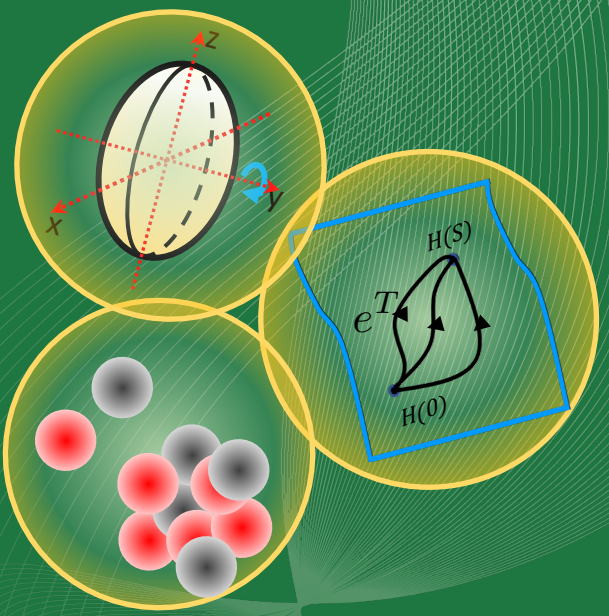
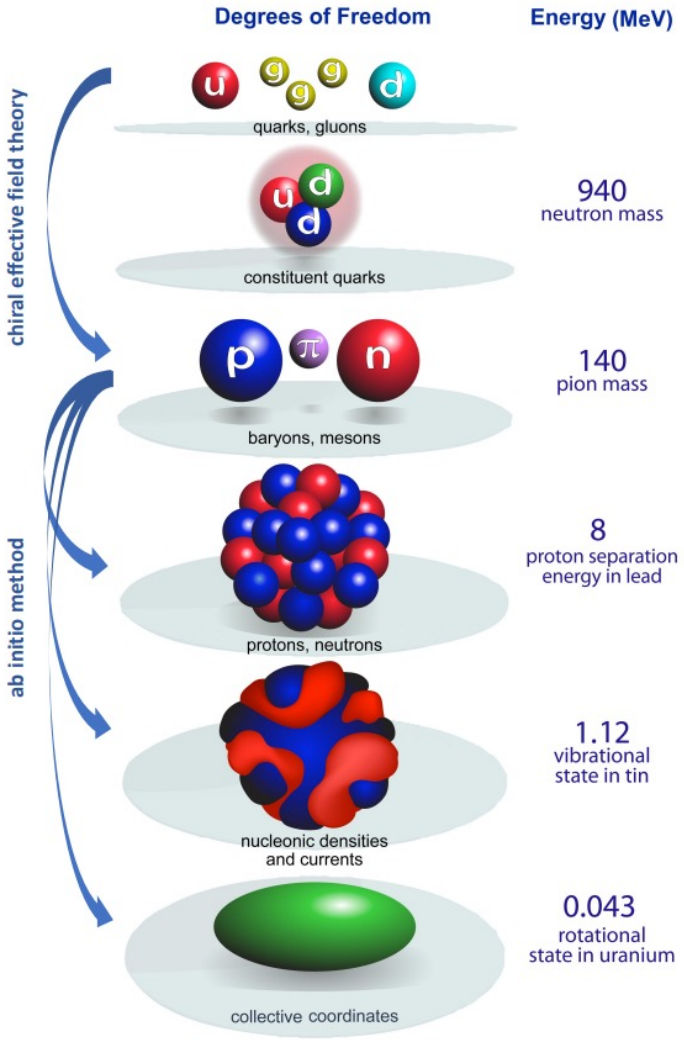
Structure of deformed nuclei on the first island of inversion

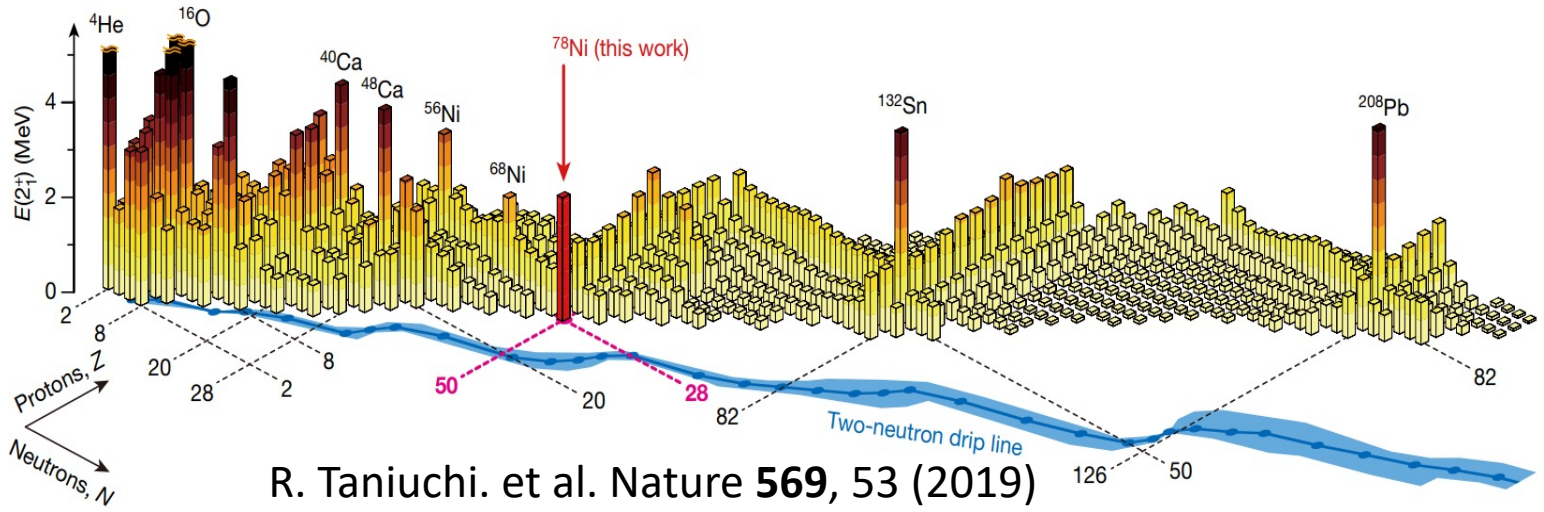
Zhonghao Sun
Gaute Hagen
Thomas Papenbrock
Oak Ridge National Laboratory



OAK RIDGE National Laboratory

Collective Phenomena from ab-initio calculations

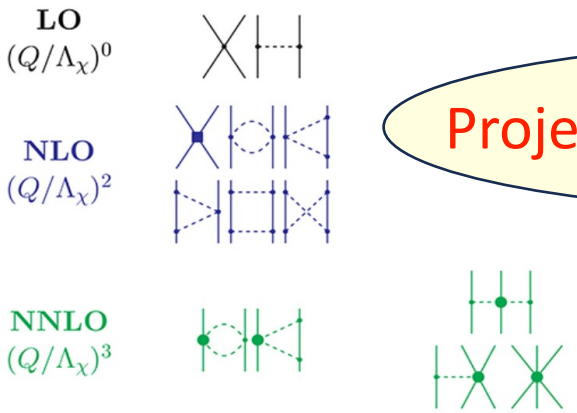




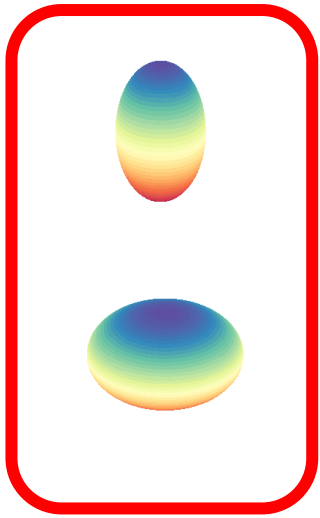
R. Taniuchi. et al. Nature **569**, 53 (2019)

Most nuclei are deformed

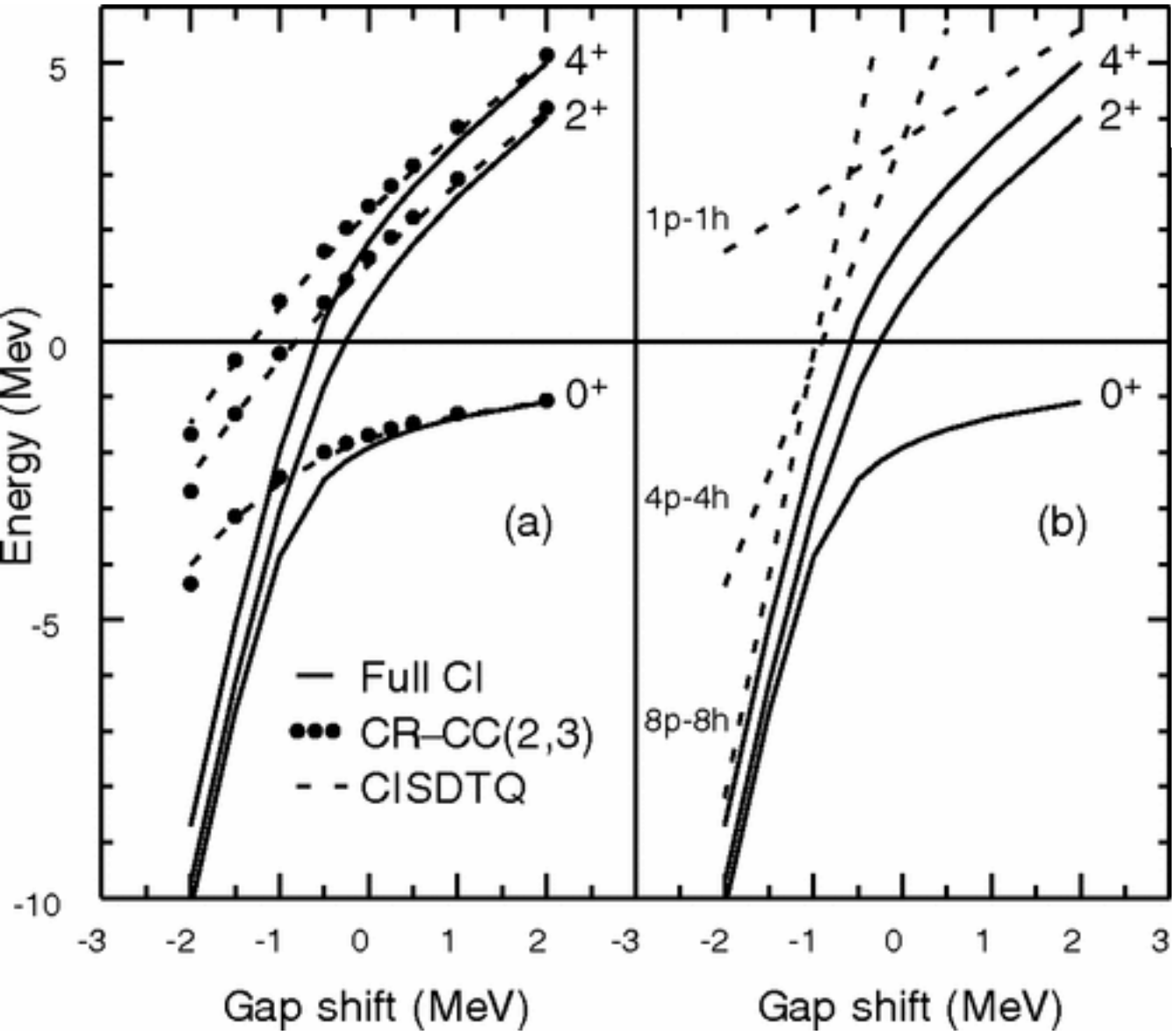
Uniform framework to computation of deformed nuclei



Projected coupled cluster theory



Single-reference coupled cluster on deformed nuclei



Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei

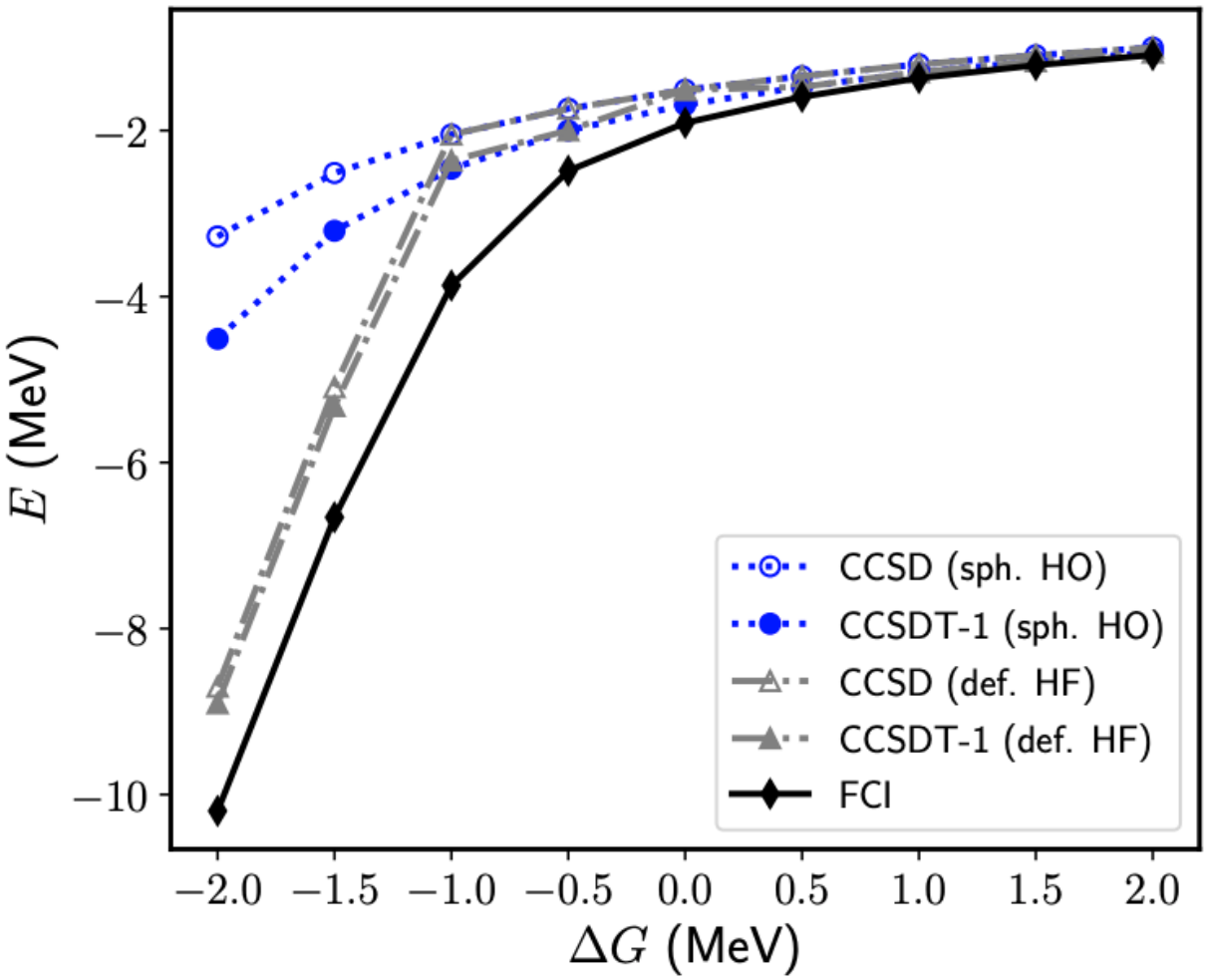
M. Horoi, J. R. Gour, M. Włoch, M. D. Lodriguito, B. A. Brown, and P. Piecuch
Phys. Rev. Lett. **98**, 112501 – Published 13 March 2007

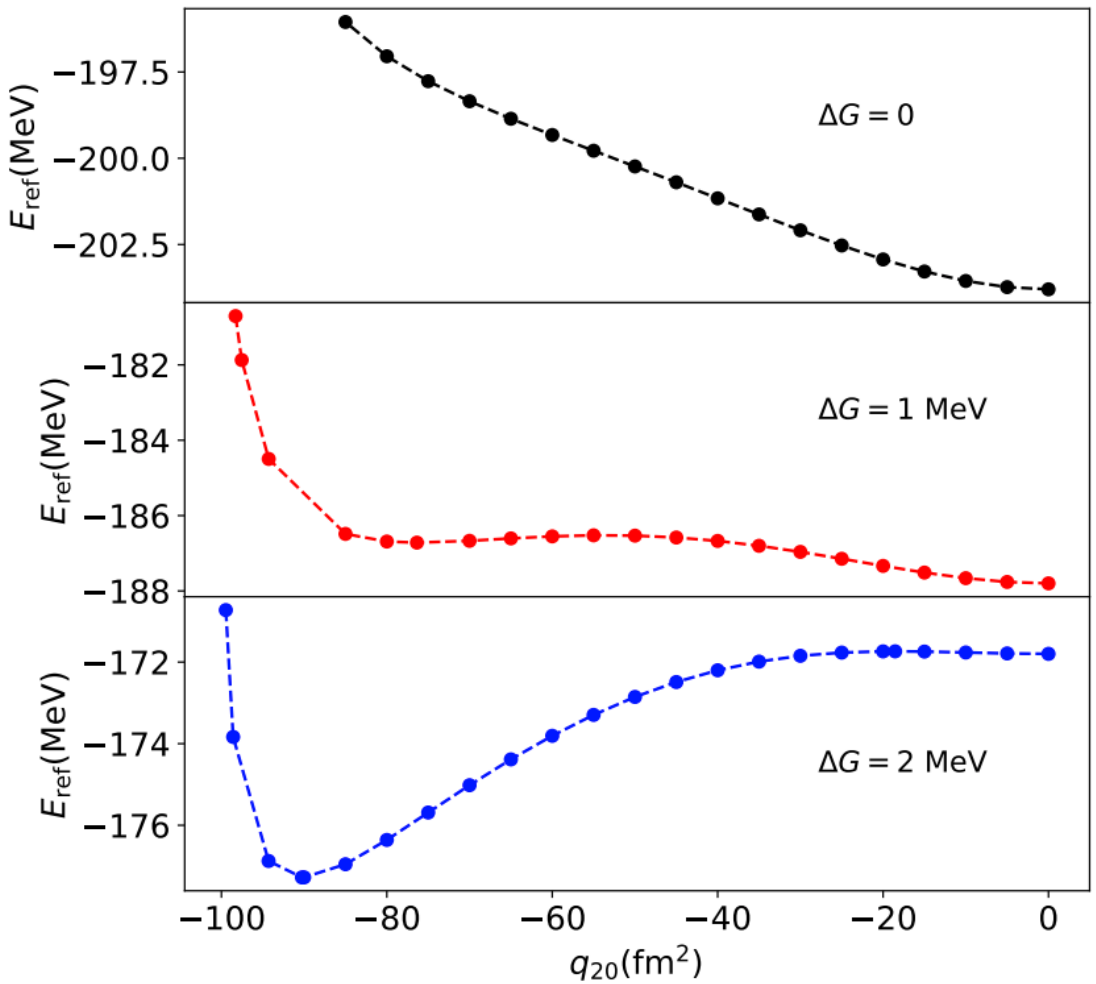
(a)The full CI, CISDTQ, and CR-CC(2,3) energies of 56Ni as functions of the shell-gap shift ΔG.

(b) Comparison of full CI energies with the trends expected for the 1p-1h, 4p-4h, and 8p-8h configurations as functions of ΔG

Coupled cluster fails at vanished shell gap

Deformation to capture correlations

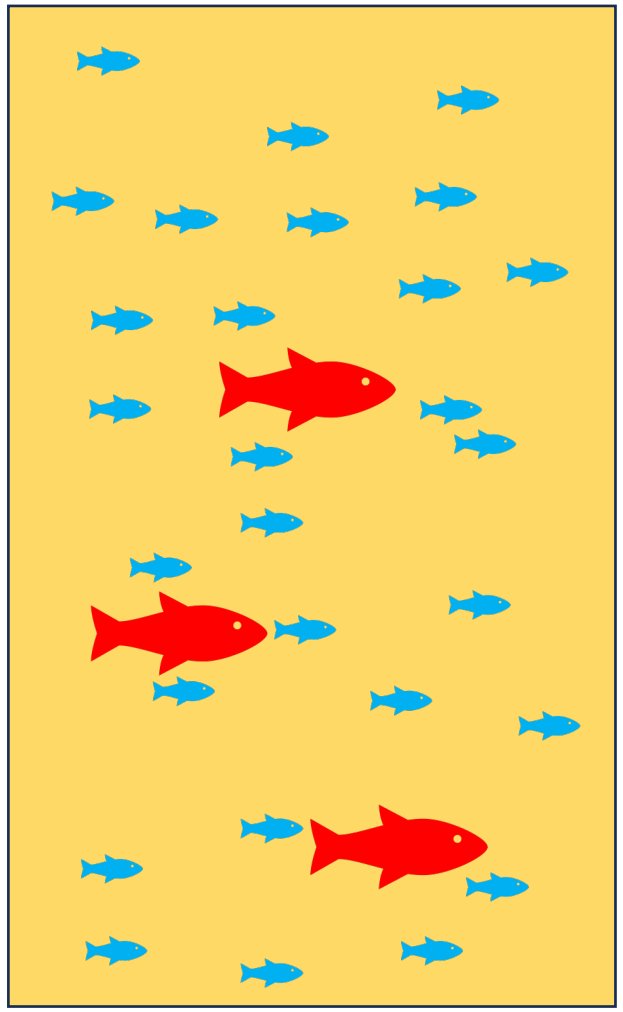




Coupled cluster fails because of

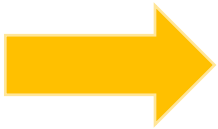
spontaneously symmetry breaking ⇌ 4p4h, 8p8h,…

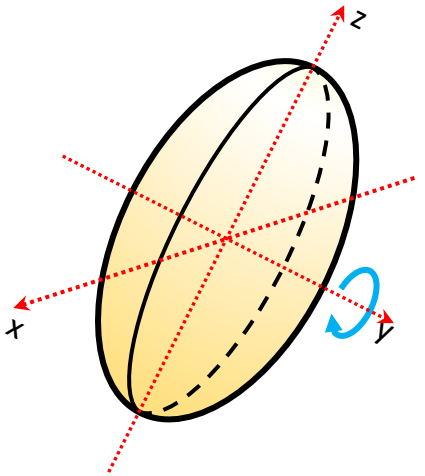
Static correlations in the atomic nuclei



Static correlations

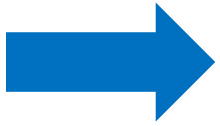
- Small number of degree of freedom
- Big contribution individually
- Exponentially scaling
- Symmetry breaking
- Responsible for the collective phenomena of the system

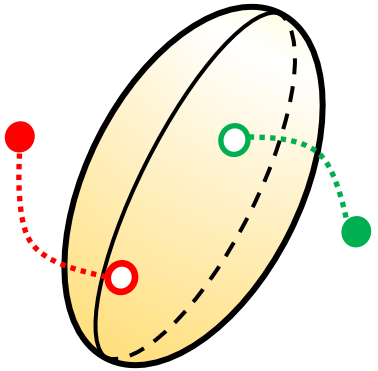




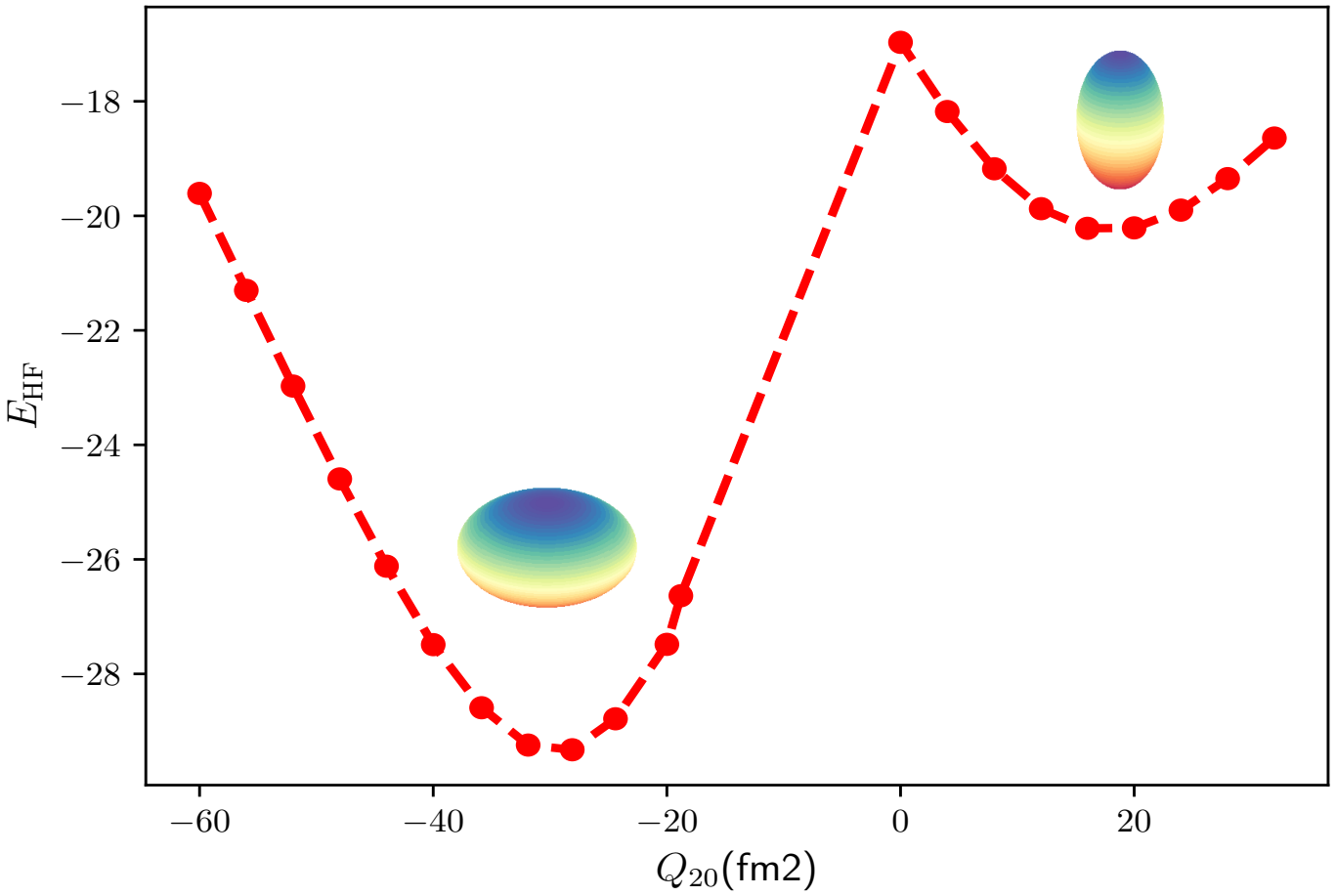
Dynamic correlations

- Large number of states, *n-particle-hole excitations*
- small contribution individually, but big contribution in a whole
- Polynomials scaling

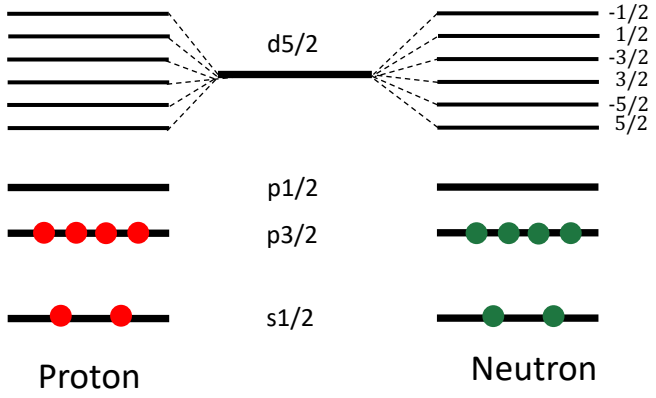


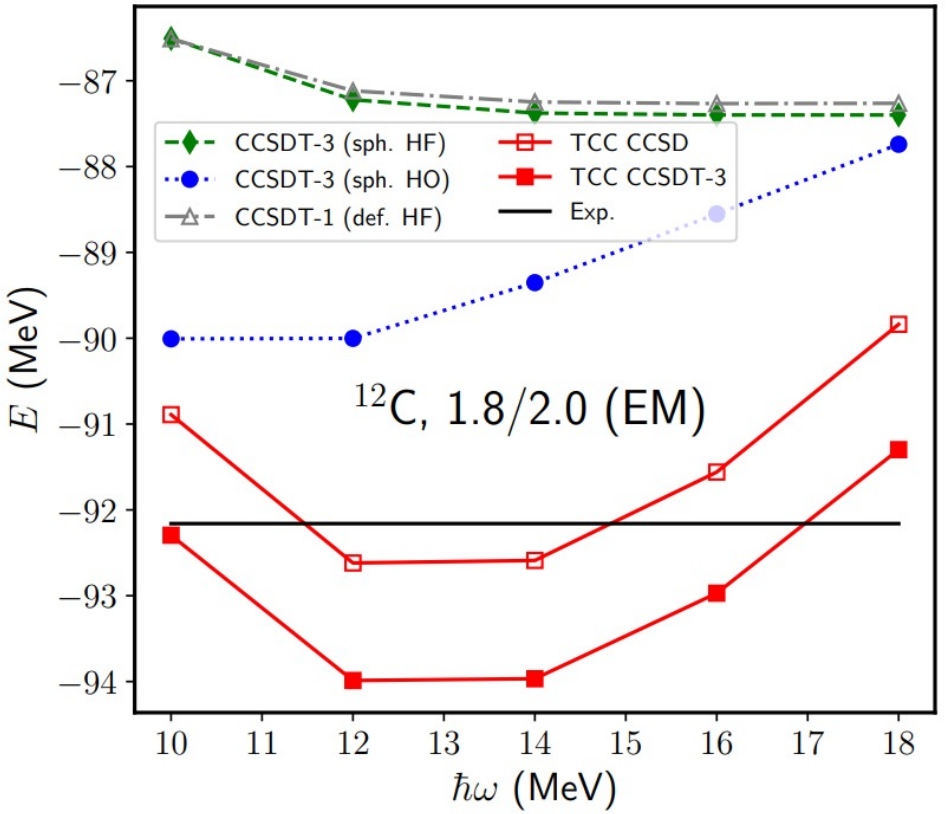


^{12}C, Strong correlation, symmetry breaking



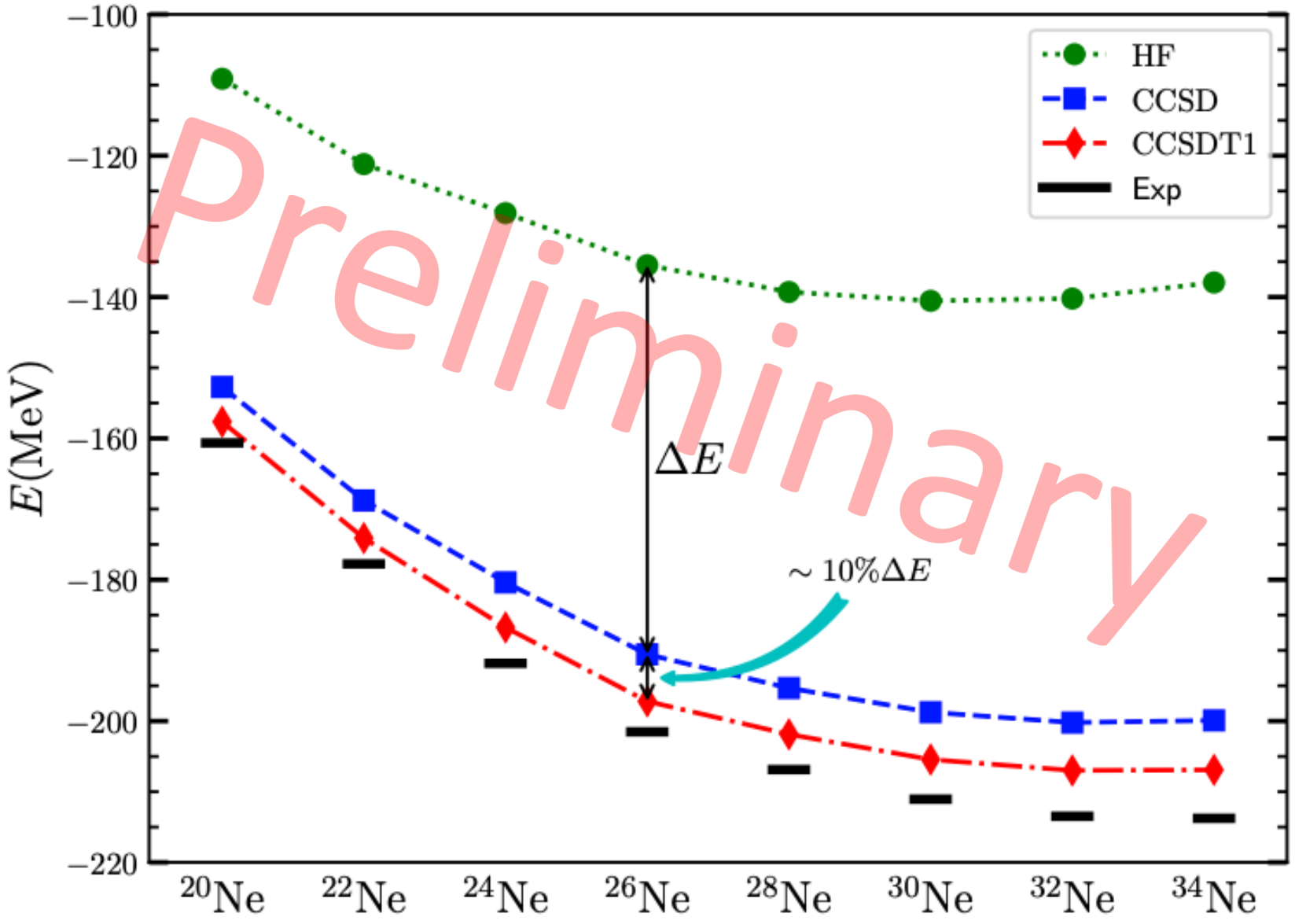
Potential surface, ^{12}C, NNLO$_{\mathrm{OPT}}$, N$_{\mathrm{MAX}}$=12





Coupled cluster on deformed basis as an alternative approach to capture high order correlations

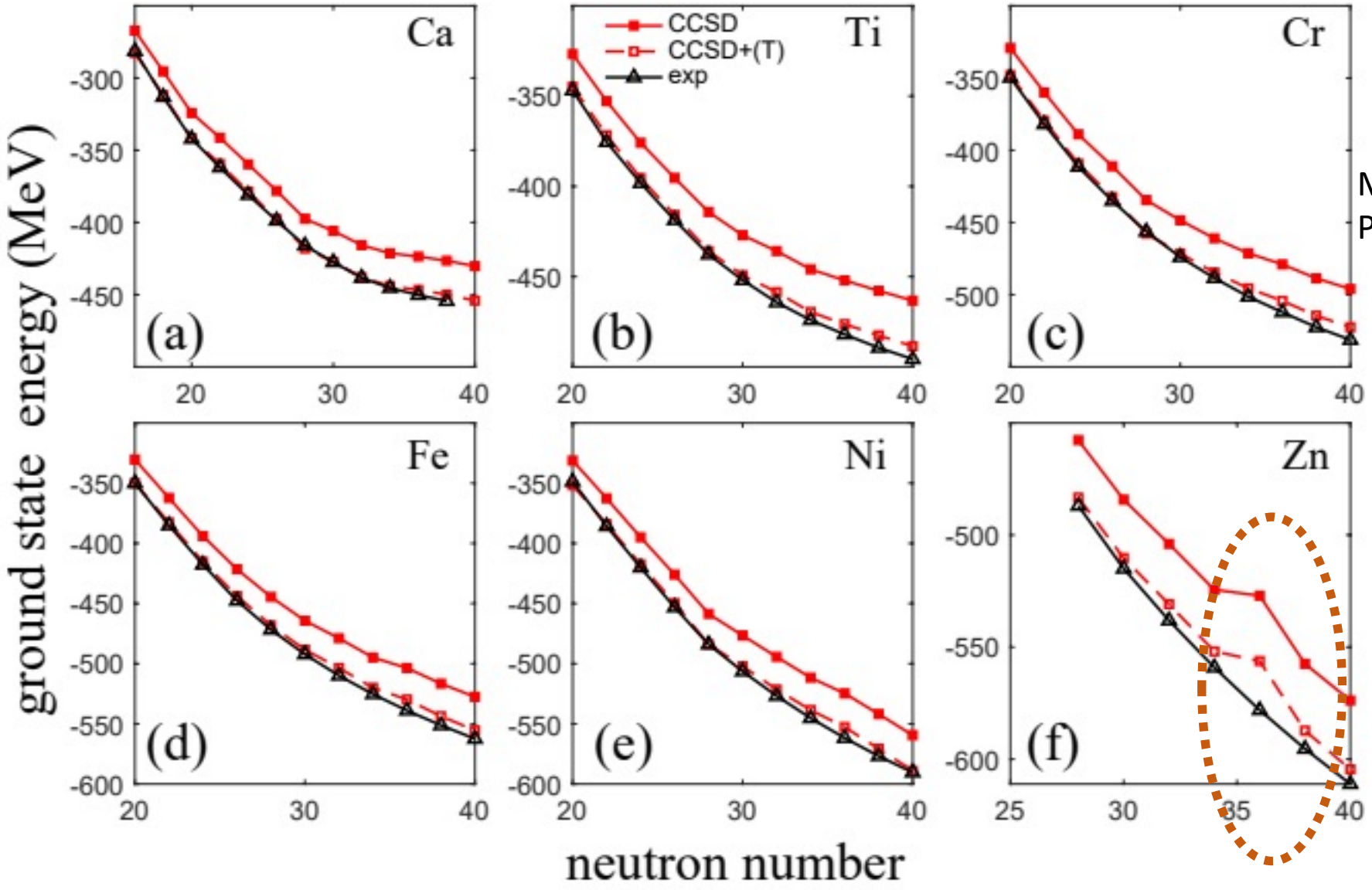
Deformed coupled cluster on open shell nuclei



Single reference CC for ”Dynamic correlations”

How to restore the broken symmetry in Coupled cluster?

Deformed coupled cluster on open shell nuclei



Markus, Sun, et al,
Phys. Rev C 105, L021303 (2022)

Projected coupled cluster theory

1. Start from a deformed reference, and perform coupled cluster calculations

$$\langle^{ab..}_{ij..}|e^{-T}He^{T}|0\rangle = 0 \qquad |\Psi\rangle = e^{T}|0\rangle$$

$$\langle\Psi| = \langle 0|(1+\Lambda)e^{-T}$$

2. Symmetry restoration

$$|\Psi^{J}\rangle = \int d\beta\omega^{J}(\beta)R(\beta)e^{T}|0\rangle$$

The true wave function is the superposition of rotated states

$$H|\Psi^{J}\rangle = E^{J}\int d\beta\omega^{J}(\beta)R(\beta)e^{T}|0\rangle$$

$$E^{J} = \frac{\int d\beta\omega^{J}(\beta)\langle 0|(1+\Lambda)e^{-T}HR(\beta)e^{T}|0\rangle}{\int d\beta\omega^{J}(\beta)\langle 0|(1+\Lambda)e^{-T}R(\beta)e^{T}|0\rangle}$$

Qiu, *et al*,
J. Chem. Phys. 147, 064111 (2017)

Disentangled cluster operator

$$\langle 0|R(\beta) = \langle 0|R(\beta)|0\rangle\langle 0|e^{V_1}$$

Thouless theorem

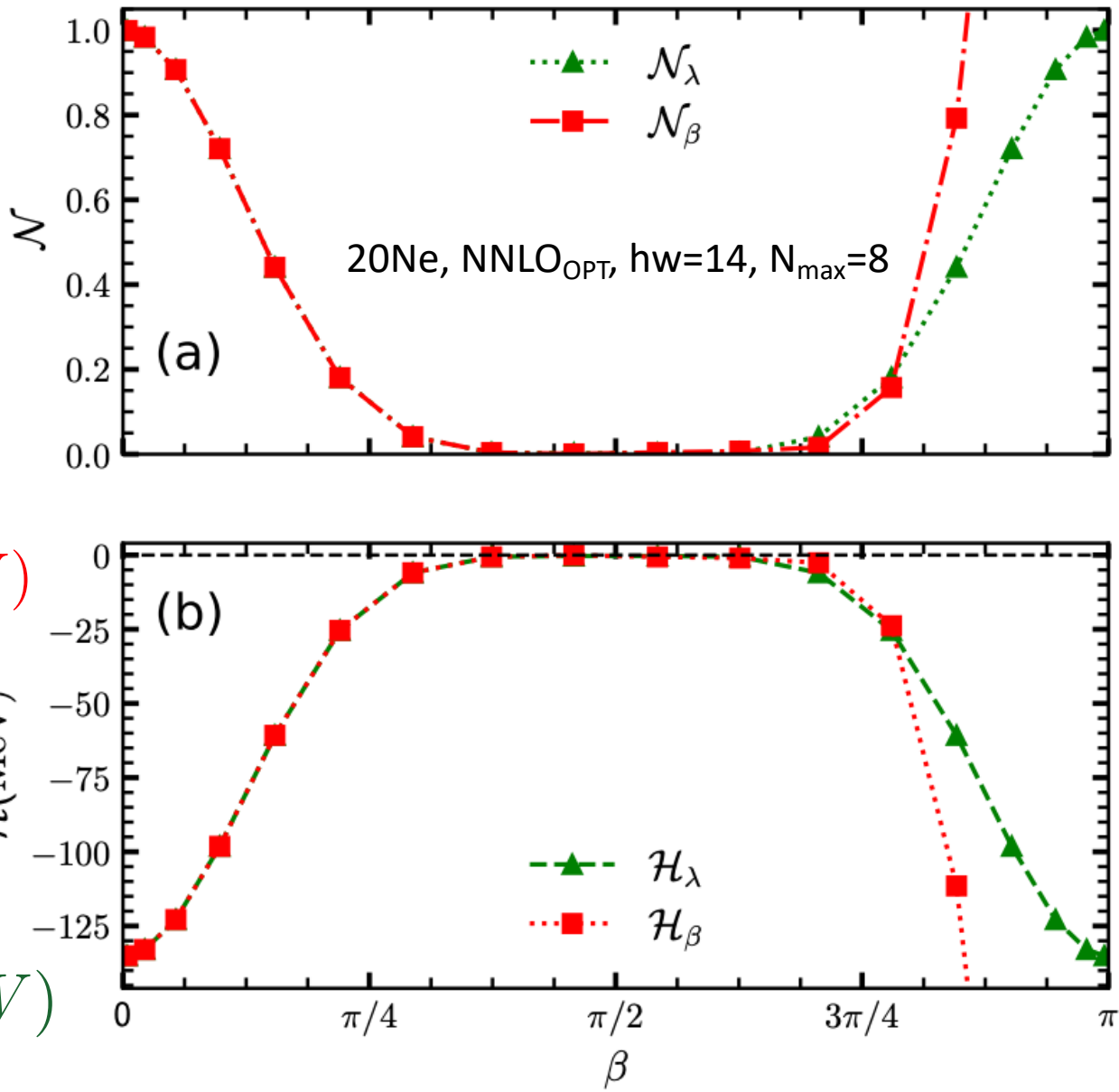
$$e^{V_1}e^{T_2} = e^{W_0}e^{W_1+W_2+\cdots}$$

Disentangled cluster operator, compute W by solving ODEs.

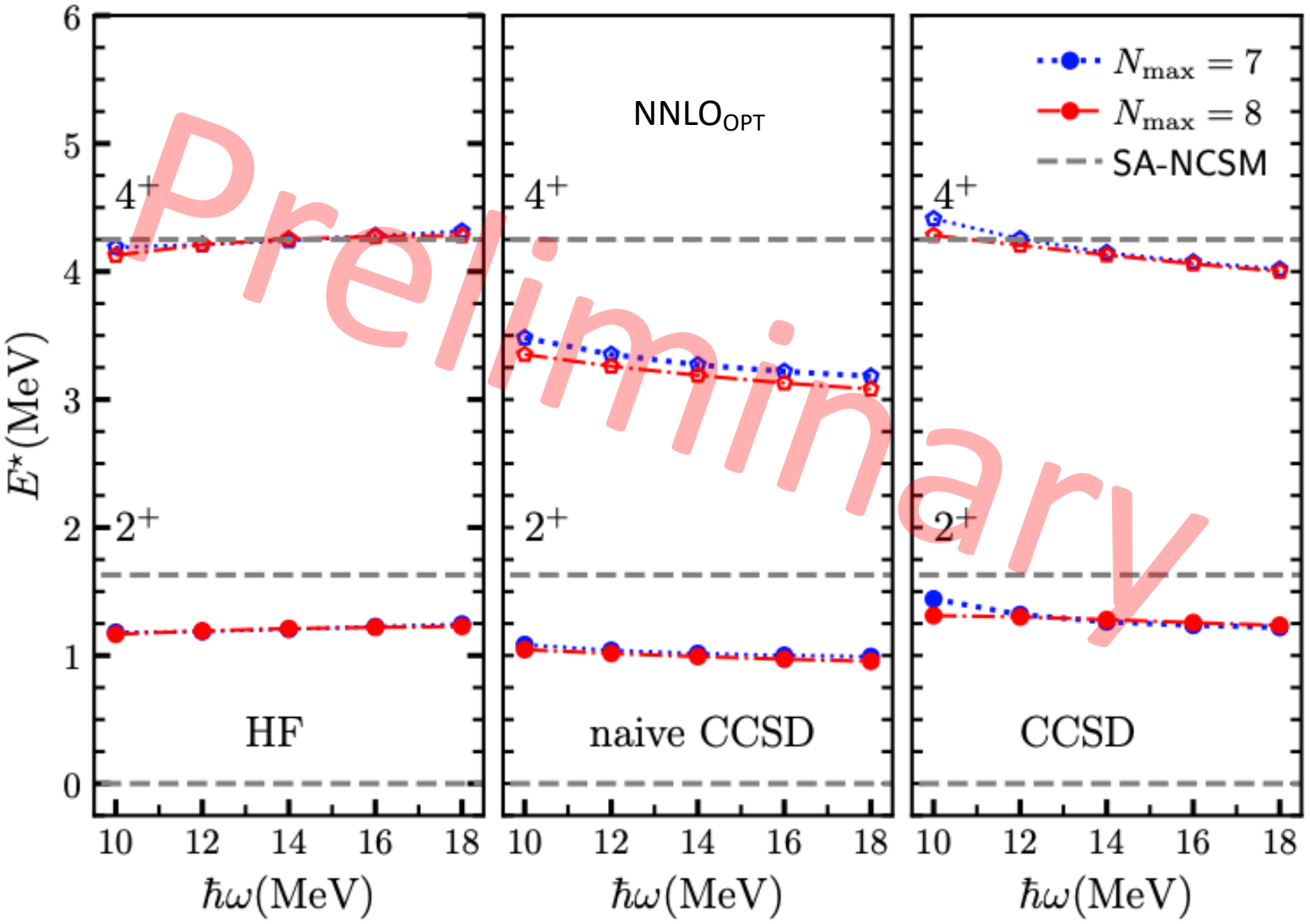
$$e^{V_1(\beta)}e^{T_2} = e^{W(\beta)} \quad \frac{dW}{d\beta} = \mathcal{F}(\frac{dV_1}{d\beta}, W)$$

- Numerical errors at large angle,
- Fail to work for odd-mass nuclei

$$e^{\lambda V_1}e^{T_2} = e^{W(\lambda)} \quad \frac{dW}{d\lambda} = \mathcal{F}(V_1, W)$$



Projected coupled cluster on ^{20}Ne

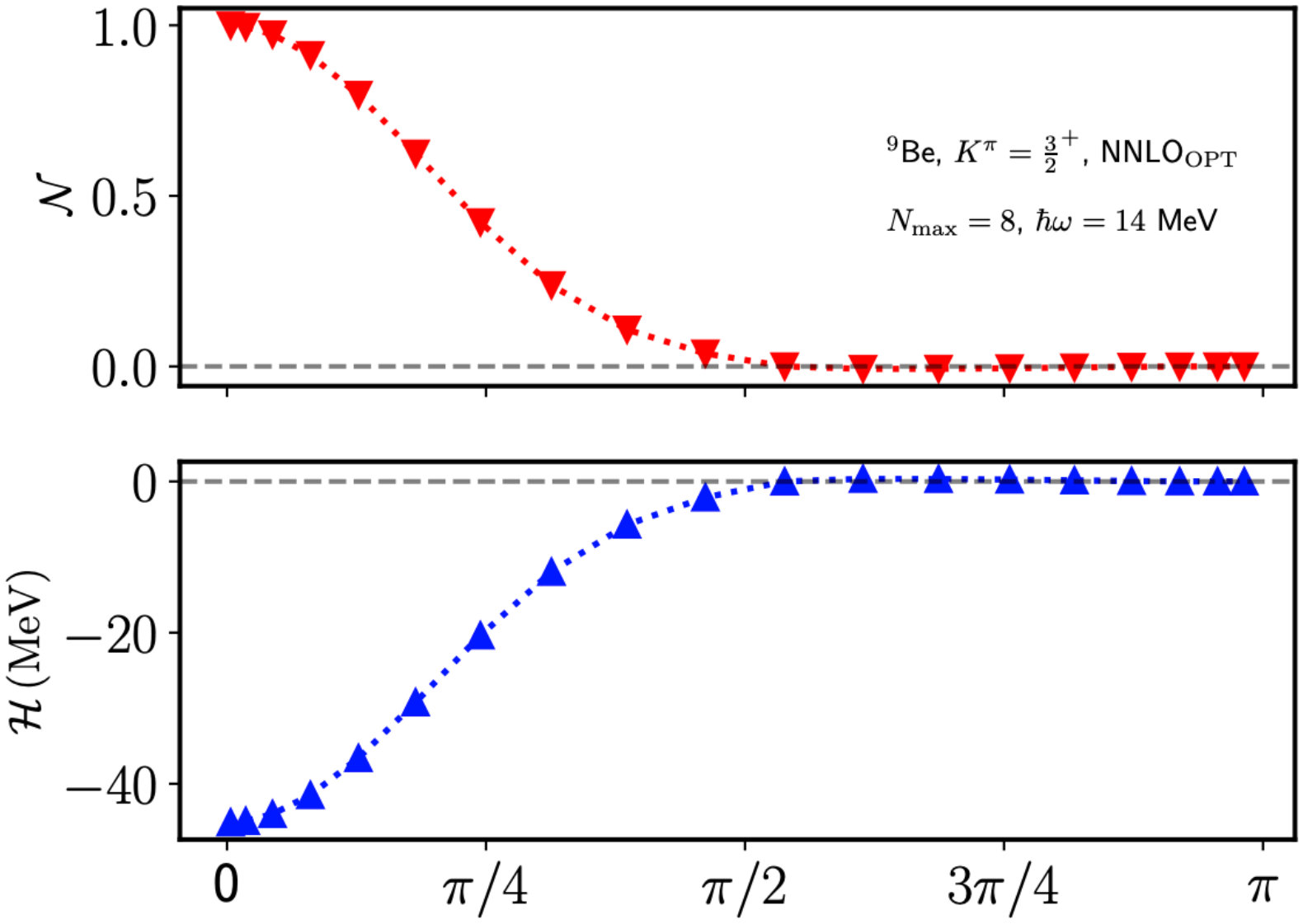


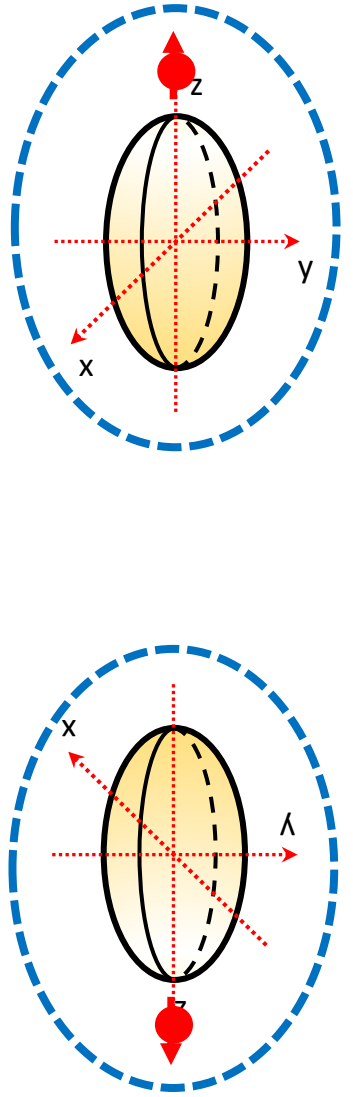
Naive CCSD: Vacuum state as the left wavefunction

Projected CC: take coupled cluster bi-orthogonal left wave function

Meet the benchmark with SA-NCSM

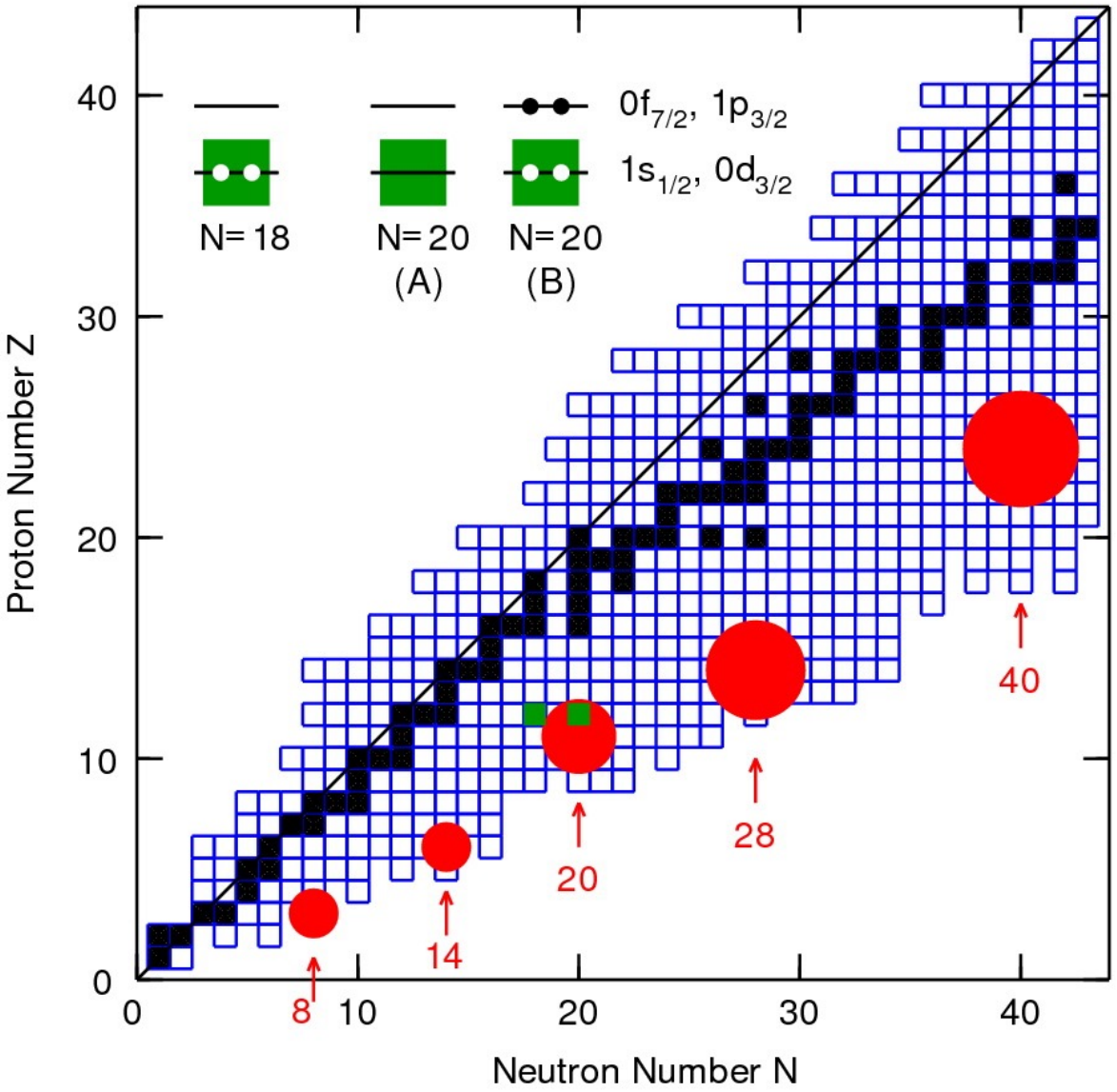
Kernels for Odd-mass nuclei

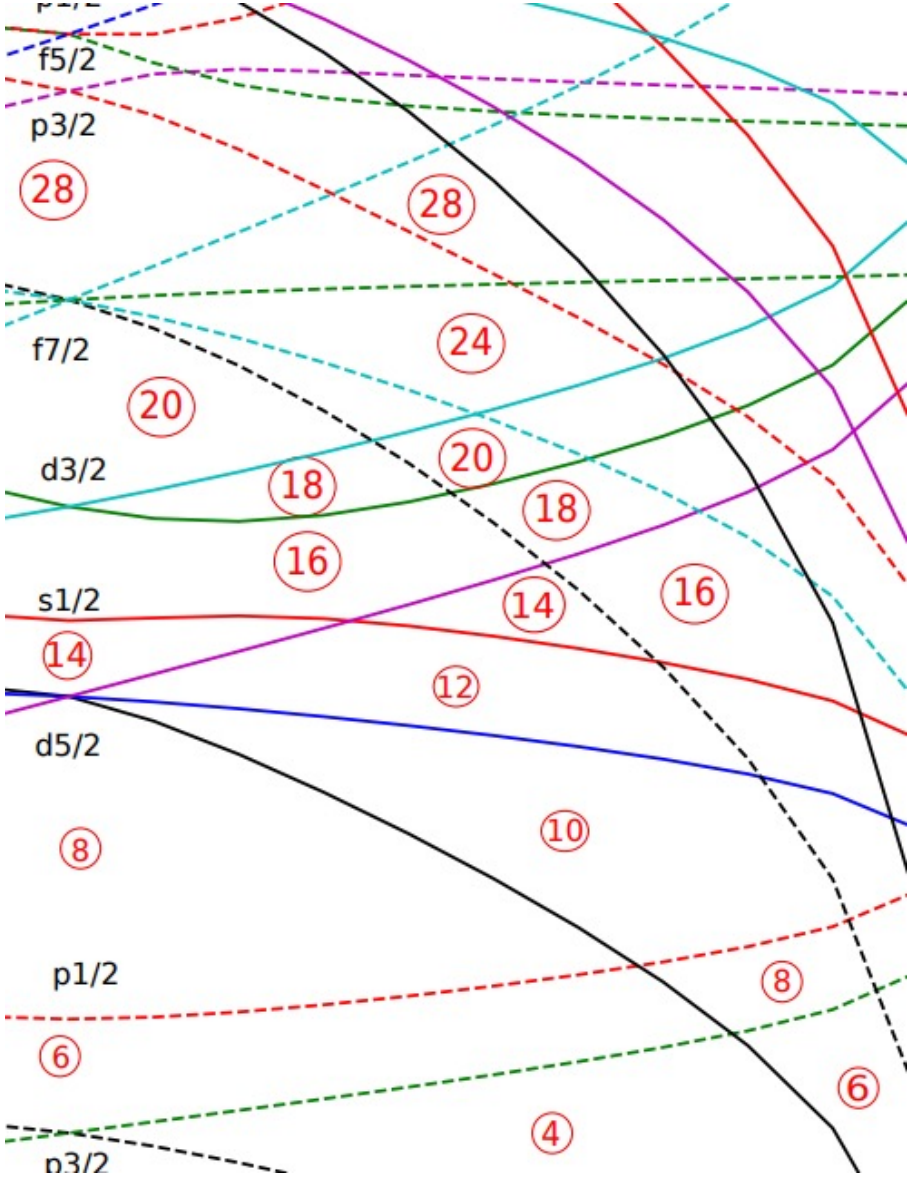




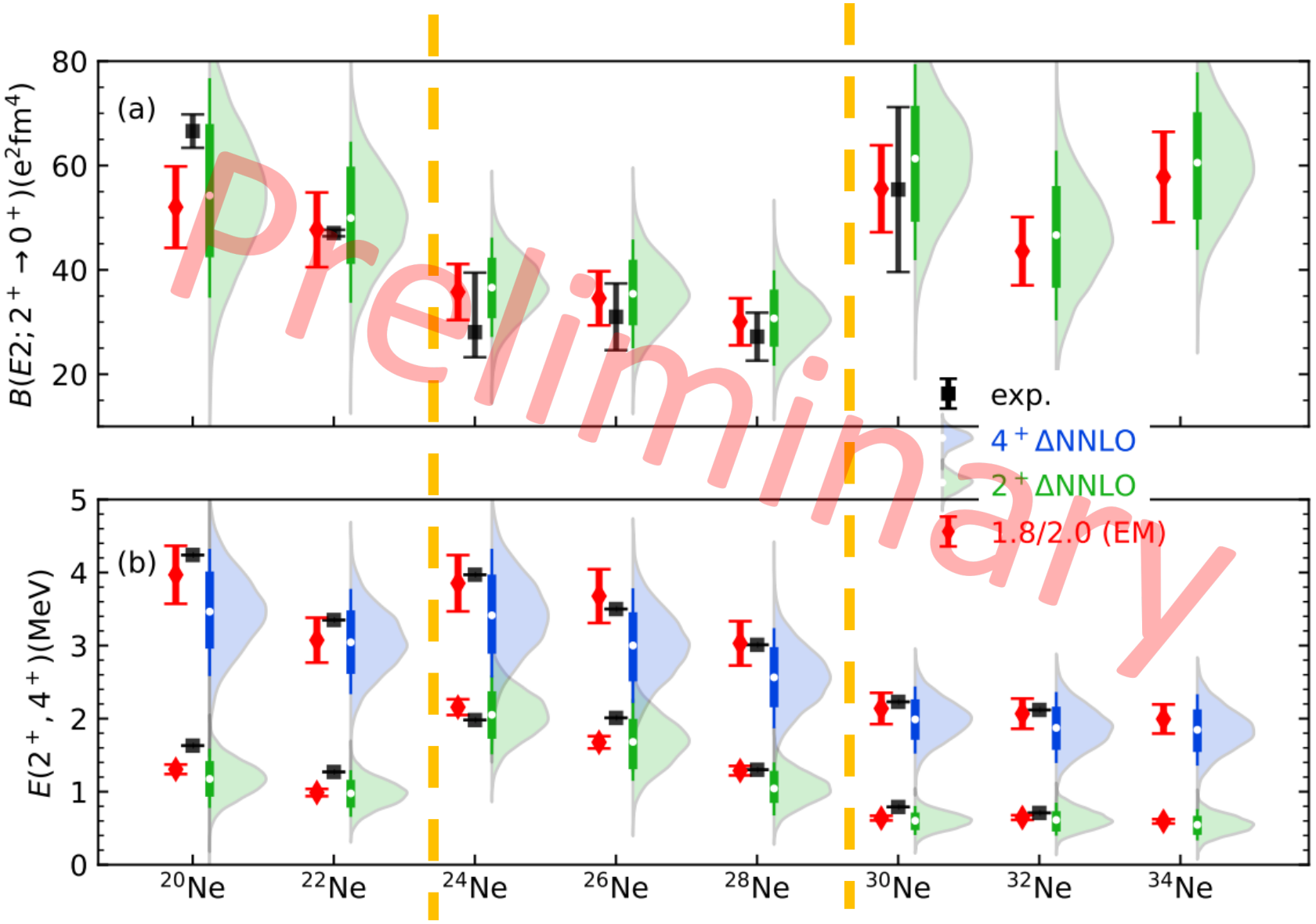
$R_y(\pi)$

Island of inversion , Ne, Na, Mg



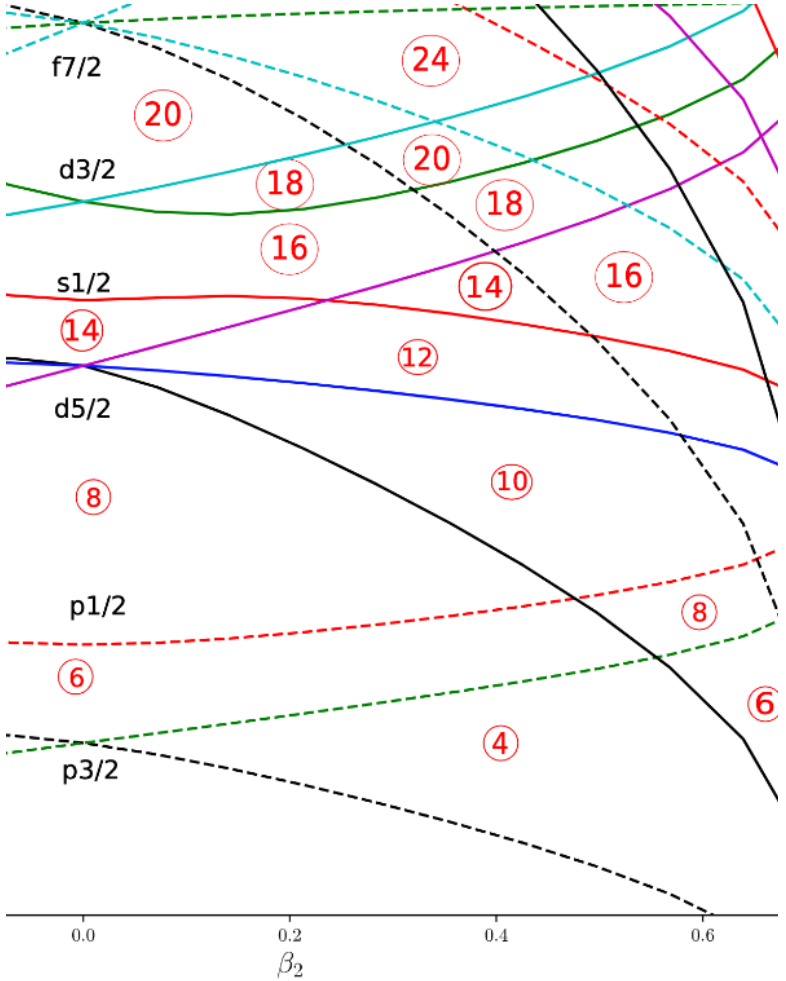


island of inversion (ioi): Ne isotopes

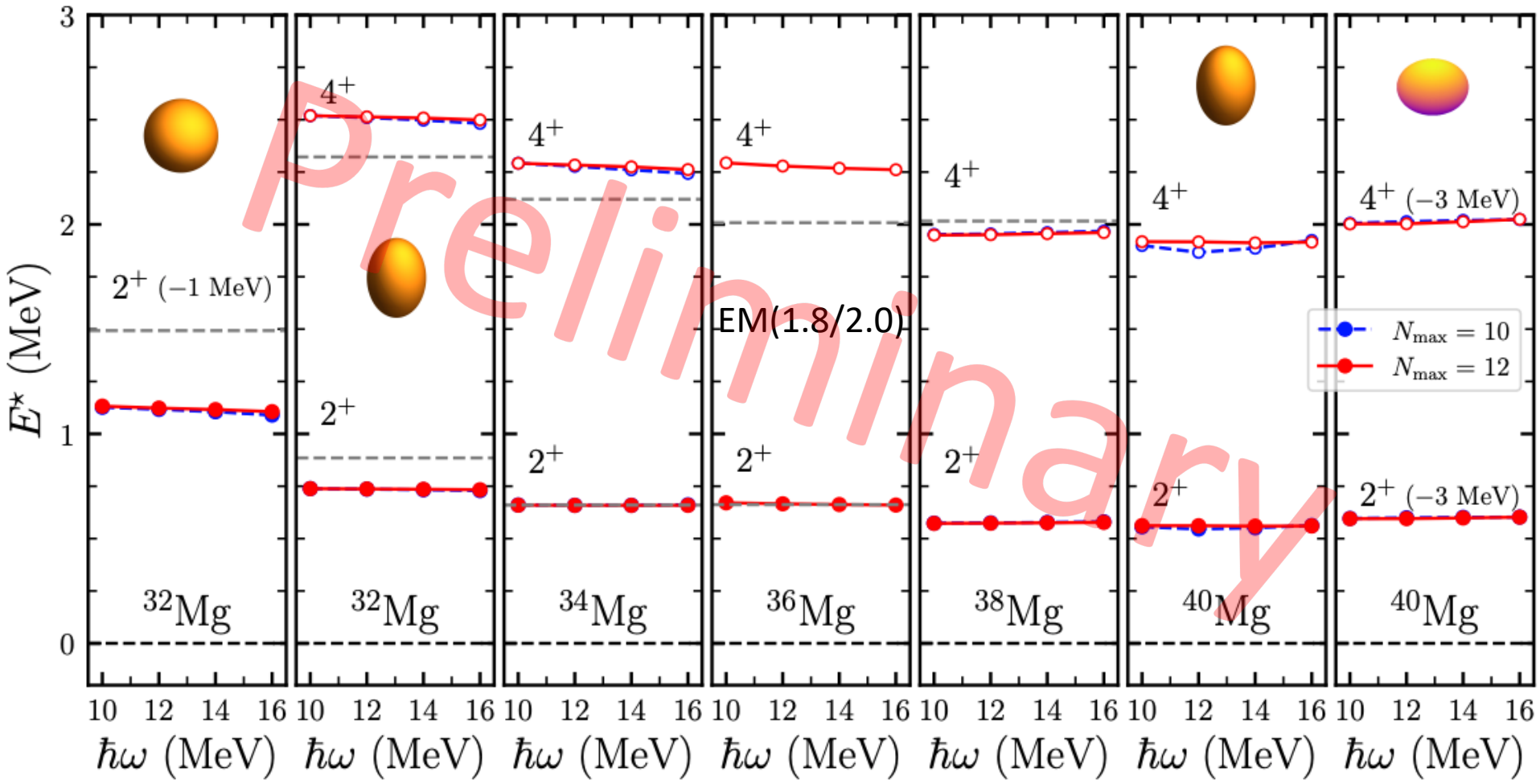


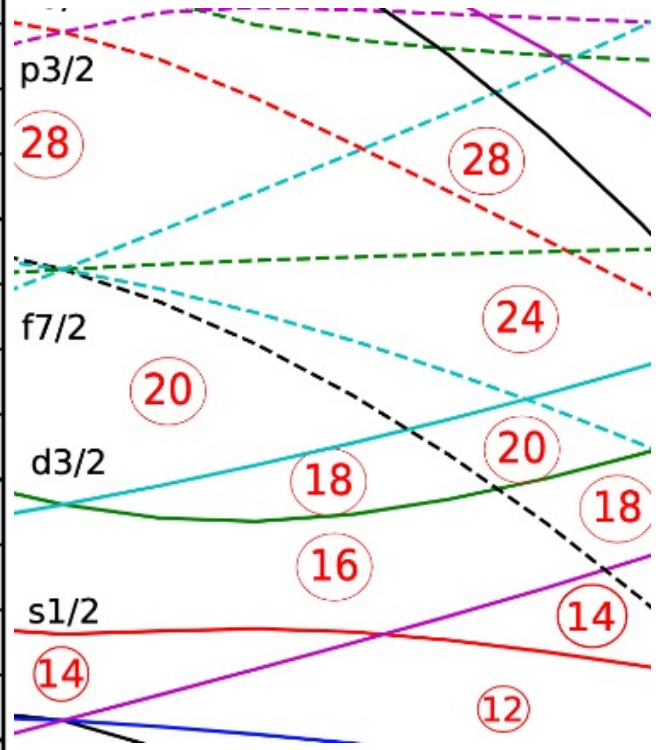
G. Hagen, S. J. Novario, Z. H. Sun et al.
Phys. Rev. C **105**, 064311 (2022)

Z. Sun, et al. "Multiscale physics of atomic nuclei from first principles ", in preparing



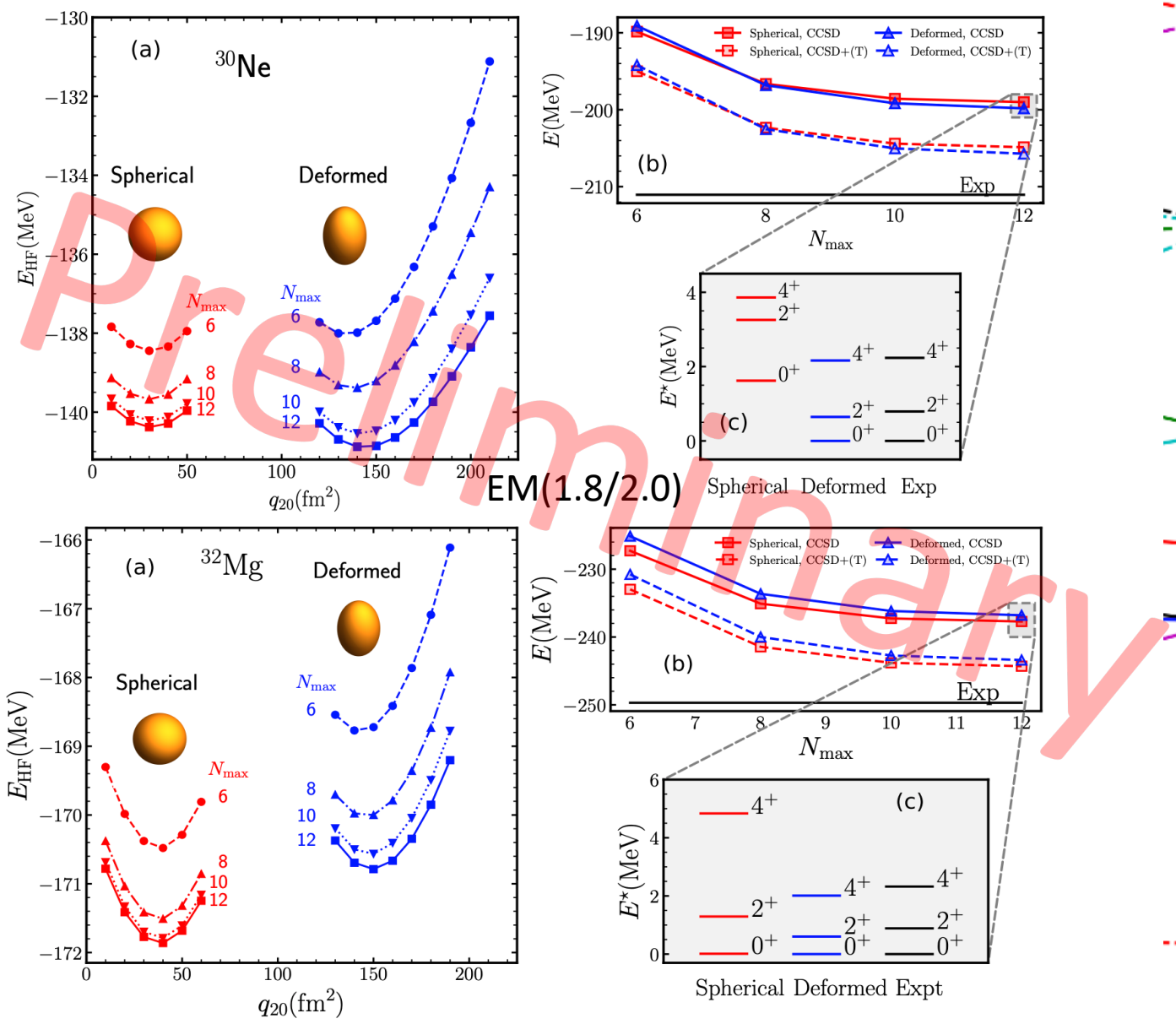
Shape evolution of Mg isotopes (projected HF)

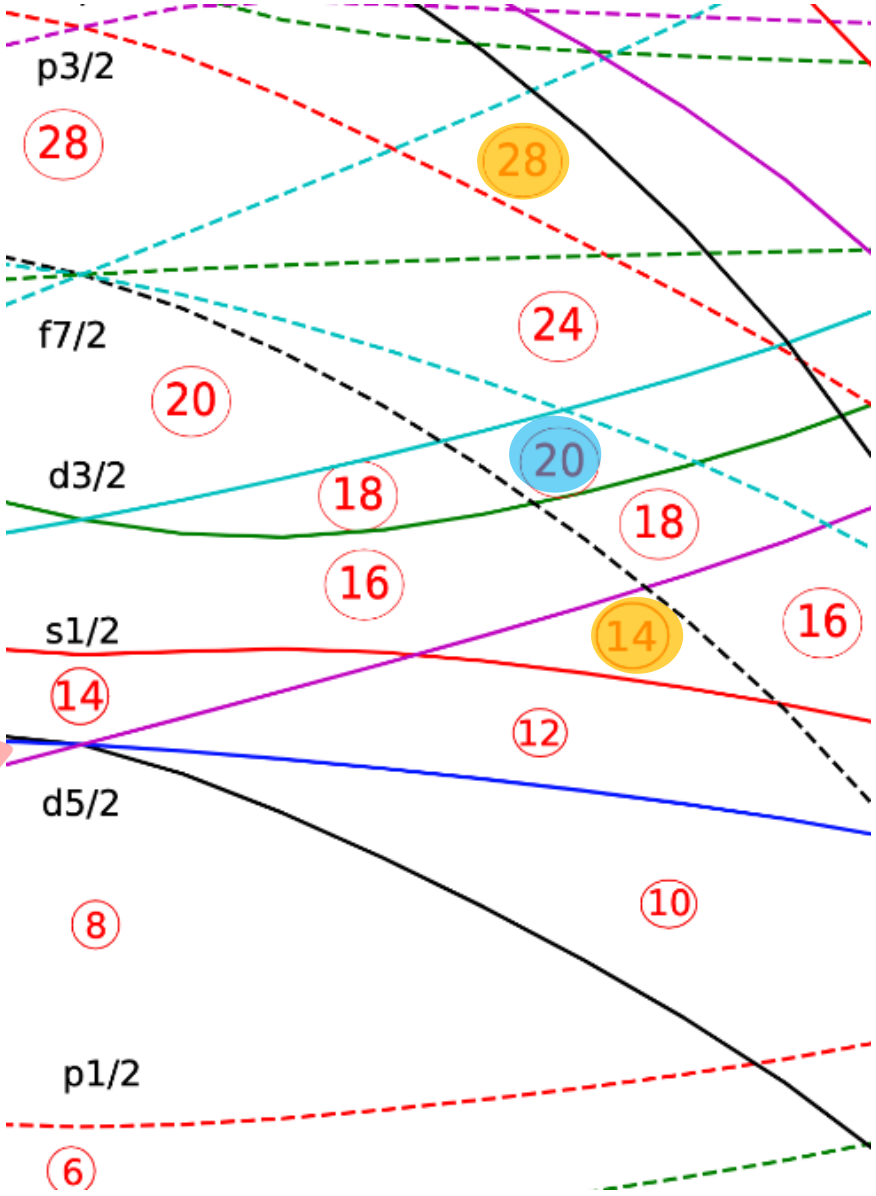




Mg isotopes beyond N=20 have similar shape

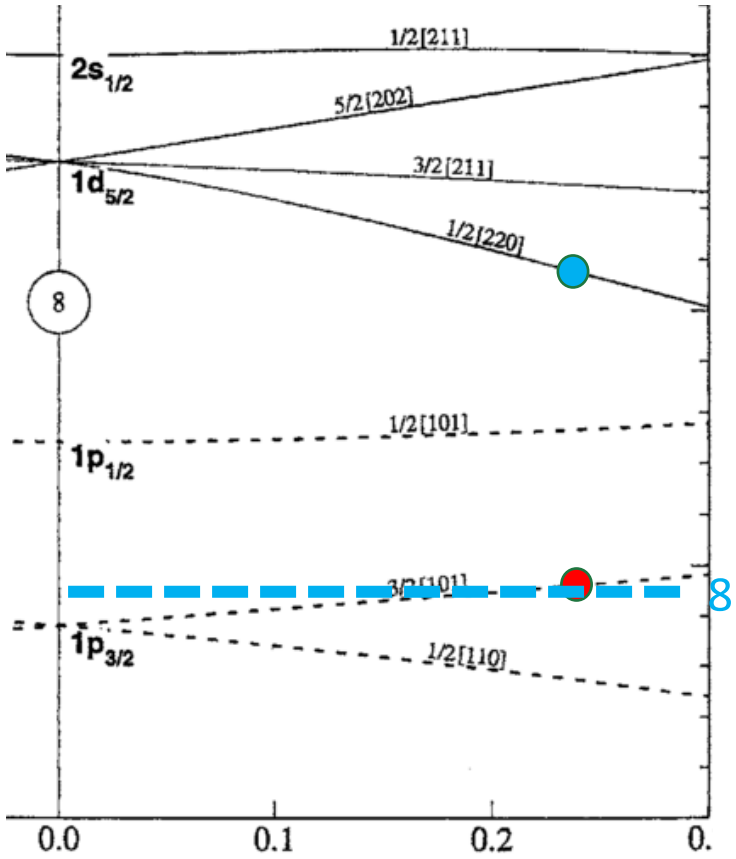
Structure of ^{30}Ne and ^{32}Mg



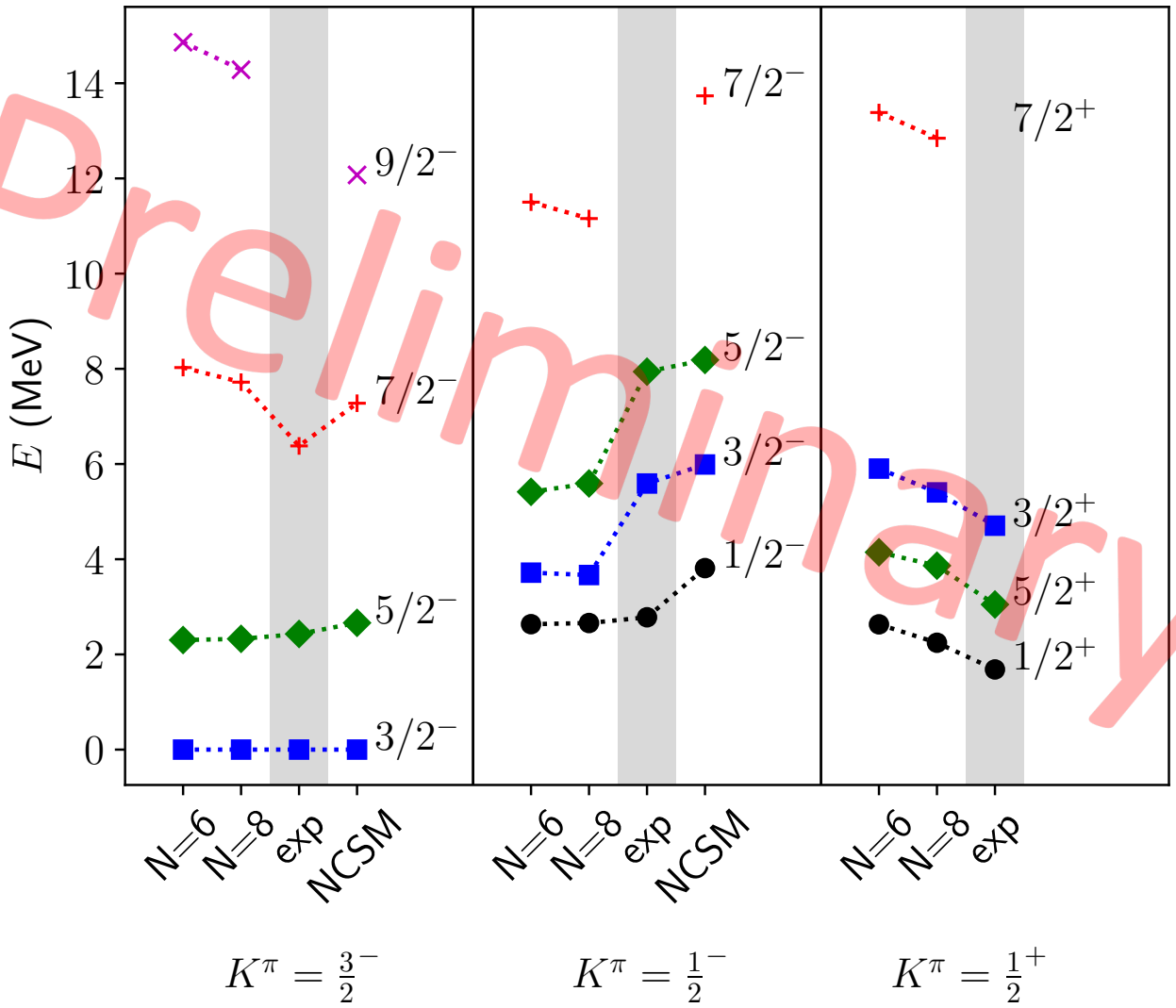


How about odd-mass nuclei,

Stand on the shoulder of deformed even-even nuclei

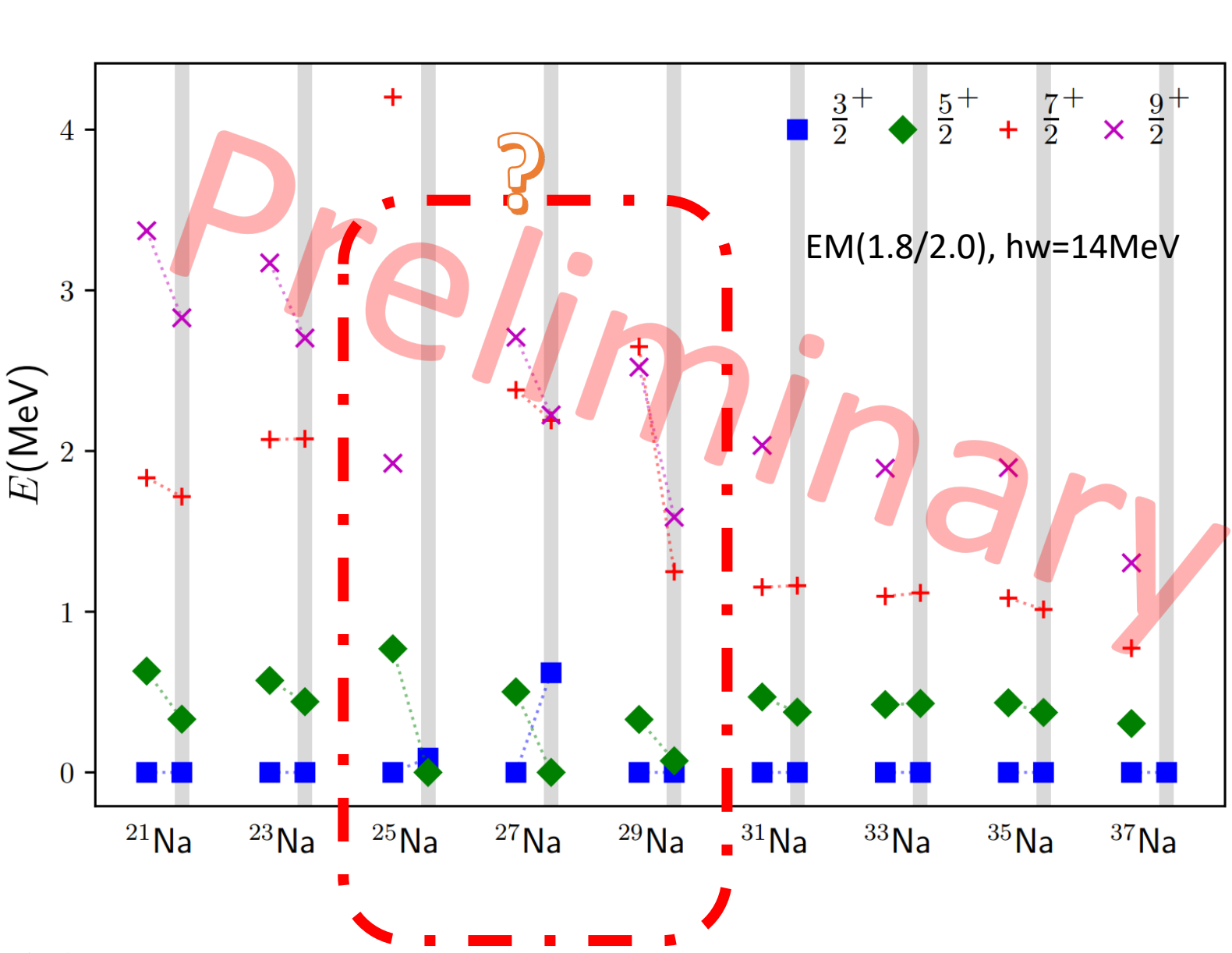


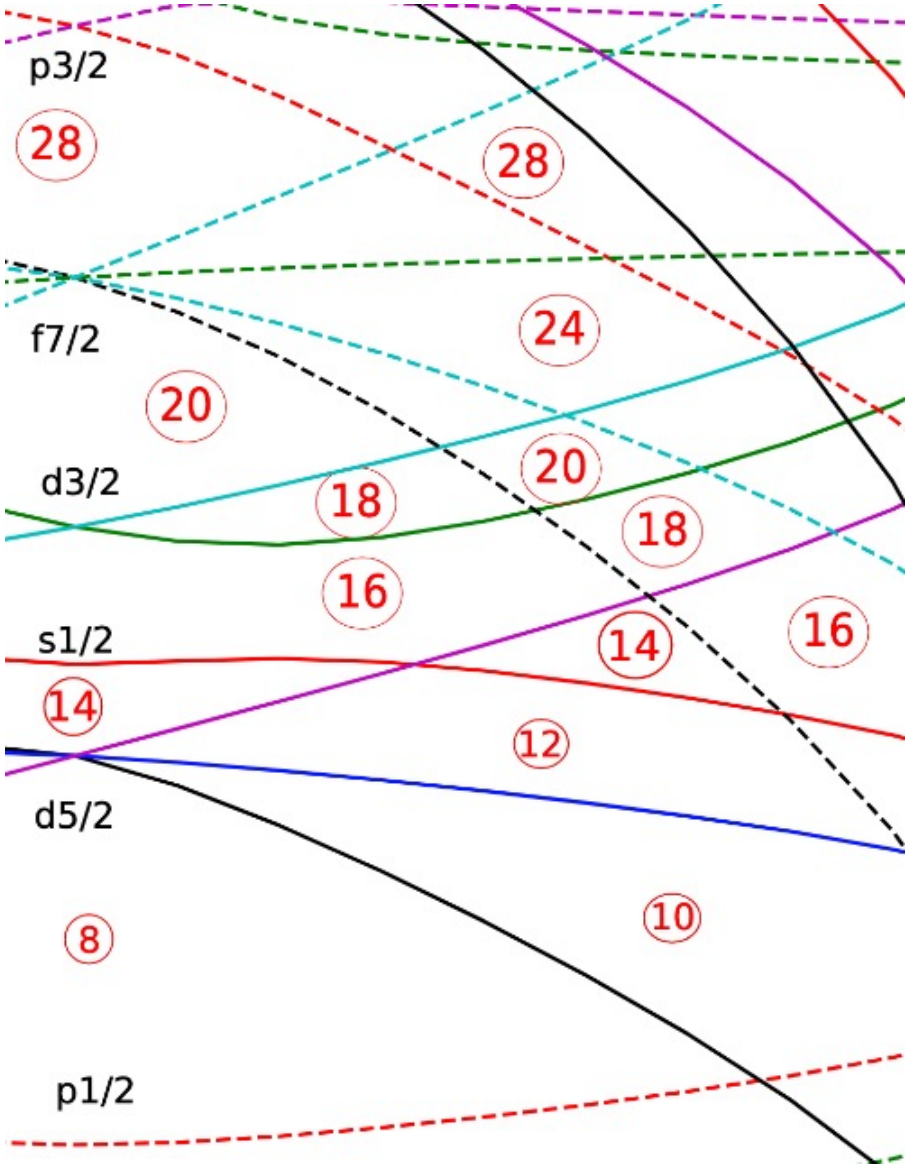
EM(1.8/2.0), hw=14 MeV



Different filling of the unpaired particle yields band heads

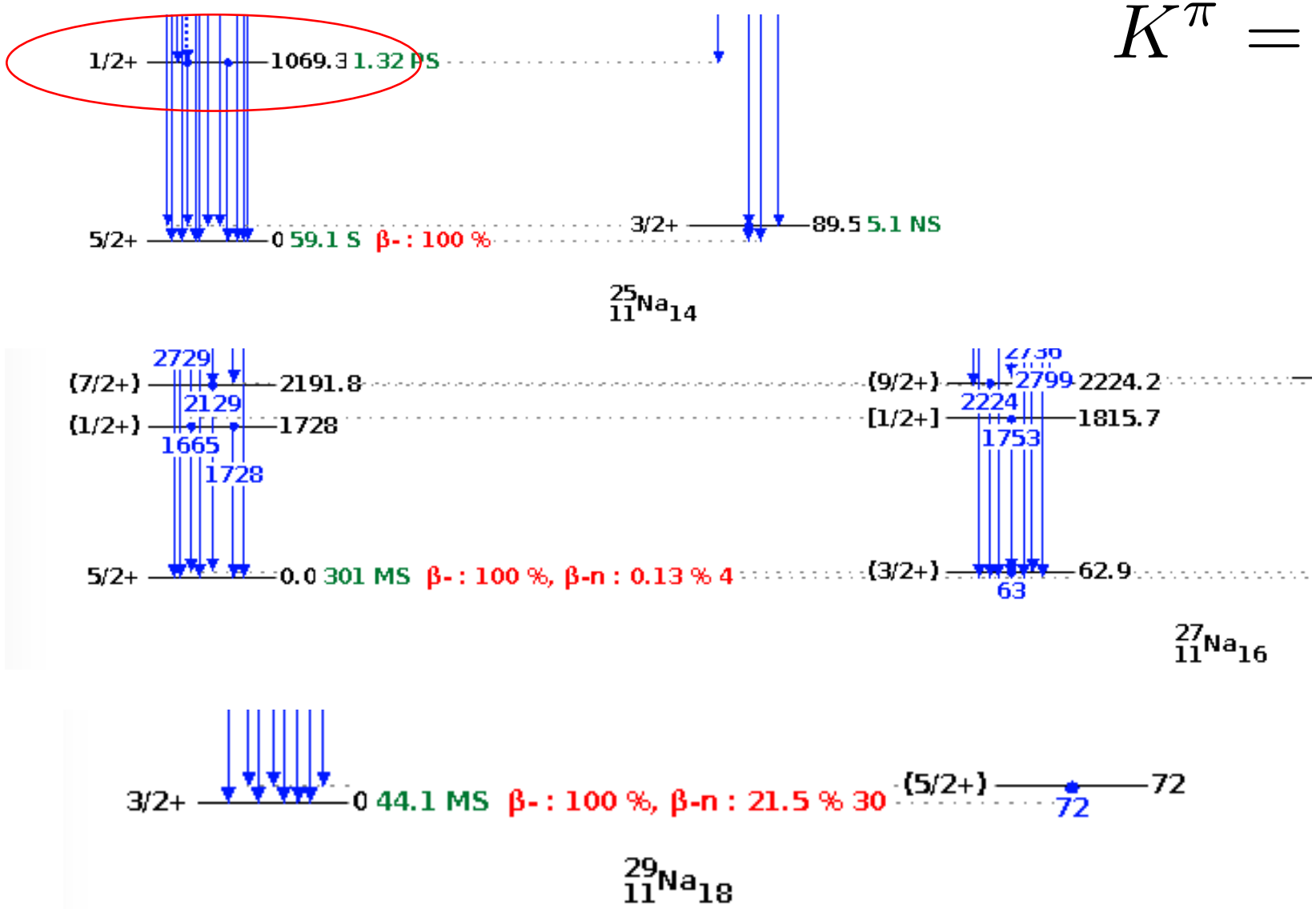
Structure of odd-mass Na isotopes

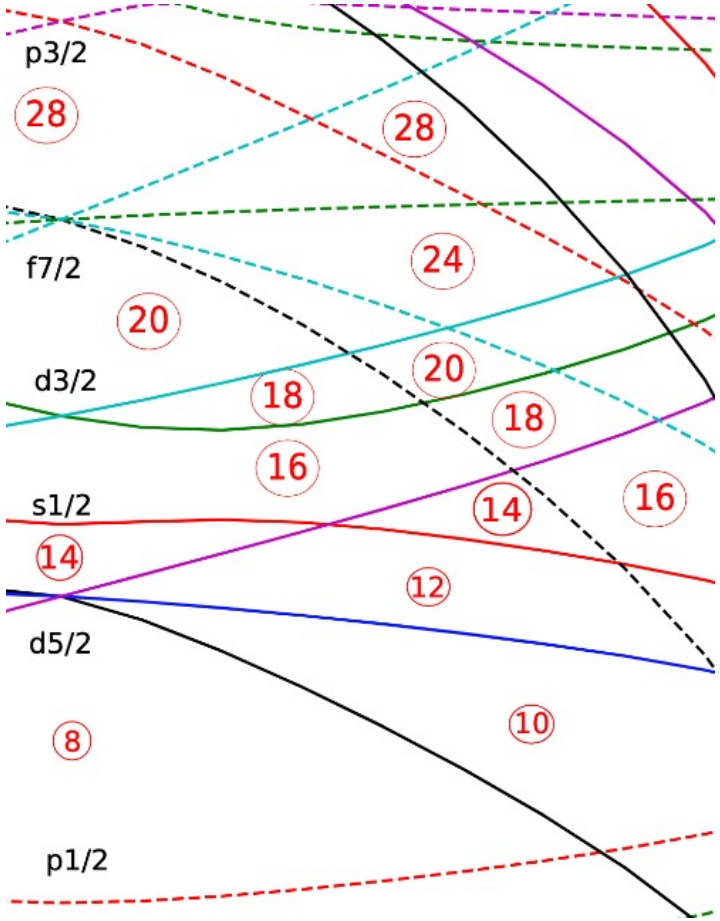




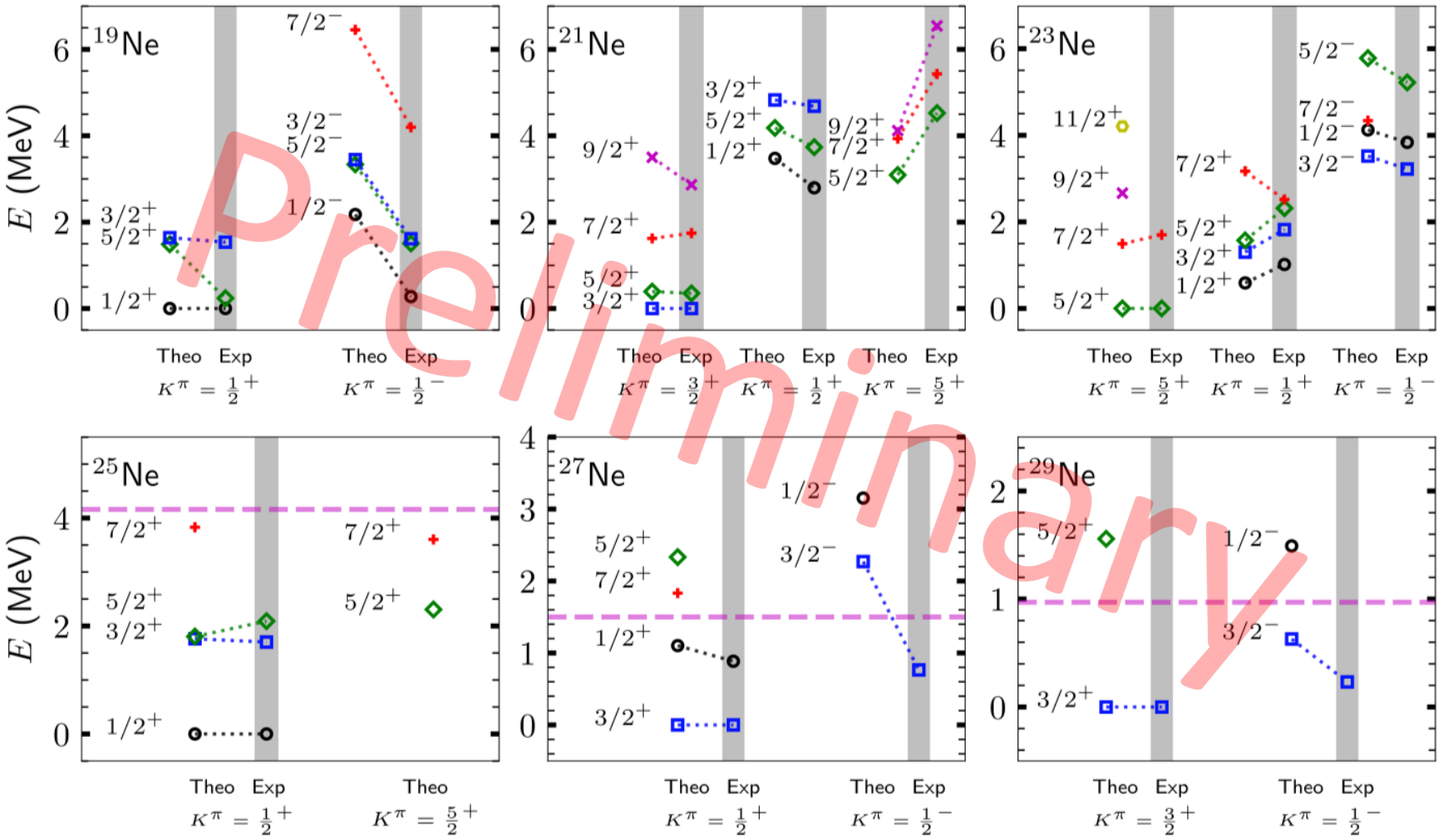
Data, ^{25,27,29}Na, band mixing

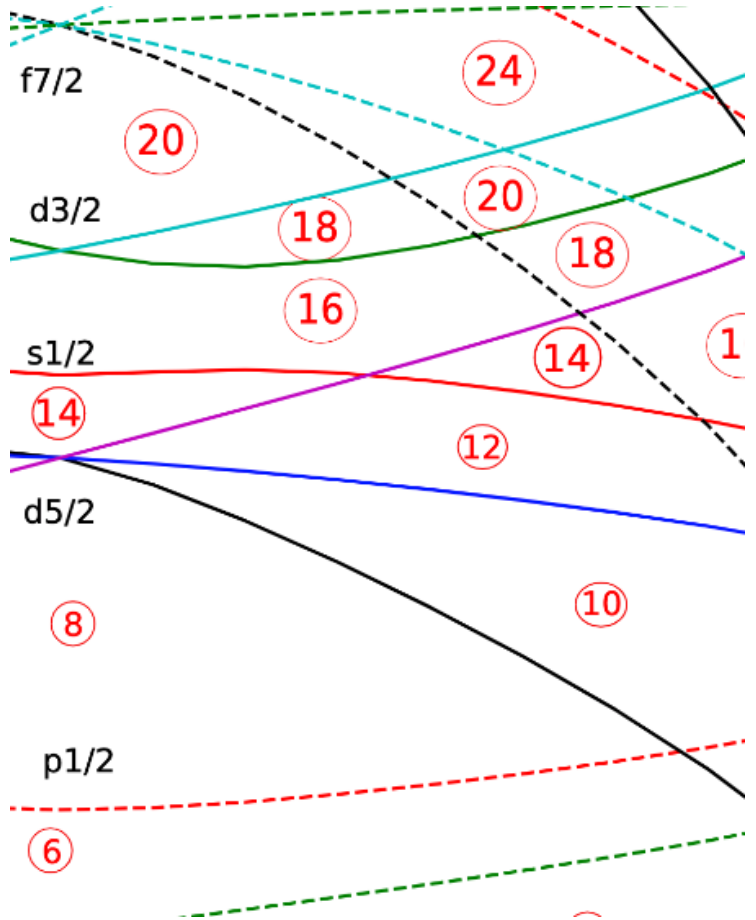
$$K^\pi = \frac{1}{2}^+ \qquad K^\pi = \frac{3}{2}^+$$





Rotational band of odd-mass Ne isotopes

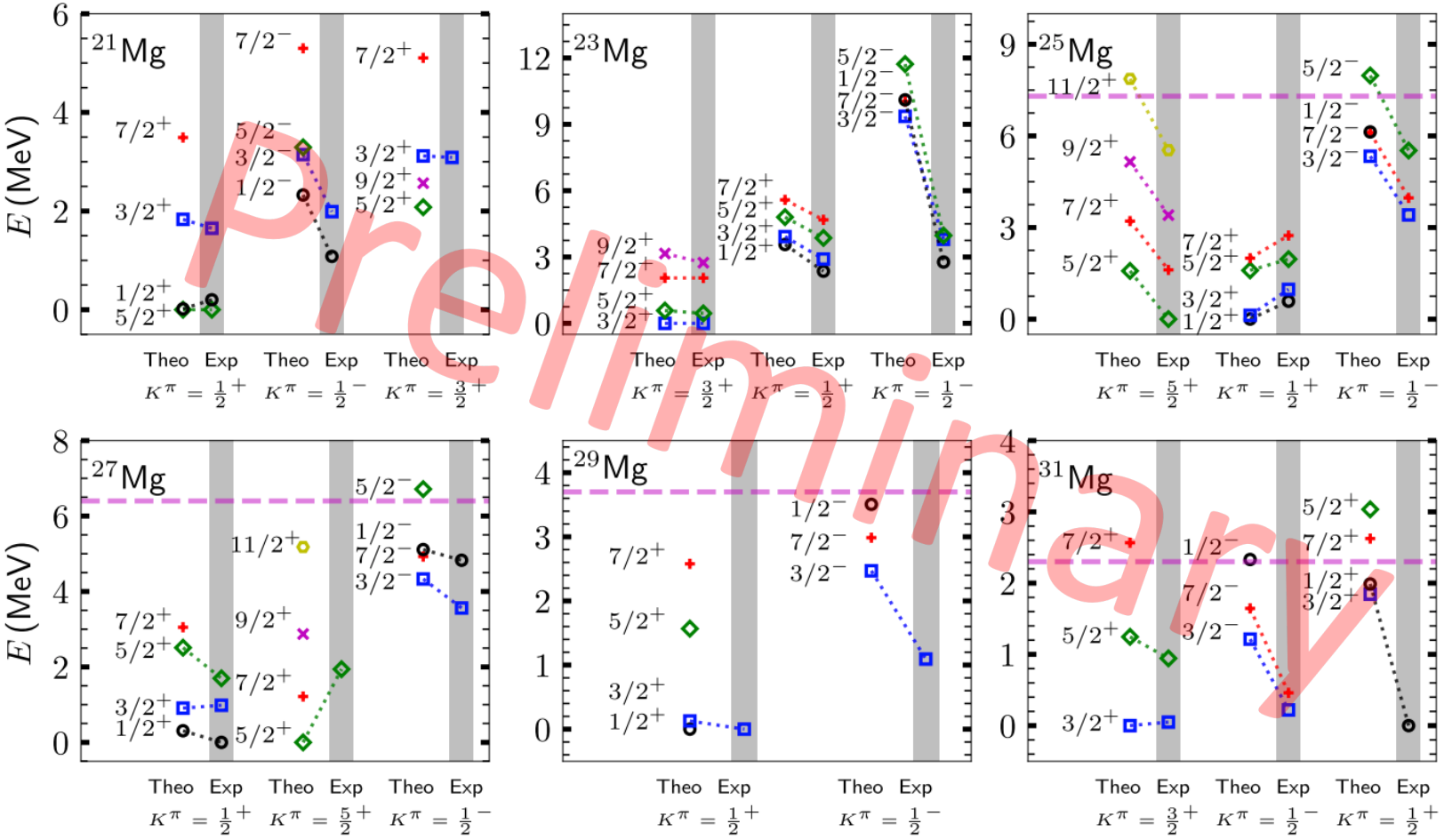


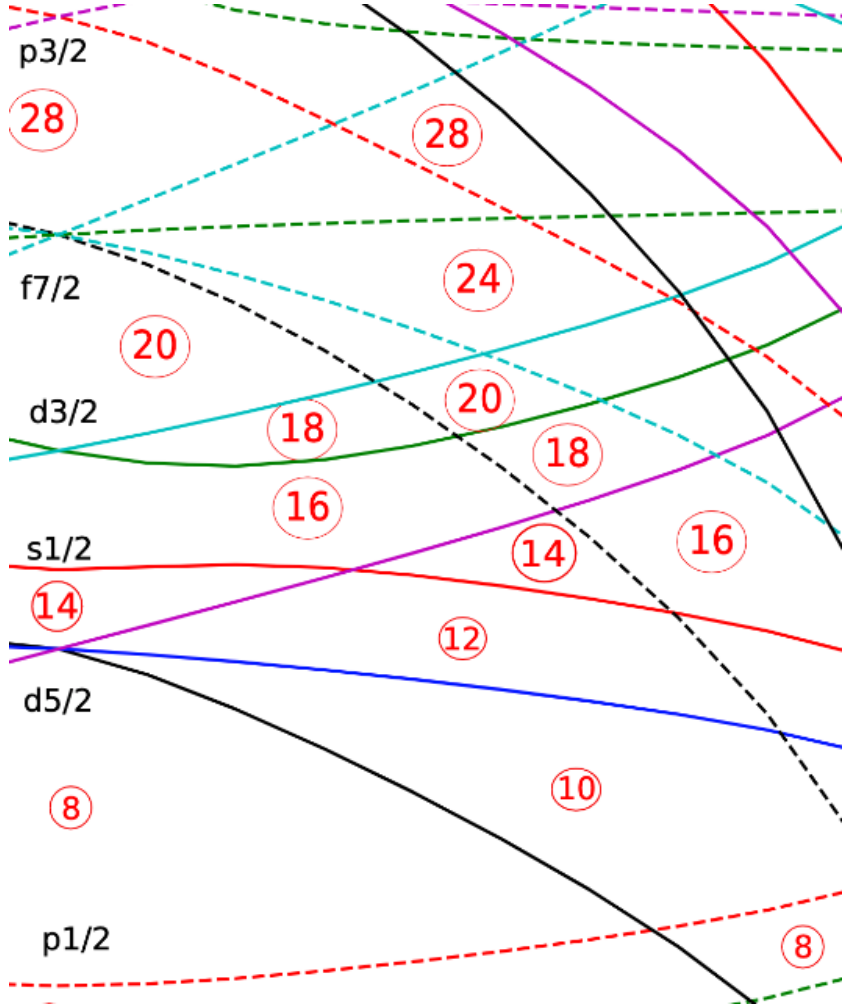


EM(1.8/2.0), hw=14MeV

The band structure of Ne determined by the unpaired neutrons

Rotational Band of odd-mass Mg isotopes

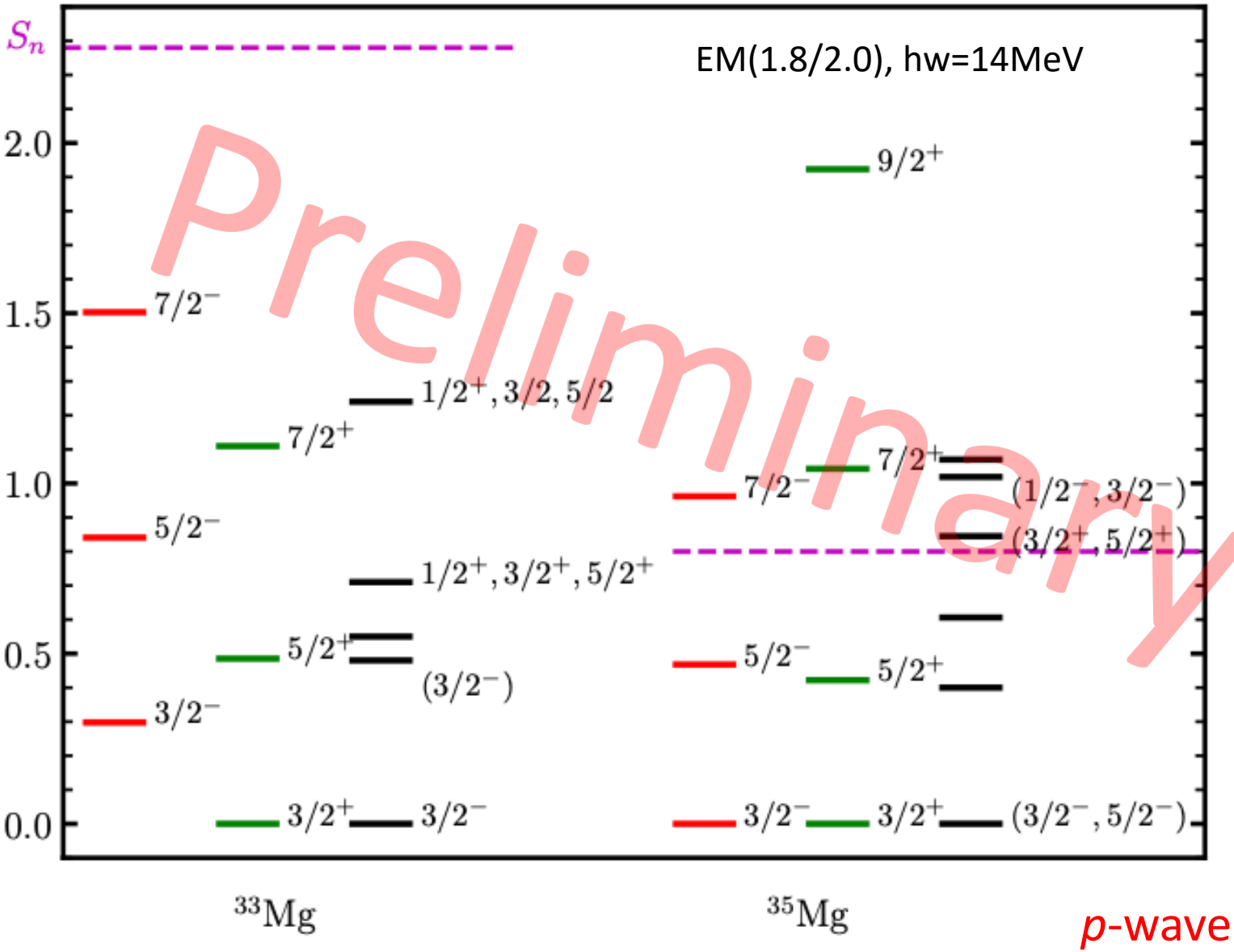


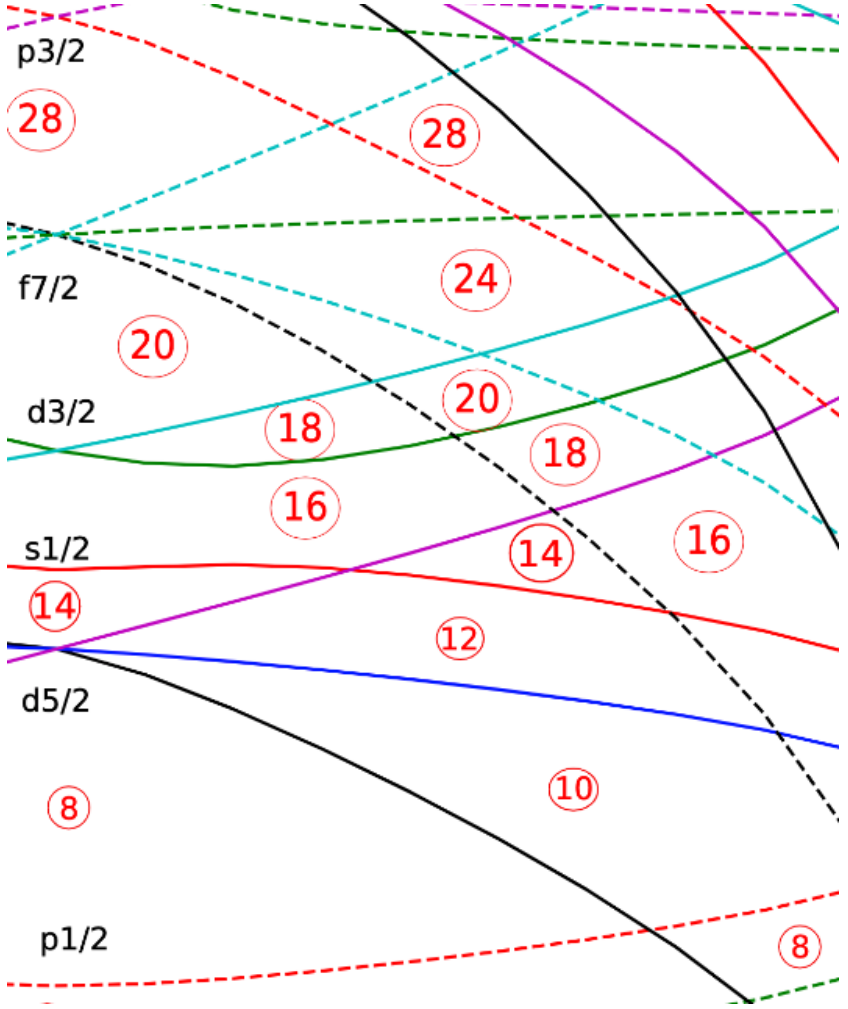


EM(1.8/2.0), hw=14MeV

The band structure of Mg determined by the unpaired neutrons

Interplay of deformation and continuum states





p-wave and *d*-wave continuum ?

Summary

- We developed a uniformed framework to calculate deformed nuclei from the ab-initio approach. even-even, odd-mass current stage.
- Static correlations lead to spontaneously symmetry breaking in the atomic nuclei. Projected coupled cluster method.
- By filling the unpaired particle to different single particle orbits, we get different rotational band.
- Preliminary result for the odd-mass, Ne, Na, and Mg.

Outlook:

- Including continuum effects to determine the g.s band head
- Developing multi-reference method.

$$\mathcal{H}\mathcal{N}\begin{pmatrix} e^{T_a}|\ \rangle \\ \cdots \\ e^{T_b}|\ \rangle \end{pmatrix} = E\mathcal{N}\begin{pmatrix} e^{T_a}|\ \rangle \\ \cdots \\ e^{T_b}|\ \rangle \end{pmatrix}$$

Thanks!