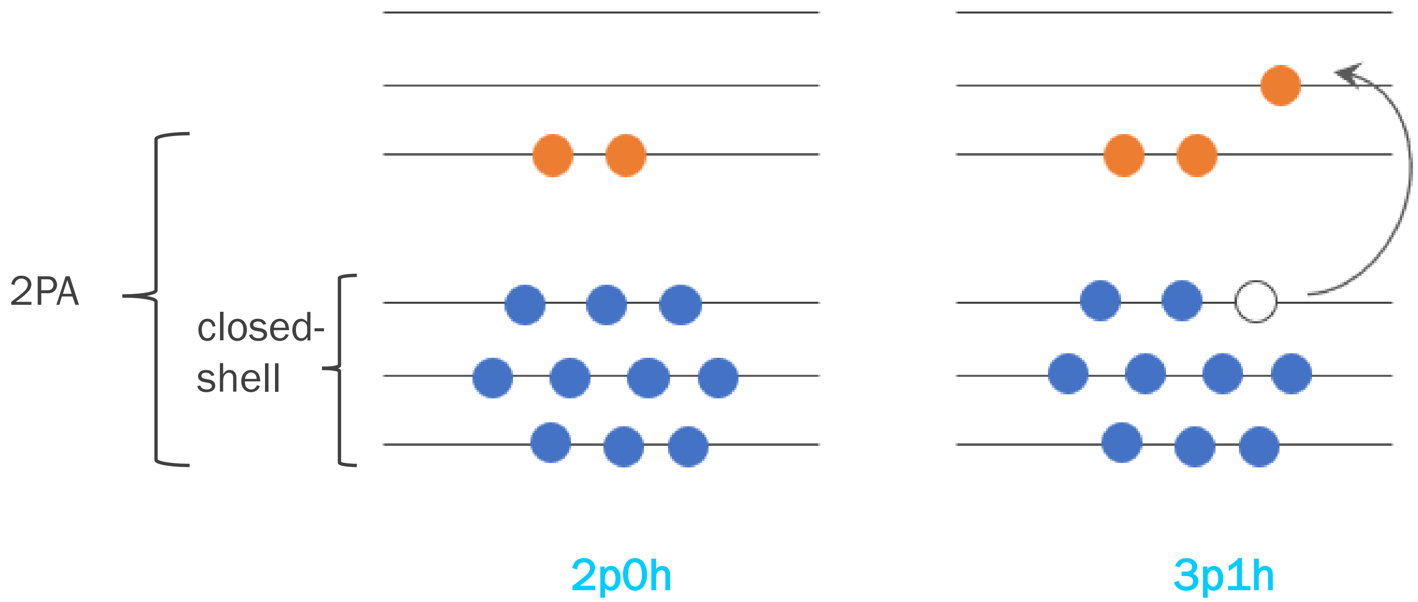
LIT-CC ansatz to solve it:

$$|\Psi_R\rangle = \mathcal{R}|\Phi_0\rangle \qquad \mathcal{R} = r_0 + \sum r_i^a a_a^\dagger a_i + \sum r_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \dots$$

LIT-CC: two-particle-attached case

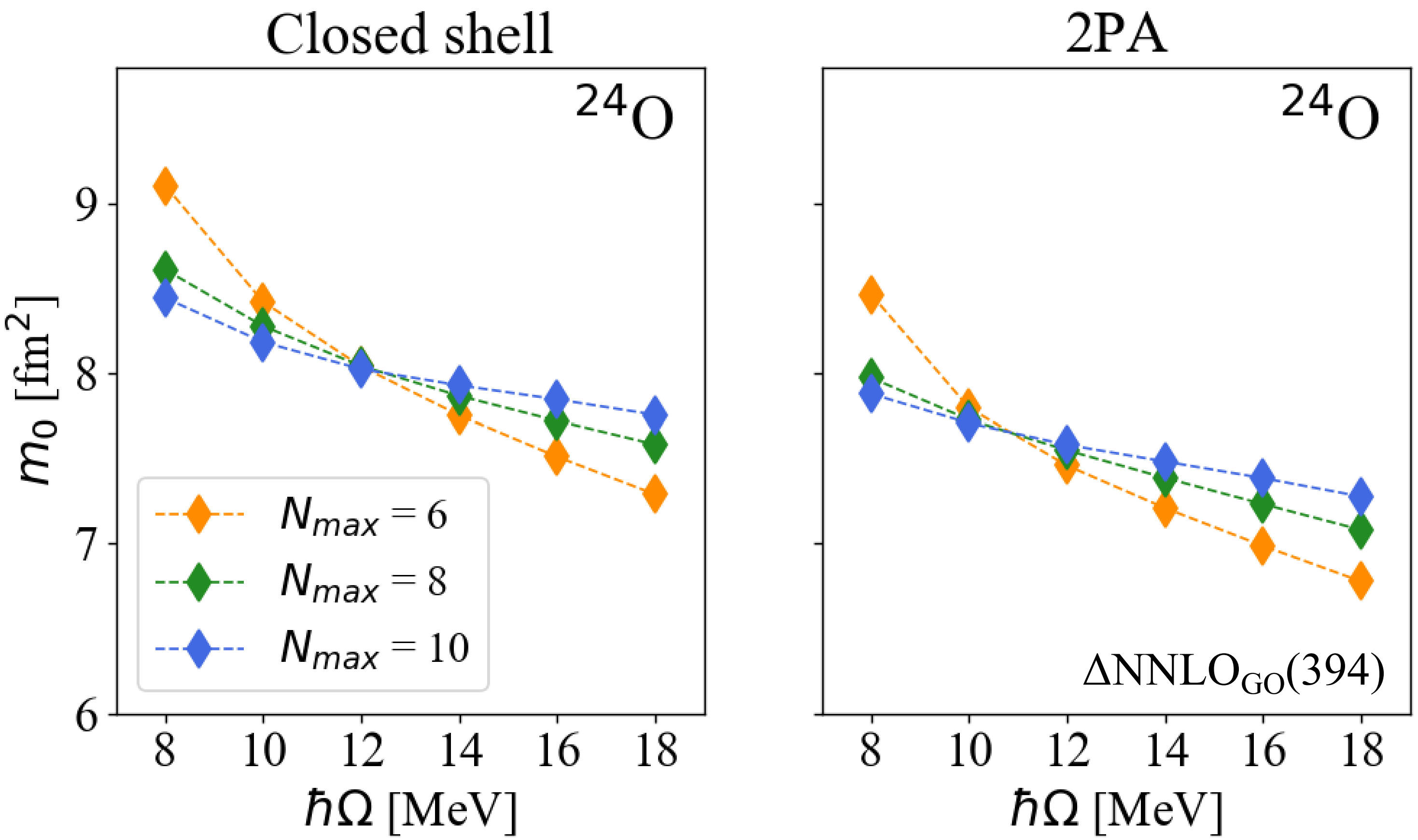
$$\mathcal{R} = \frac{1}{2}\sum r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \dots$$

$$|\Psi_R\rangle = \mathcal{R}|\Phi_0\rangle$$



Non-energy-weighted dipole sum rule

$$m_0 = \int d\omega\, R(\omega) = \langle \Psi_{0,L}^{2PA} | \overline{\Theta^\dagger} \overline{\Theta} | \Psi_{0,R}^{2PA} \rangle$$



Electric dipole polarizability

$$\alpha_D = 2\alpha \int d\omega \frac{R(\omega)}{\omega}$$