

The static correlations in nuclear structure

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RM 150, BLDG 6008

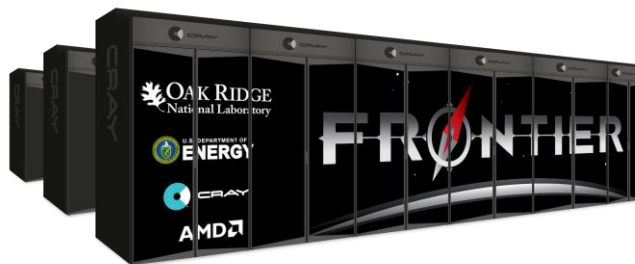
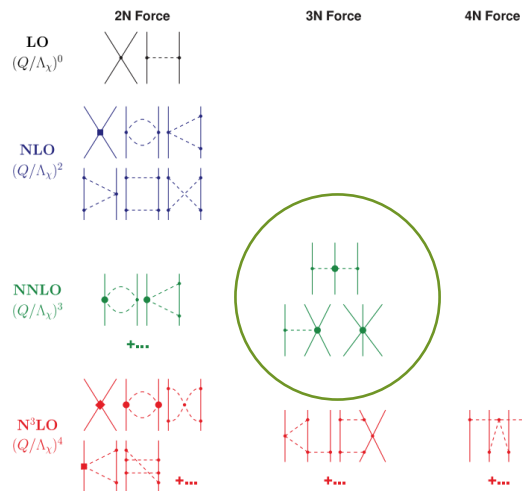
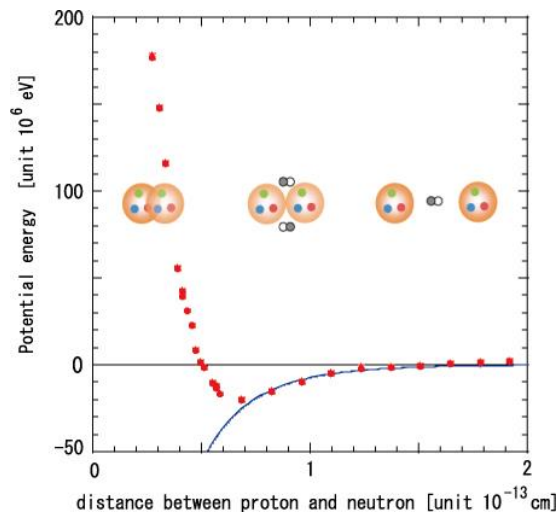


Status of Ab-initio calculations of nuclei, from QCD to the neutron star

$$\mathcal{L}_{\text{QCD}}^0 = \bar{q}i\gamma^\mu \mathcal{D}_\mu q - \frac{1}{4} g_{\mu\nu,a} g_a^{\mu\nu}.$$

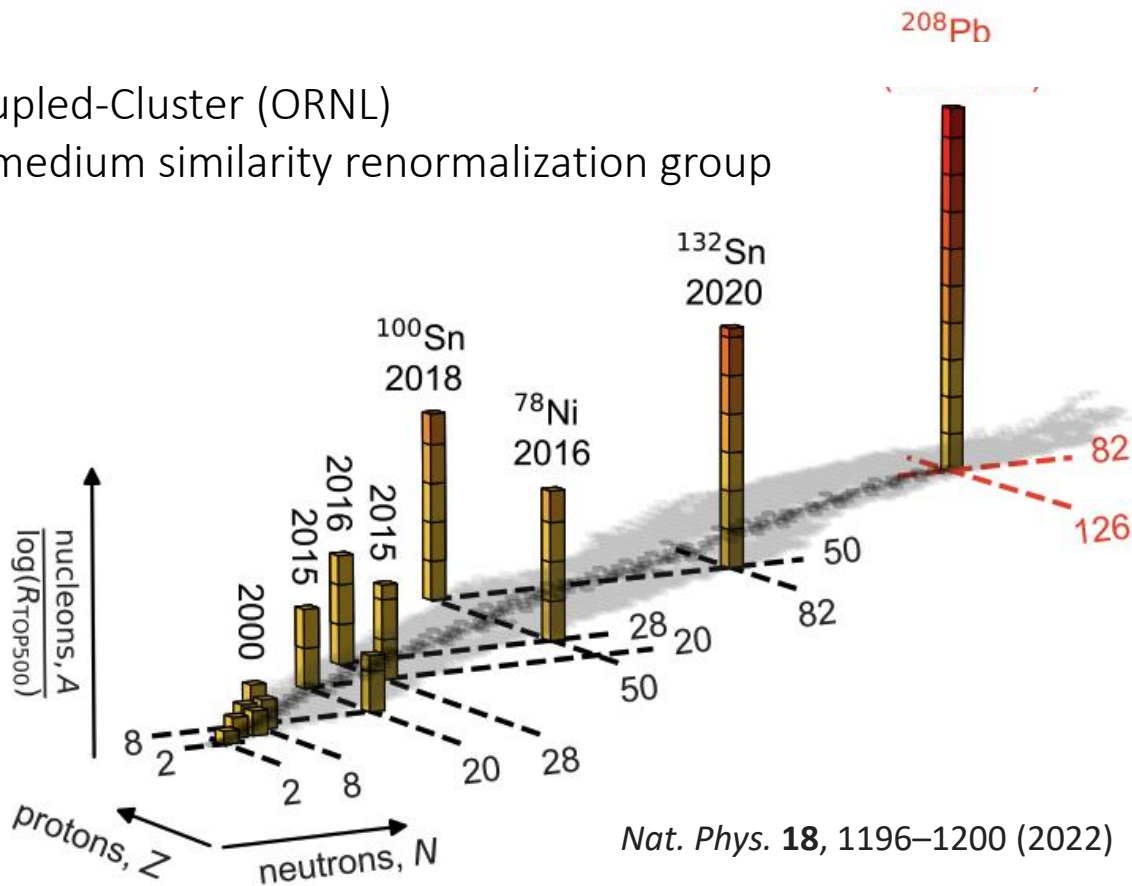
QCD lagrangian at vanished quark mass

Chiral symmetry
breaking



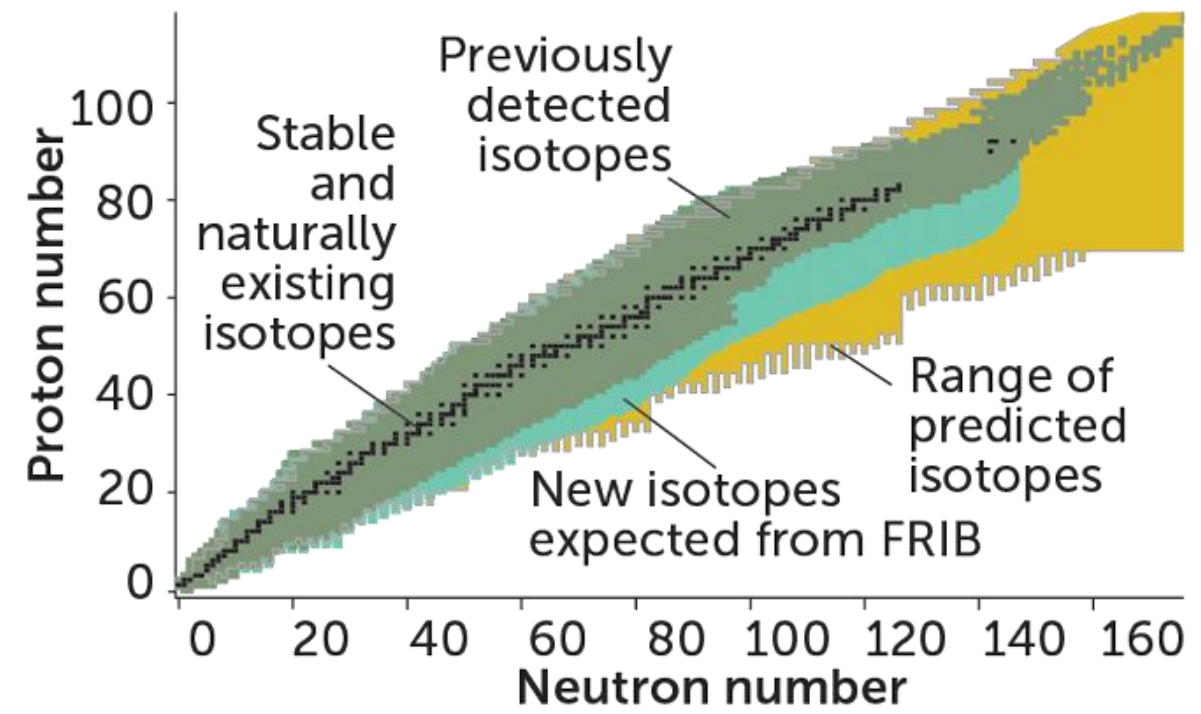
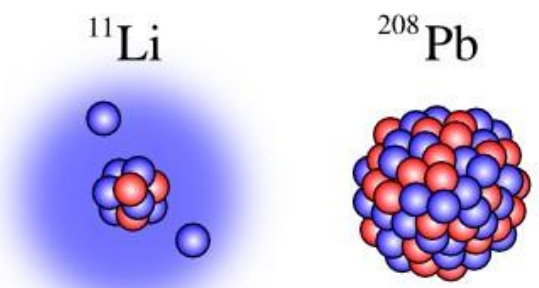
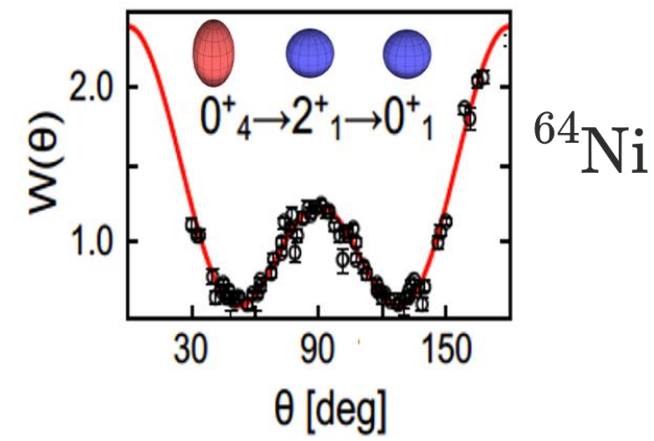
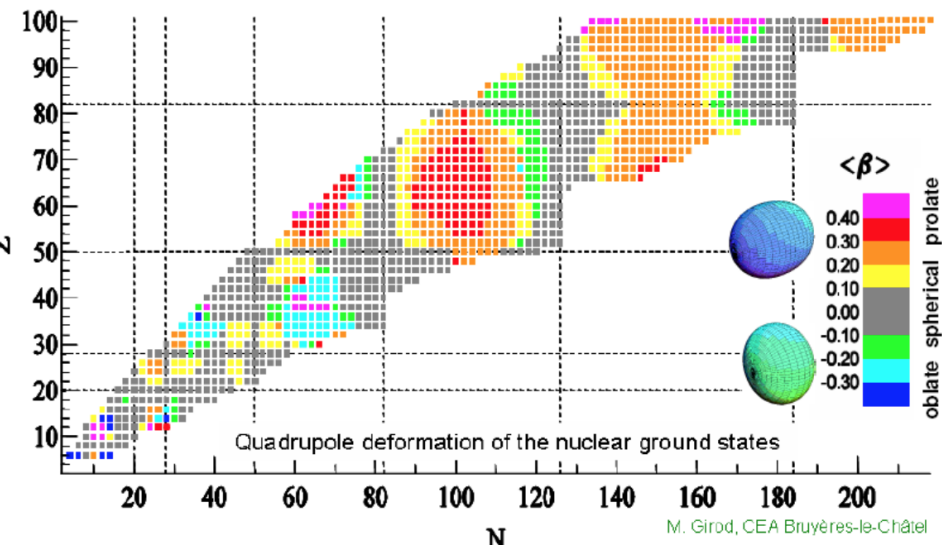
Coupled-Cluster (ORNL)

In-medium similarity renormalization group

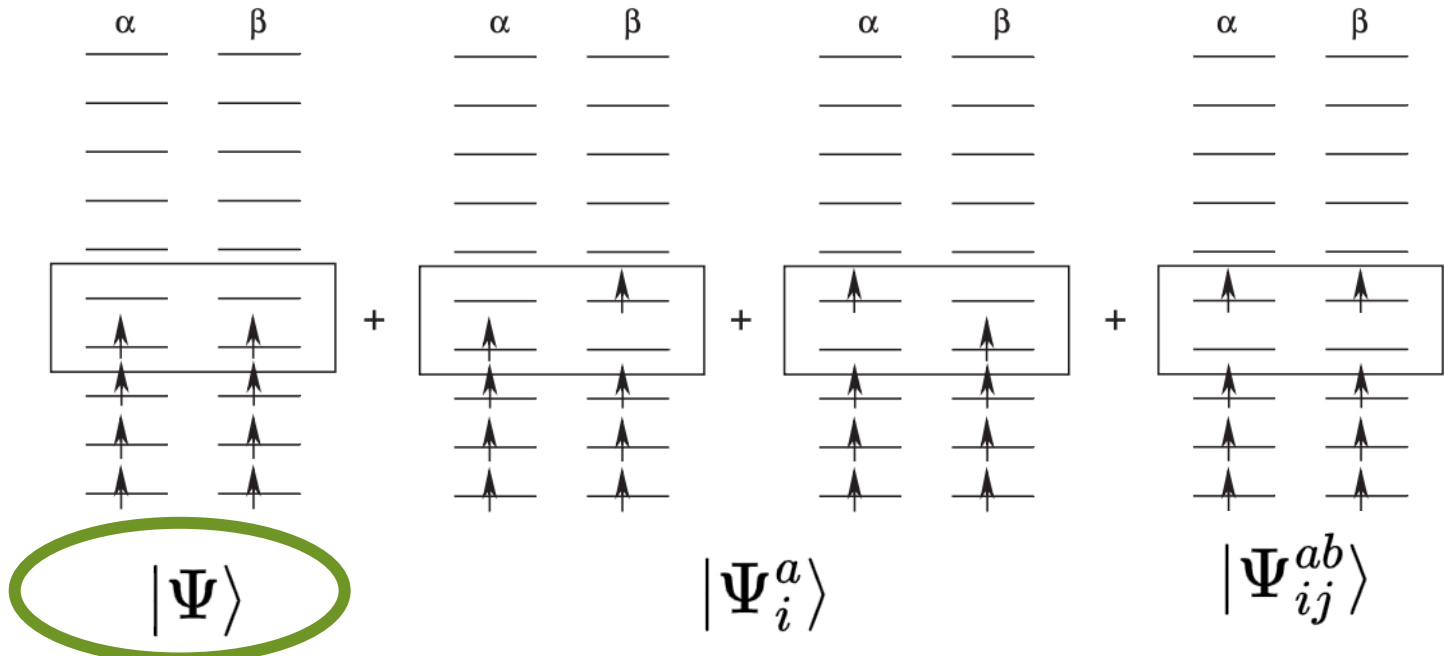


Nat. Phys. **18**, 1196–1200 (2022)

Most nuclei are deformed



Many-body correlations in the atomic nuclei, Coupled-cluster method



Reference state
e.g., HF mean field

Particle-hole excitation on top of the reference

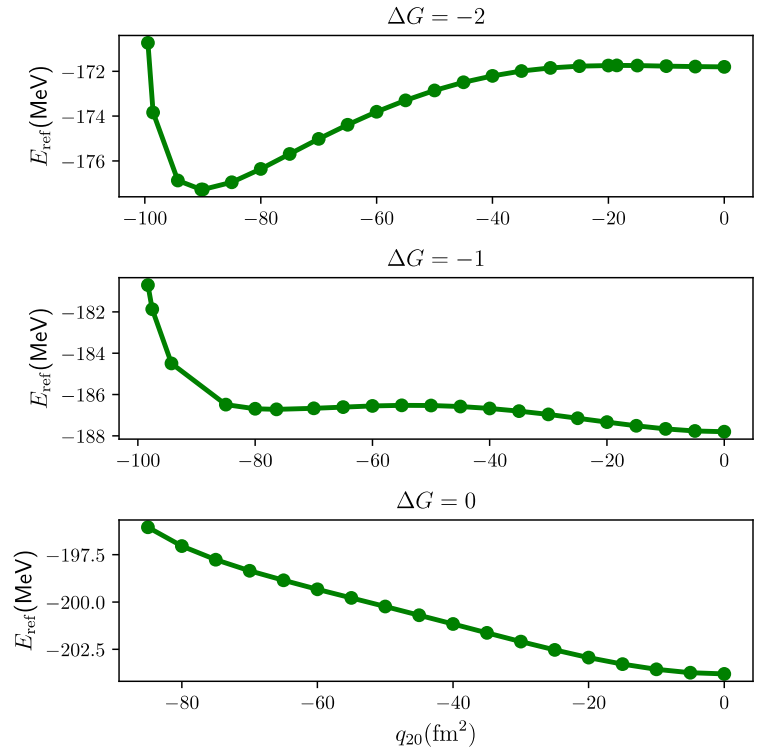
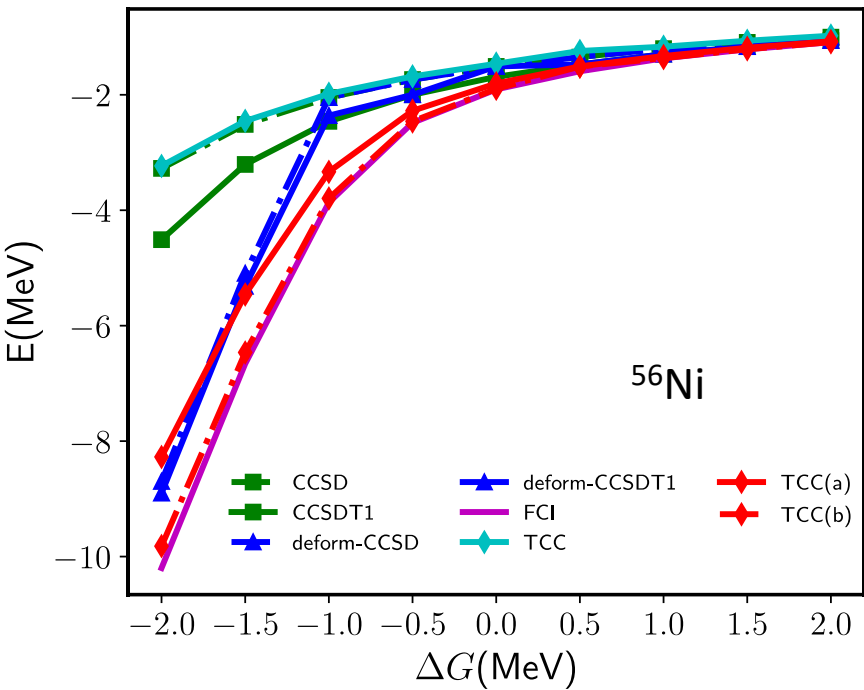
$$\langle \Psi_{i\dots}^{a\dots} | e^{-T} H e^T | \Phi_0 \rangle = 0$$

$$E = E_{ref} + E_{corr}$$

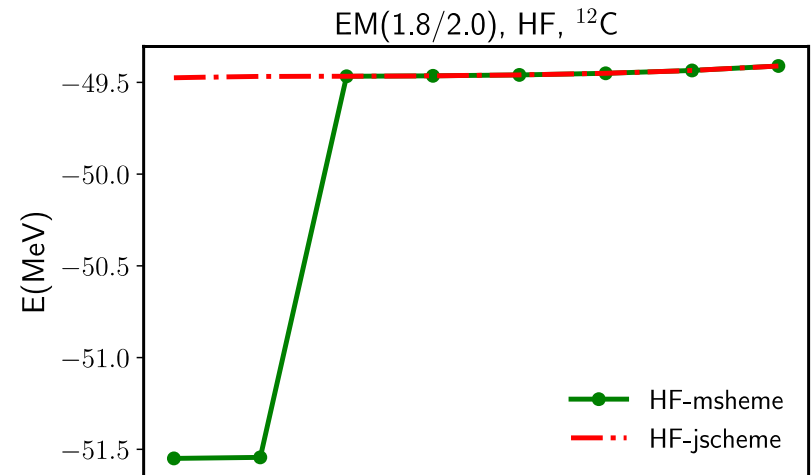
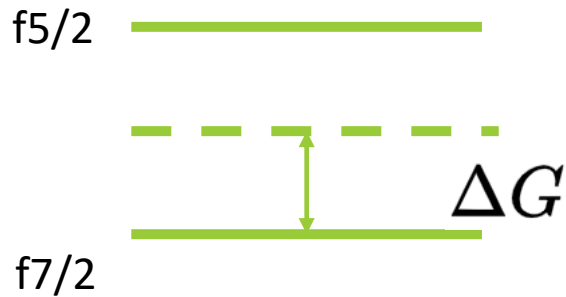
$$T_n = \frac{1}{(n!)^2} \sum_{\substack{a_1, a_2, \dots, a_n \\ i_1, i_2, \dots, i_n}} t_{i_1, i_2, \dots, i_n}^{a_1, a_2, \dots, a_n} \hat{a}_1^\dagger \hat{a}_2^\dagger \dots \hat{a}_n^\dagger \hat{i}_1 \hat{i}_2 \dots \hat{i}_n$$

Reference state = New Vacuum (void particle-hole excitations)

Failure of Coupled cluster



The nuclei have a deformed mean-field (multi-reference)



Static correlation (non-dynamic) and dynamic correlation

$$E_{corr} = E_{static} + E_{dyn}$$

Static correlation

A few state coupled to the reference, but individually, have big contribution to correlation energy.

Scales exponentially

$$H = \begin{array}{c} |1\rangle \\ |2\rangle \\ |3\rangle \\ \vdots \\ \vdots \\ |N\rangle \end{array} \begin{bmatrix} E & t & 0 & 0 & 0 & 0 \\ t' & E & t & 0 & 0 & 0 \\ 0 & t' & E & t & 0 & 0 \\ 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 0 & \cdot & \cdot & t \\ 0 & 0 & 0 & 0 & t' & E \end{bmatrix}$$

- Shell model, treat all correlations
- in a static way
- Limited to $A < 18$

Dynamic correlation

Many states, small contribution individually, large contribution in total

Polynomial scale

Coupled cluster, treat all correlations, as dynamic correlation

Up to $A=208$

Deformation, rotation, shape co-existence ...

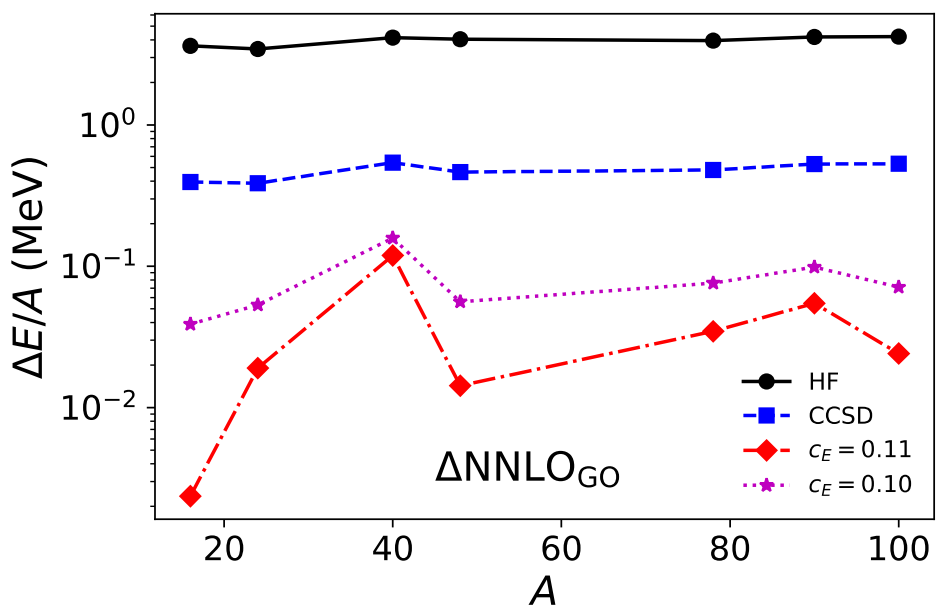
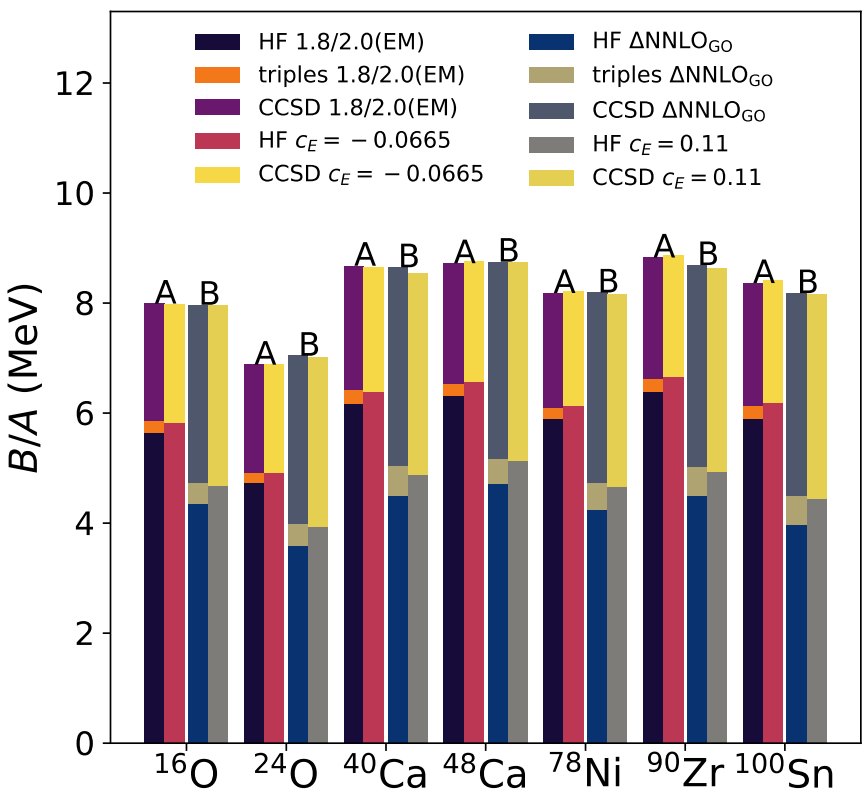
Static correlations

Challenge to Coupled cluster

Dynamic correlations in CC

All dynamic correlations, three-particle-three-hole
Can be renormalized to CCSD

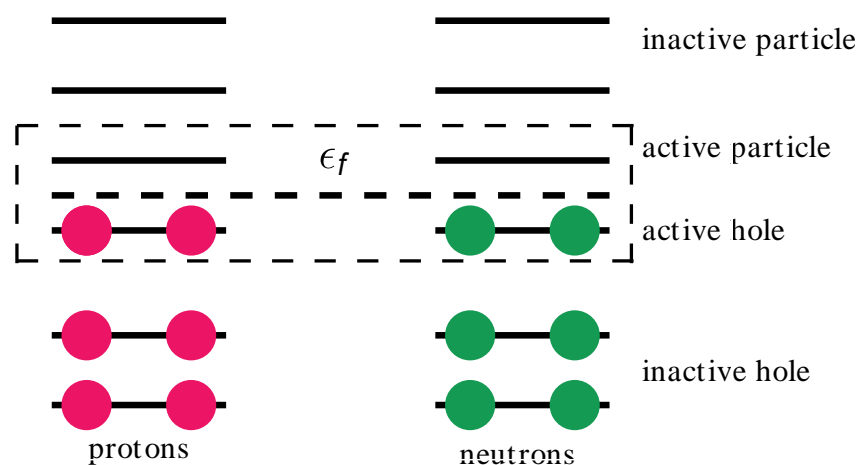
Dynamic correlations from 3p3h can be replaced by a short-range three-body force



“How to renormalize the coupled cluster”,
ZH Sun, Thomas P, G Hagen arXiv:2205.12990

We get CCSDT energy on CCSD level with renormalized CC

The tailored coupled cluster method, static correlations



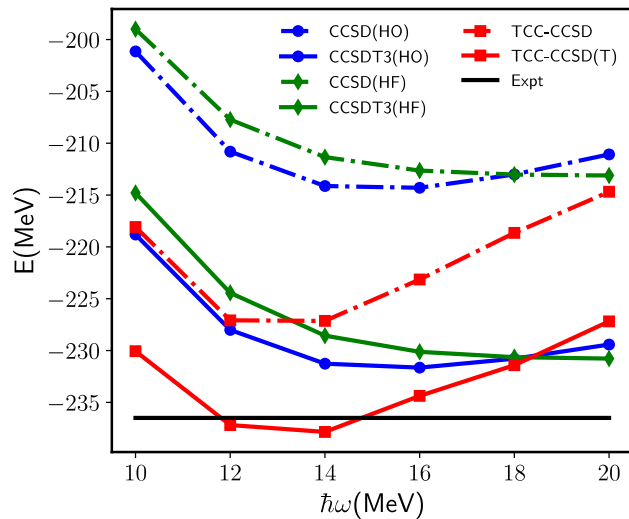
Static correlation,
configuration interaction

$$|\Psi_{\text{TCC}}\rangle = e^{T_{\text{ext}} + T_{\text{act}}} |\Psi_0\rangle.$$

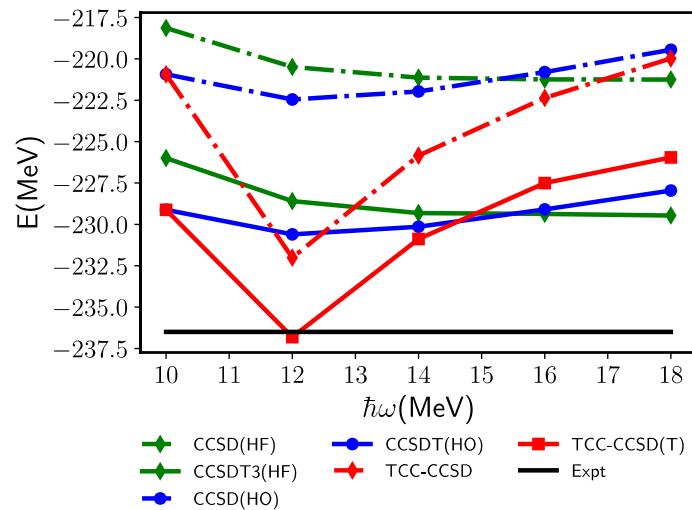
Dynamic correlations,
CC size-extensive, polynomial scale

NNLO_{OPT}

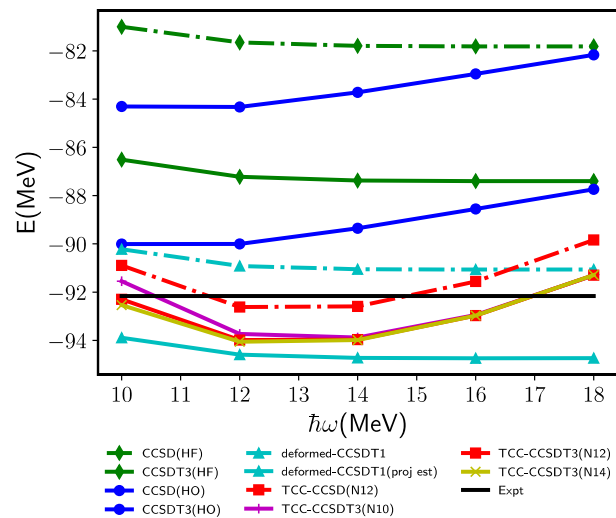
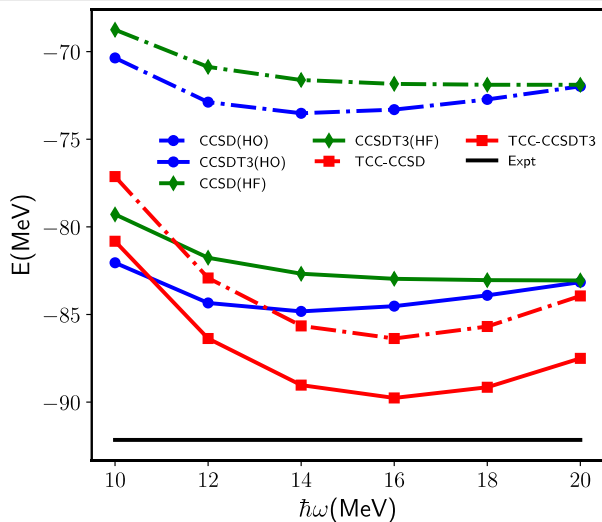
²⁸Si



EM(1.8/2.0)



¹²C



“Static correlations in nuclear many-body system”, ZH Sun, GH, TP, in preparing.

Summary

- We find, Dynamic correlations from high-order particle-hole excitations, can be efficiently captured by renormalized CC (short-range three-body)
- Static correlation are responsible for the spontaneous symmetry breaking, failure of CC. efficient approach still desired for the ab-initio calculation of the whole nuclei chart

Work in progress

- Find ansatz in nuclear physics that can be solve on quantum computer (QC)
- TCC(static correlations) is not suit for QC, for the large dimension
- Working on CC-GCM, to treat the multi-reference nuclei and port to QC

Thanks !