Multi-Configurational Many-Body Perturbation Theory and *Ab Initio* Nuclear Structure

Alexander Tichai
Institut für Kernphysik

TECHNISCHE UNIVERSITÄT DARMSTADT

Many-Body Perturbation Theory

Motivation

- access nuclear observables in the **medium-mass regime**
- methods like coupled cluster, self-consistent Green's function and in-medium SRG have been successfully applied
- alternative: use a conceptual simple approach

$\Rightarrow$ **many-body perturbation theory**

Concept

- definition of **unperturbed basis**

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1 \qquad \hat{H}_0 |\Phi_n\rangle = E_n |\Phi_n\rangle$$

- **power-series expansion**

$$E_n(\lambda) = \sum_{p=0}^{\infty} E_n^{(p)} \lambda^p$$

- determine expansion coefficients order by order
- problem: need to control the **convergence behaviour**

Multi-Configurational MBPT

- **reference state** from diagonalization in a small model space $\mathcal{M}_{\text{ref}}$

$$|\psi_{\text{ref}}\rangle = \sum_{J \in \mathcal{M}_{\text{ref}}} c_J |J\rangle$$

- generalization of Fock operator via **1B density matrix**

$$f_{pq} = h_{pq} + \sum_{rs} \langle pr|\hat{H}|qs\rangle \cdot \gamma^r_s$$

- set $\hat{H}_0 = \hat{f}^{\text{diag}}$ and define **single-particle energies** $\epsilon_p = f_{pp}$
- investigate high-order corrections via **recursive scheme**

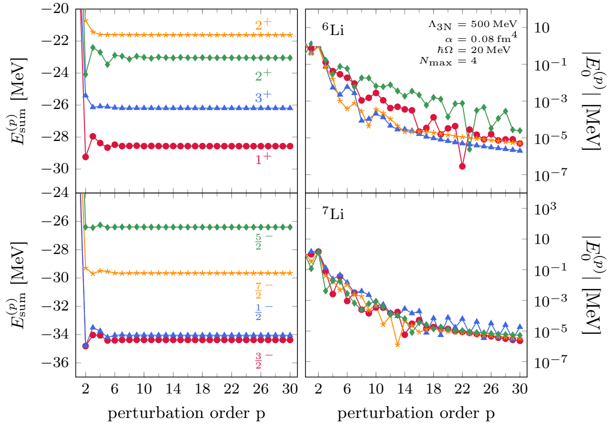
$\longrightarrow$ convergent series motivates use of low-order partial sums

- evaluate **second-order energy correction** explicitly

$$E^{(2)} = \sum_{I,J} c_I c_J^\star \sum_K \frac{\langle I|\hat{H}|K\rangle\langle K|\hat{H}|J\rangle}{E^{(0)} - E_K}$$

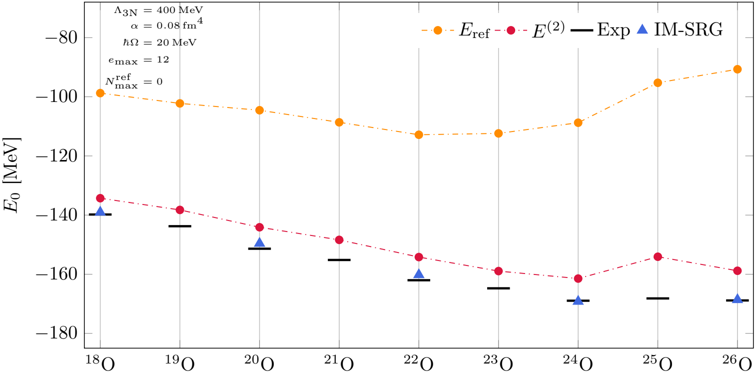
- application of **normal-ordering** techniques

Convergence Behaviour - ^{6}Li and ^{7}Li



- perturbation series **converges exponentially** fast for all reference states
- low-order partial sums yield good approximation to converged result

Low-Order Results - Oxygen Chain



- second-order correction accounts for a large part of correlation energy
- small deviation due to missing higher-order corrections
- computationally **very cheap** technique (<1% of IM-SRG runtime)
- allows for investigation of **odd nuclei** in the medium-mass regime