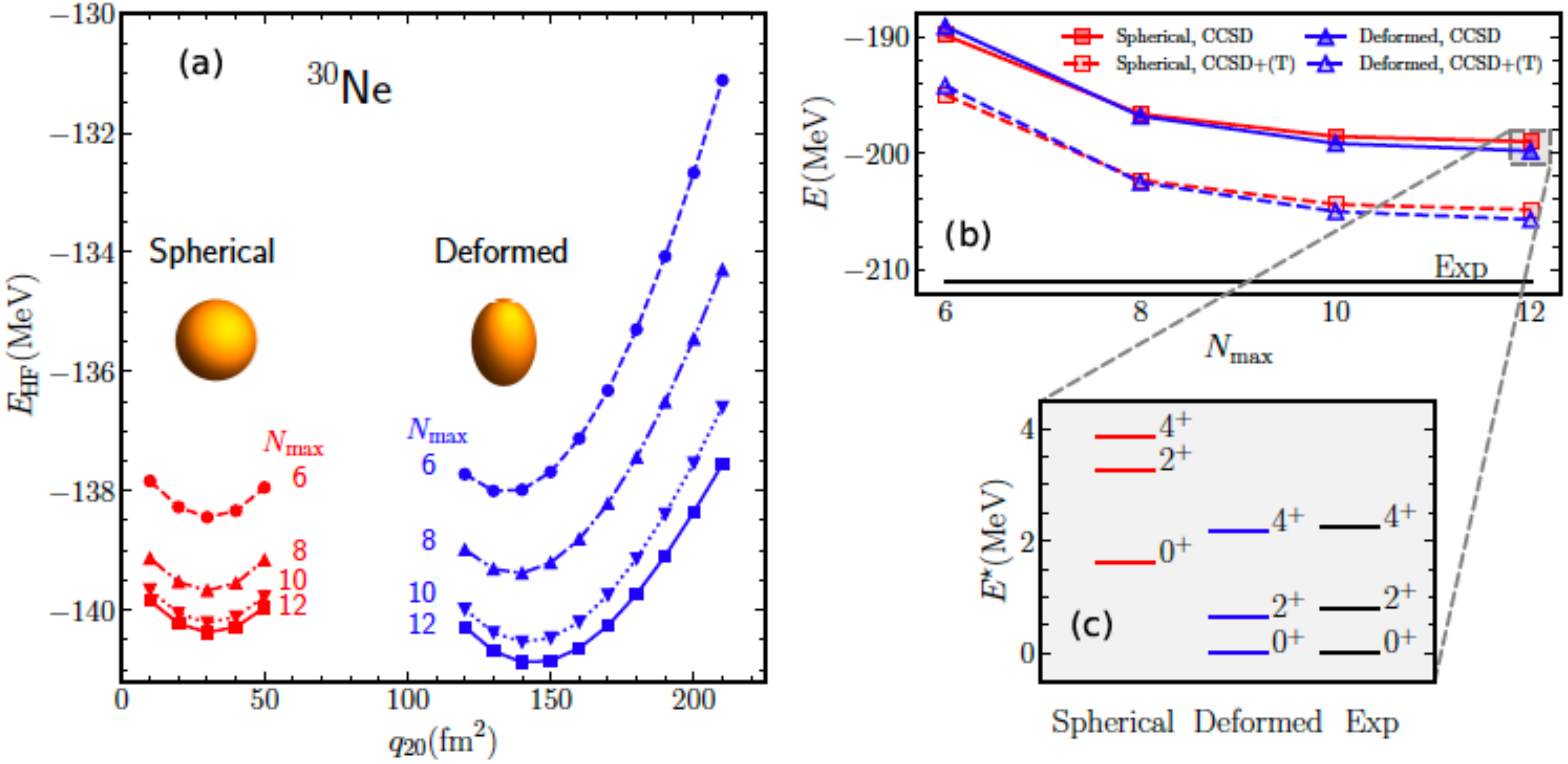
Low-lying spectroscopy of nuclei via coupled cluster techniques



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ESNT workshop on **"Nuclear ab initio spectroscopy"**

May 21-24, 2024

Work supported by the US Department of Energy

SciDAC Scientific Discovery through Advanced Computing

NUCLEI Nuclear Computational Low-Energy Initiative

Happy Birthday, Gaute!

Thank you for two decades of most exciting and productive collaboration!

Today’s menu

- Baishan Hu, Zhonghao Sun, G. Hagen, TP, *Ab initio computations of strongly deformed nuclei around ^{80}Zr*, arXiv:2405.05052
- Zhonghao Sun, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, TP, *Multiscale physics of atomic nuclei from first principles*, arXiv:2404.00058
- B. Acharya, B. S. Hu, S. Bacca, G. Hagen, P. Navrátil, TP, *The magnetic dipole transition in ^{48}Ca*, arXiv:2311.11438

→ Zhonghao Sun’s talk

Multiscale problem:

The bulk of the binding energy is from short-range correlations
Symmetry projection accounts for small details

Coester and Kümmel (1960), "Short-range correlations in nuclear wave functions"
Lipkin (1960): "Collective motion in many-particle systems: Part 1. the violation of conservation laws"

	E_{HF}	$E_{CCSD(T)}$	$E_{Proj.}$	$\langle J_{HF}\rangle$	$\langle J_{CCSD(T)}\rangle$
^{8}Be	-16.74	-50.24	-53.57	11.17	5.82
^{20}Ne	-59.62	-161.95	-164.21	21.26	12.09
^{34}Mg	-90.21	-264.34	-265.84	22.62	15.03

Data from Hagen et al., Phys. Rev. C 105, 064311 (2022)

Energy gain from symmetry projection is small and not size extensive

Multiscale problem:

The bulk of the binding energy is from short-range correlations
Symmetry projection accounts for small details

Nuclear superfluidity

	E_{BHF}	E_{BCC}	$E^{estim.}_{Proj.}$	$\langle \Delta N^2 \rangle$
^{74}Ni	-447.7	-608.3	-609.0	5.1
^{124}Sn	-759.9	-1034.3	-1034.7	6.0

Data from Tichai, Demol, Duguet (2023)

Energy gain from symmetry projection is small and not size extensive

Emergent symmetry breaking is great

Points out the existence of universal long-range physics (“Nambu-Goldstone modes”)

1. Deformation (HF) → rotational bands
2. Broken phases (BHF) → pairing rotational bands
3. Broken parity → bands with opposite parities close in energy

Separation of scales enable construction of effective theories

Broken symmetry	Tool	Phenomena	Low-lying excitations	Energy gain from symmetry projection	Energy scale (rare earth region)	Number of participating nucleons
SO(3)	HF	Deformation Rotational bands	$\frac{1}{2a}I(I+1)$	$\frac{1}{2a}\langle I^2\rangle$	$\frac{1}{2a}\sim 13\text{keV}$	A
U(1)	HFB	Superfluidity Pairing rotational bands	$\frac{1}{2a}(n-n_0)^2$	$\frac{1}{2a}\langle\Delta n^2\rangle$	$\frac{1}{2a}\sim 0.2\text{ MeV}$	$A^{1/3}\dots A^{2/3}$

Short-range correlations yield the bulk of the binding energy

… because the nuclear force is short ranged (Bethe 1936)

$$E_{\rm corr} = \sum_{ia} t_i^a \langle i|H_{\rm no}|a\rangle + \frac{1}{4}\sum_{ijab}\left(t_{ij}^{ab} + t_i^a t_j^b - t_i^b t_j^a\right)\langle ij|H_{\rm no}|ab\rangle$$

$\propto \delta_{x_i}^{x_a}$ ← locality

$\sum_{ijab}$ ← effectively $\sum_{j=1}^{A} \cdots$

$\propto \delta_{x_i}^{x_j}\delta_{x_b}^{x_a}\,\delta_{x_i}^{x_a}$ ← short range ($\delta_{x_i}^{x_j}$, $\delta_{x_b}^{x_a}$), locality ($\delta_{x_i}^{x_a}$)

$\propto A$

How do long-range parts of T_2 or $T_3, T_4, \cdots$ contribute: They modify the short-range part of T_2

$$\left(e^{-T} H e^{T}\right)\Big|_{ij}^{ab} = H_{ij}^{ab} + [H,T] + \cdots = 0$$

Consequence: The long-range parts of T_α contribute little to the energy and are hard to get.
→ Failure of spherical coupled cluster and VS-IMSRG to account for $B(E2)$.

Nuclear deformation

Spherical shell model vs Nilsson model

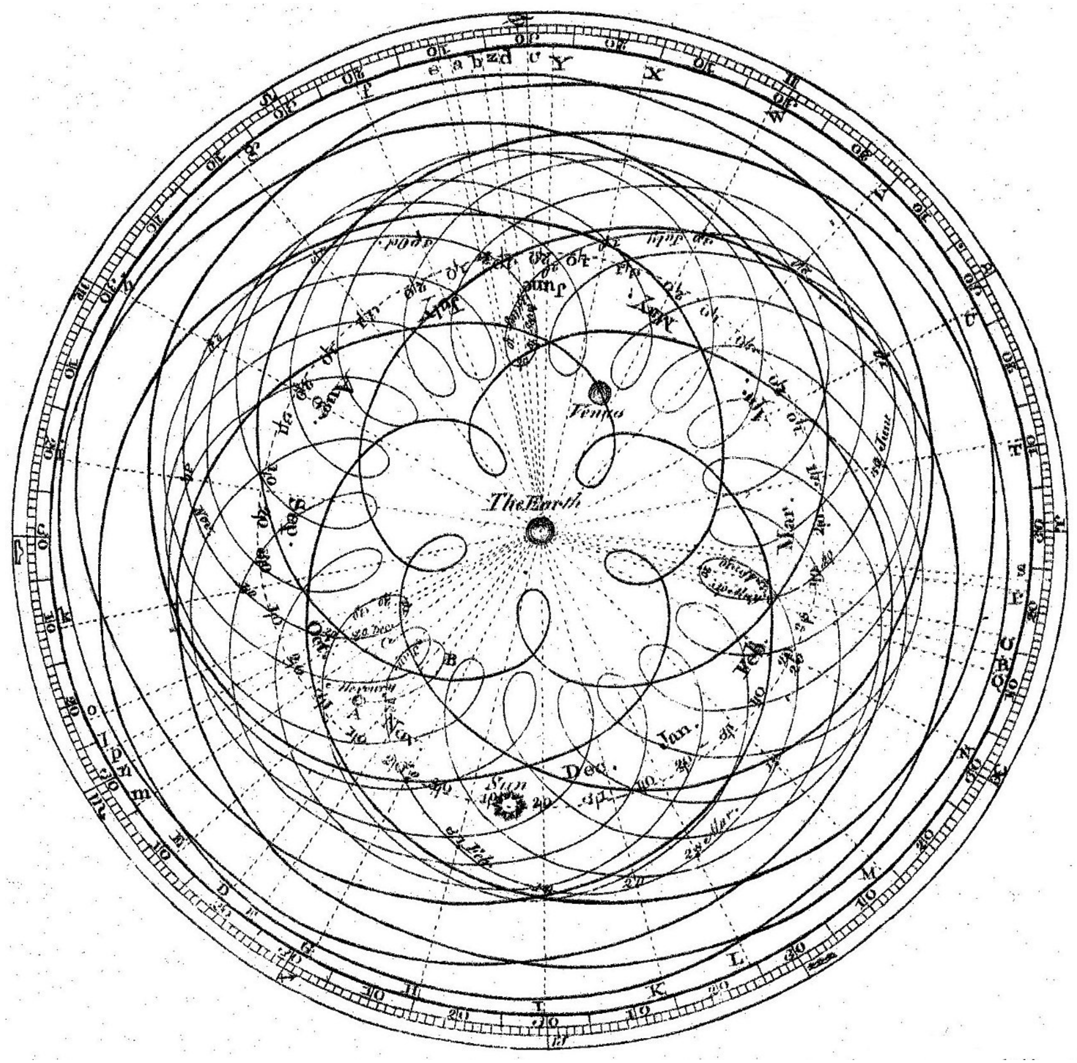
- 🙂 Predicts excitations and spins of closed-shell nuclei +/- 1 nucleon
- 🙂 Provides us with a basis
- 🙂 Elliott's SU(3) explains how quadrupole collectivity arises in a spherical HO basis
- 😩 Not simple: Uses SU(3) Clebsch-Gordan coefficients and coefficients of fractional parentage to construct SU(3) states
- 😩 Complicates interpretation of deformation: "np-nh excitations, parity inversion, monopole vs multipole"

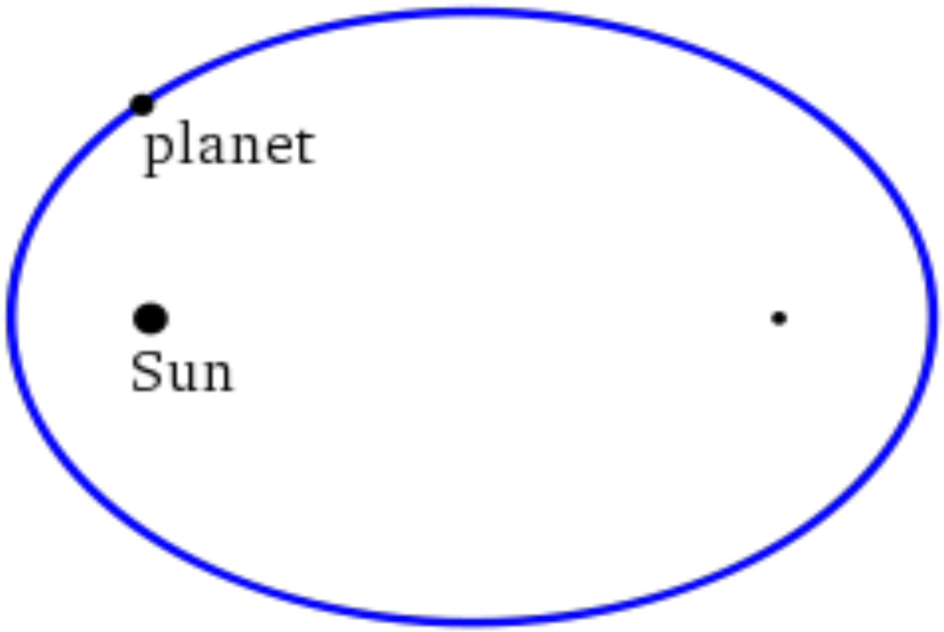
- 😌 Predicts spins of odd-mass nuclei and deformations of any nucleus
- 😌 Explains shape coexistence
- 😌 Based on an adiabatic picture: fast intrinsic degrees of freedom vs slow overall rotations → effective theories
- 😌 Conceptually simple for most nuclei on the chart
- 😩 Requires symmetry projection

Allez les Bleus!

Nuclear deformation

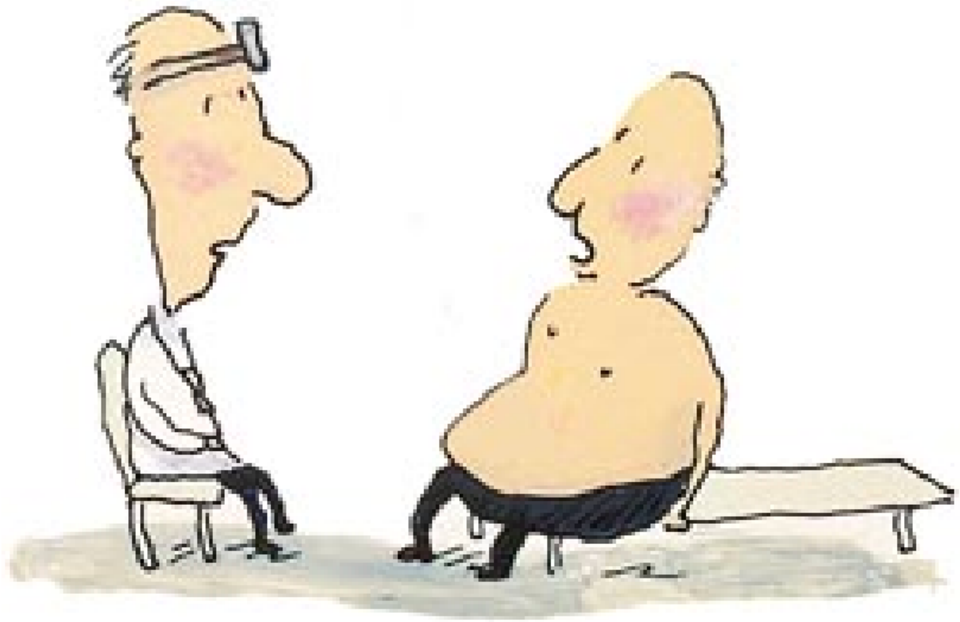
Spherical shell model vs Nilsson model





Low resolution makes physics easier + efficient

- Weinberg's Third Law of Progress in Theoretical Physics: *"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"*
- There's an old joke about a doctor and patient . . .



Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.

Our approach

Short-range correlations followed by long-range ones

1. Start from an axially symmetric reference state (wished we broke more)
2. Include short-range (“dynamical”) correlations via coupled cluster method
   - captures UV physics right

😩 Symmetry projection includes collective effects
   - captures IR physics

Bally, Duguet, Ebran, Frosini, Hergert, Porro, Rodriguez, Soma, Yao, …

1. Start from a symmetry broken (J, J_z, N, Z, Π) reference state
2. Perform GCM and restore symmetries (“ab initio to long-range physics”)
   - captures IR physics

😩 MBPT2 includes dynamical correlations
   - captures UV physics

Shape coexistence

States with different shapes that are close in energy

Reviews: Heyde and Wood, Rev. Mod. Phys. 83, 1467 (2011); Gade and Liddick, J. Phys. G 43, 024001 (2016); Bonatsos, et al., Atoms 11, 117 (2023).

Observed in ^{30}Mg by Schwerdtfeger et al., Phys. Rev. Lett. 103, 012501 (2009) and in ^{32}Mg by Wimmer et al., Phys. Rev. Lett. 105, 252501 (2010).

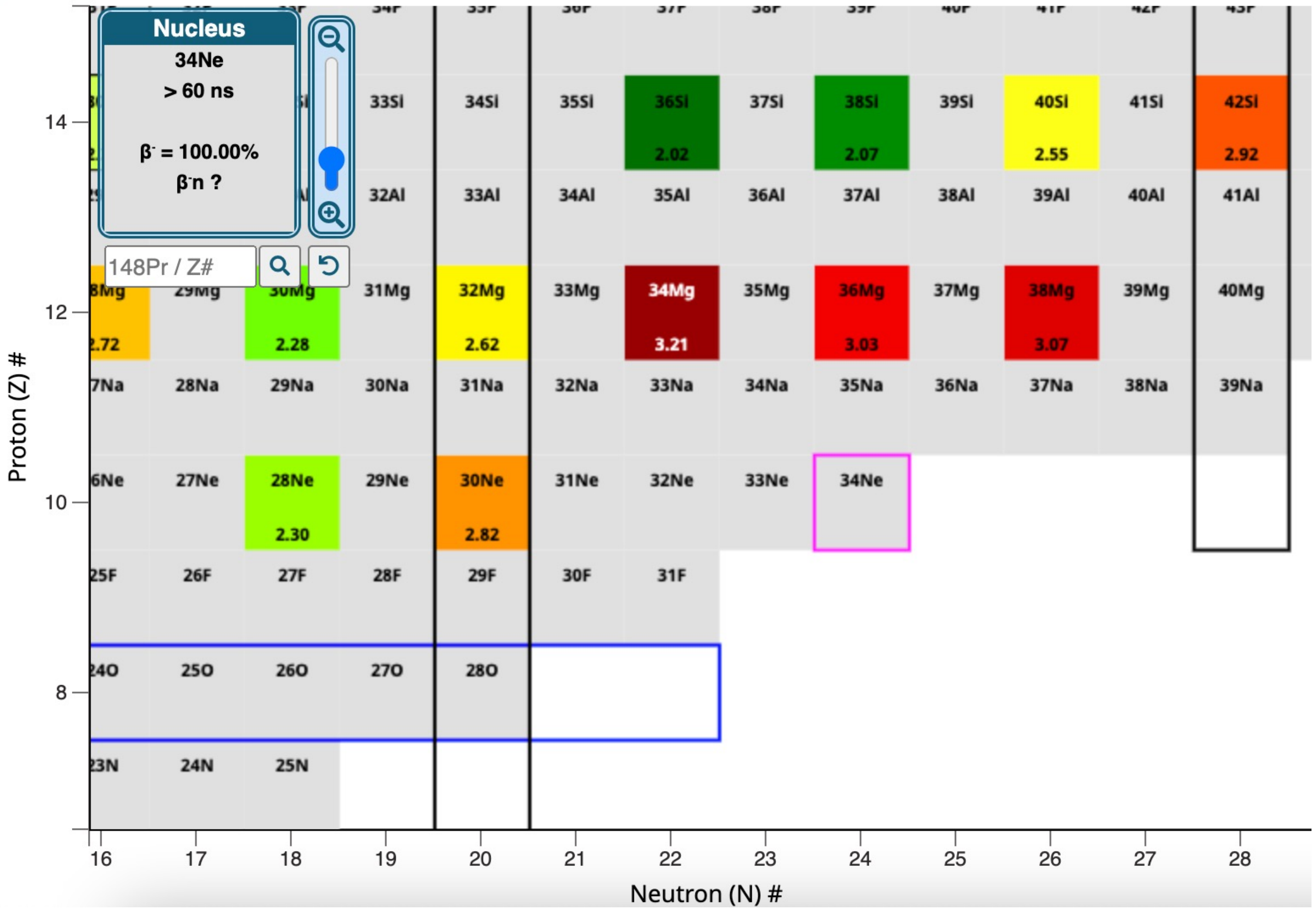
Theoretical descriptions: Reinhard et al., Phys. Rev. C 60, 014316 (1999); Rodríguez-Guzmán, Egido, and Robledo, Nucl. Phys. A 709, 201 (2002); Péru and Martini, Eur. Phys. J. A 50, 88 (2014); Caurier, Nowacki, and Poves, Phys. Rev. C 90, 014302 (2014); see also Tsunoda et al., Nature 587, 66 (2020).

Neutron-rich nuclei beyond $N \geq 20$ are deformed

$$R_{4/2} \equiv \frac{E_{4^+}}{E_{2^+}}$$

$R_{4/2} = 10/3$ for a rigid rotor

Simple picture: Spherical states (magic $N = 20$ number in the traditional shell model) coexist with deformed ground states



Poves & Retamosa (1987); Warburton, Becker, and Brown (1990); …

How do we compute these nuclei?

Input: Nucleon-nucleon and three-nucleon forces from chiral effective field theory: 1.8/2.0(EM) from [Hebeler at al, Phys Rev C (2011)]; and an ensemble of interactions used for computations of ^{28}O [Kondo et al, Nature 2023]; large model space consisting of 13 harmonic oscillator shells

1. Axially-symmetric Hartree-Fock computations with quadrupole constraint
2. Normal-ordered two-body approximation [Hagen et al 2007; Roth et al 2012; Ripoche et al 2020]
3. Coupled-cluster computations based on deformed reference state
4. Angular momentum projection of deformed coupled-cluster state

Projection onto good angular momentum

Projected energies

$$E^{(J)} = \frac{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{H}(\beta)}{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{N}(\beta)}$$

We follow:

- Qiu, Henderson, Scuseria, …
- Tsuchimochi & Ten'no
- Duguet, …

Approach: Kernels from coupled cluster theory;
Thouless theorem: $\langle\Phi|R(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V$ with de-excitation operator V.

$$\mathcal{N}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V e^T|\Phi\rangle\,,$$

$$\mathcal{H}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V He^T|\Phi\rangle$$

Key: Disentangled formalism [Qiu et al] $\quad e^V e^T|\Phi\rangle \equiv e^{W_0+W_1+W_2+\cdots}|\Phi\rangle$

How to compute $e^{V(\beta)}e^{T} = e^{W_0(\beta)+W_1(\beta)+W_2(\beta)+\dots}$?

Qiu, Henderson, Zhao, Scuseria, JCP (2017):
Take derivative w.r.t. β and solve differential equatio
with $W_i(\lambda = 0) = T_i$; integrate from $\beta = 0 \rightarrow \pi$

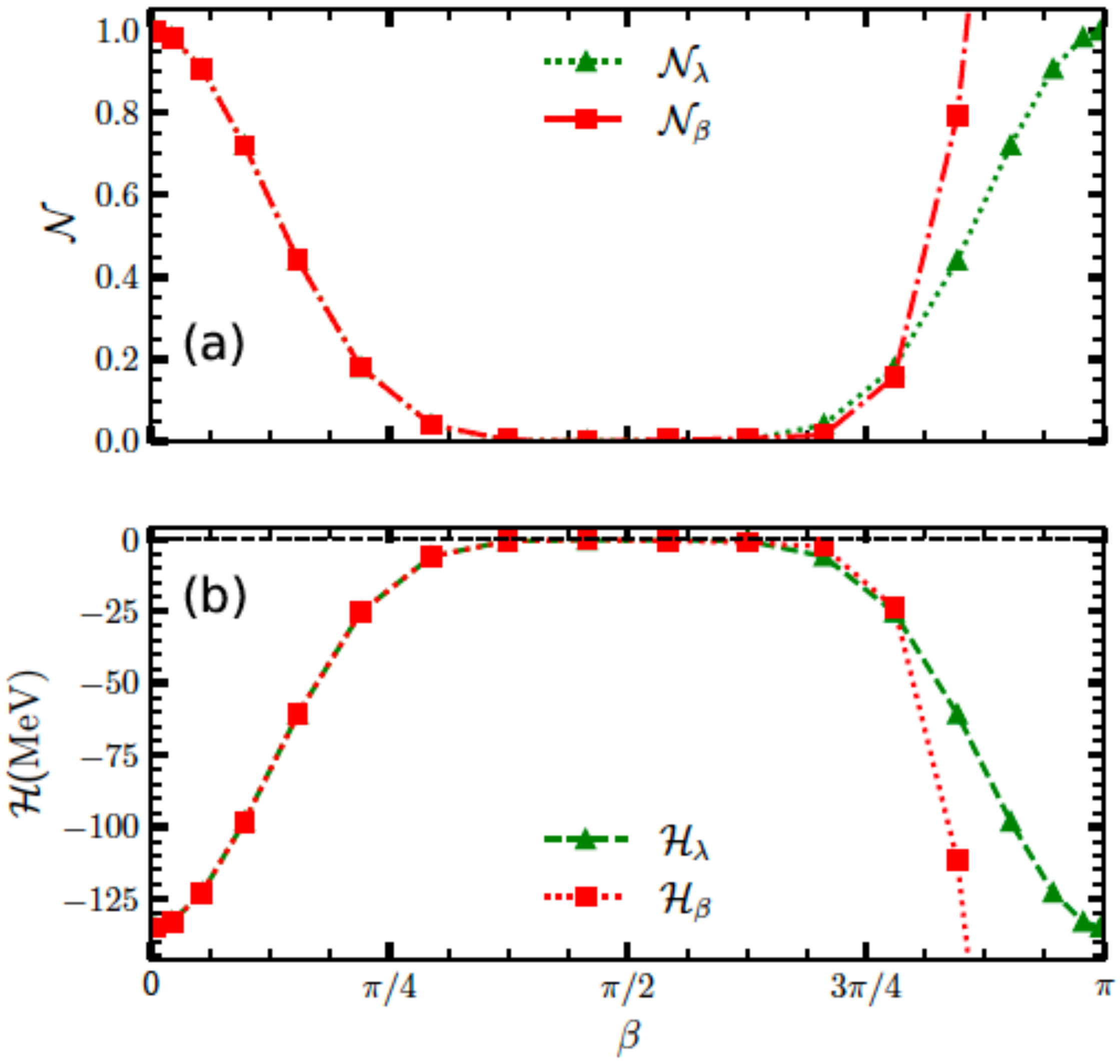
$$e^{V(\beta)}e^{T} = e^{W_0(\beta)+W_1(\beta)+W_2(\beta)+\dots}$$

This leads to unsymmetric kernels.

Better: Zhonghao Sun et al. (2024)

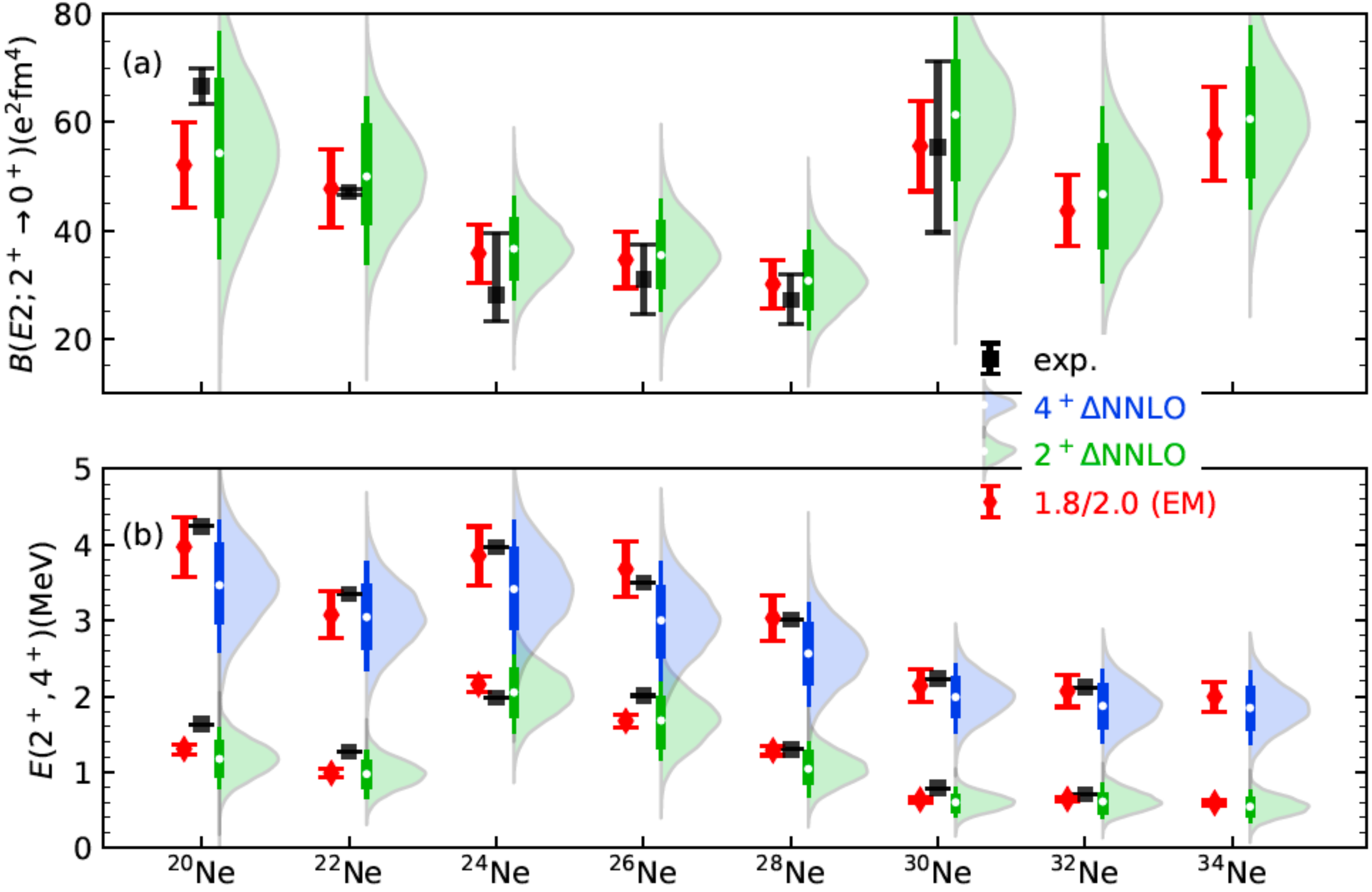
$$e^{\lambda V}e^{T} = e^{W_0(\lambda)+W_1(\lambda)+W_2(\lambda)+\dots}$$

For fixed β, take derivative w.r.t. λ and solve differential equations with $W_i(0) = T_i$; integrate from $\lambda = 0 \rightarrow 1$.

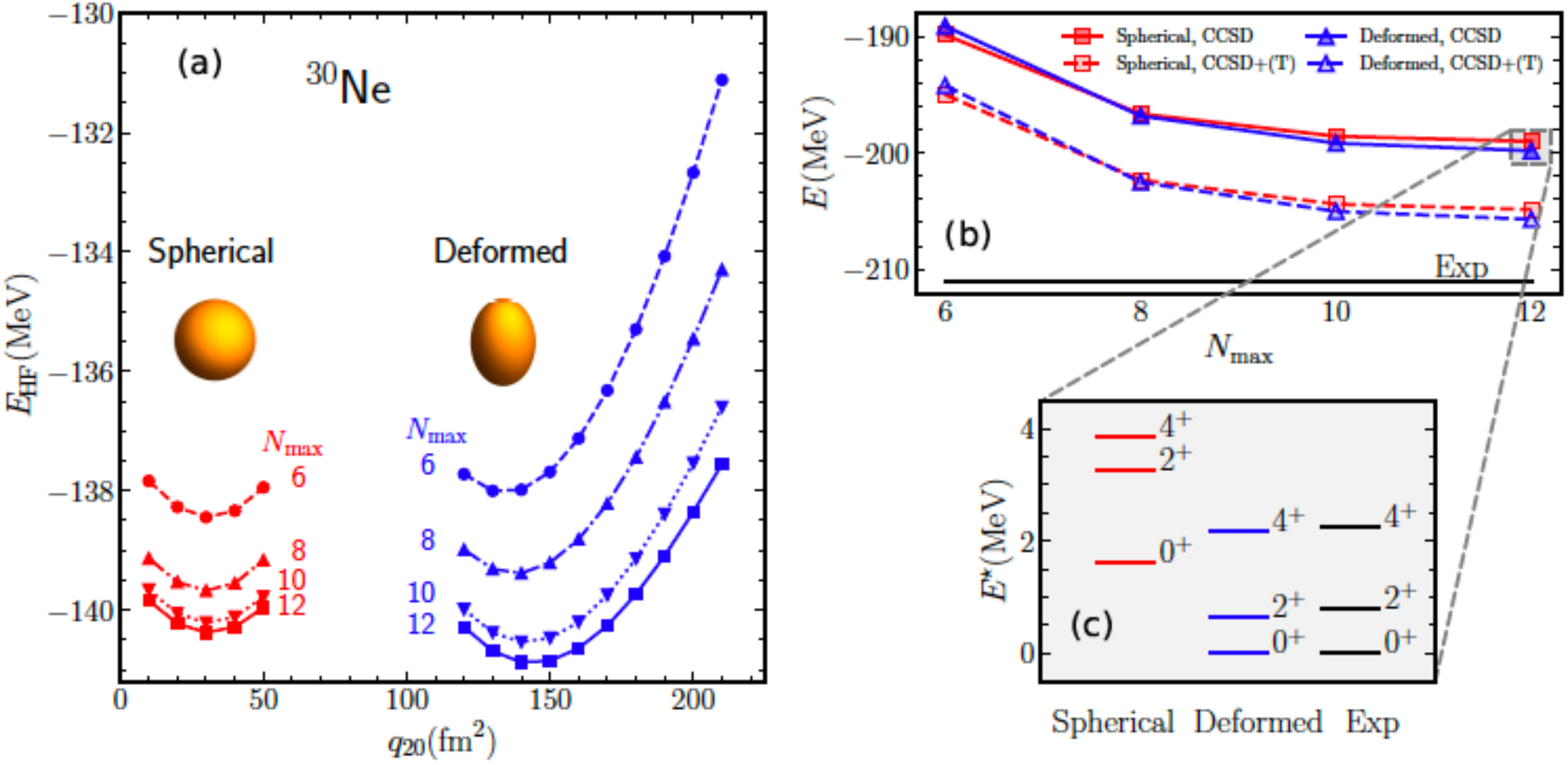


Zhonghao Sun et al., arXiv:2404.00058

Collectivity of neon nuclei

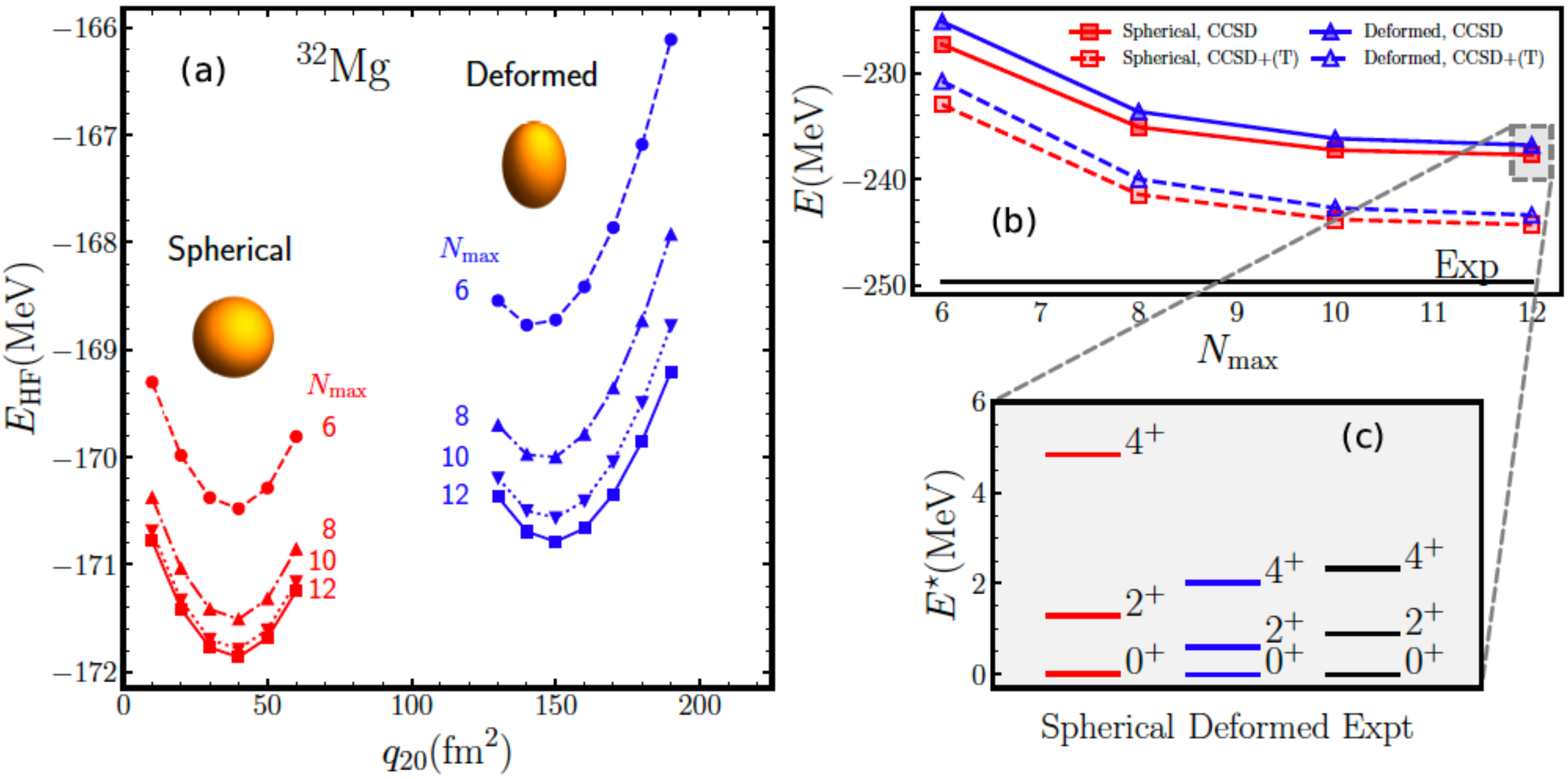


Prediction: Shape coexistence in ^{30}Ne



Zhonghao Sun et al., arXiv:2404.00058

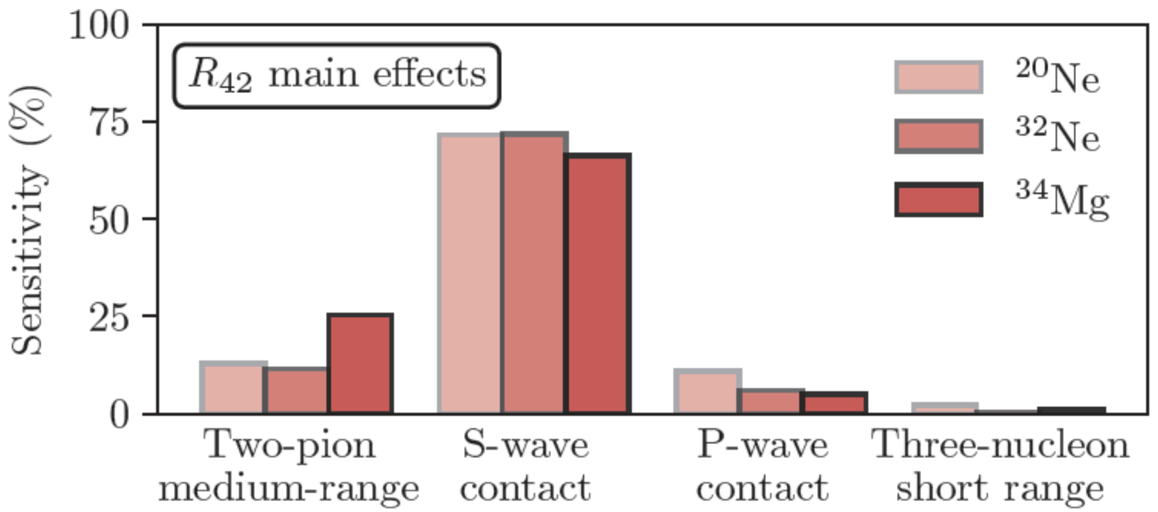
Confirmation: Shape coexistence in ^{32}Mg



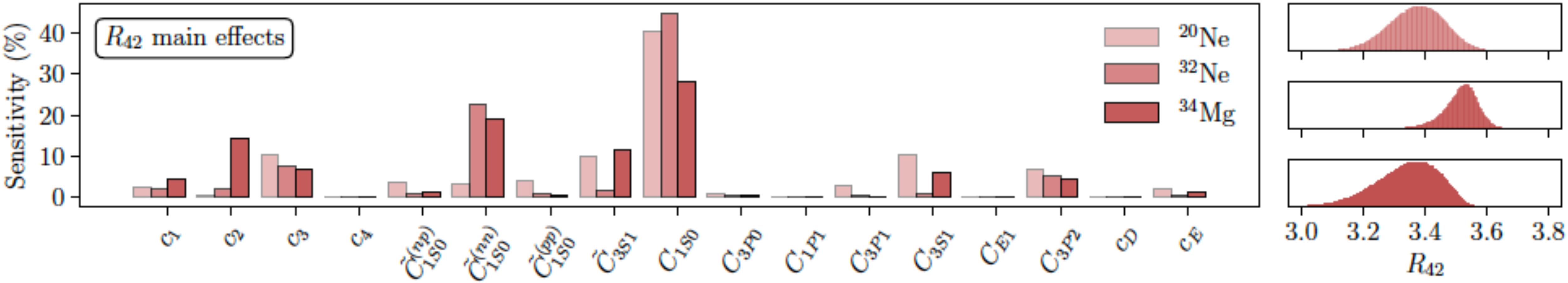
Zhonghao Sun et al., arXiv:2404.00058

What drives nuclear deformation?

Executive summary

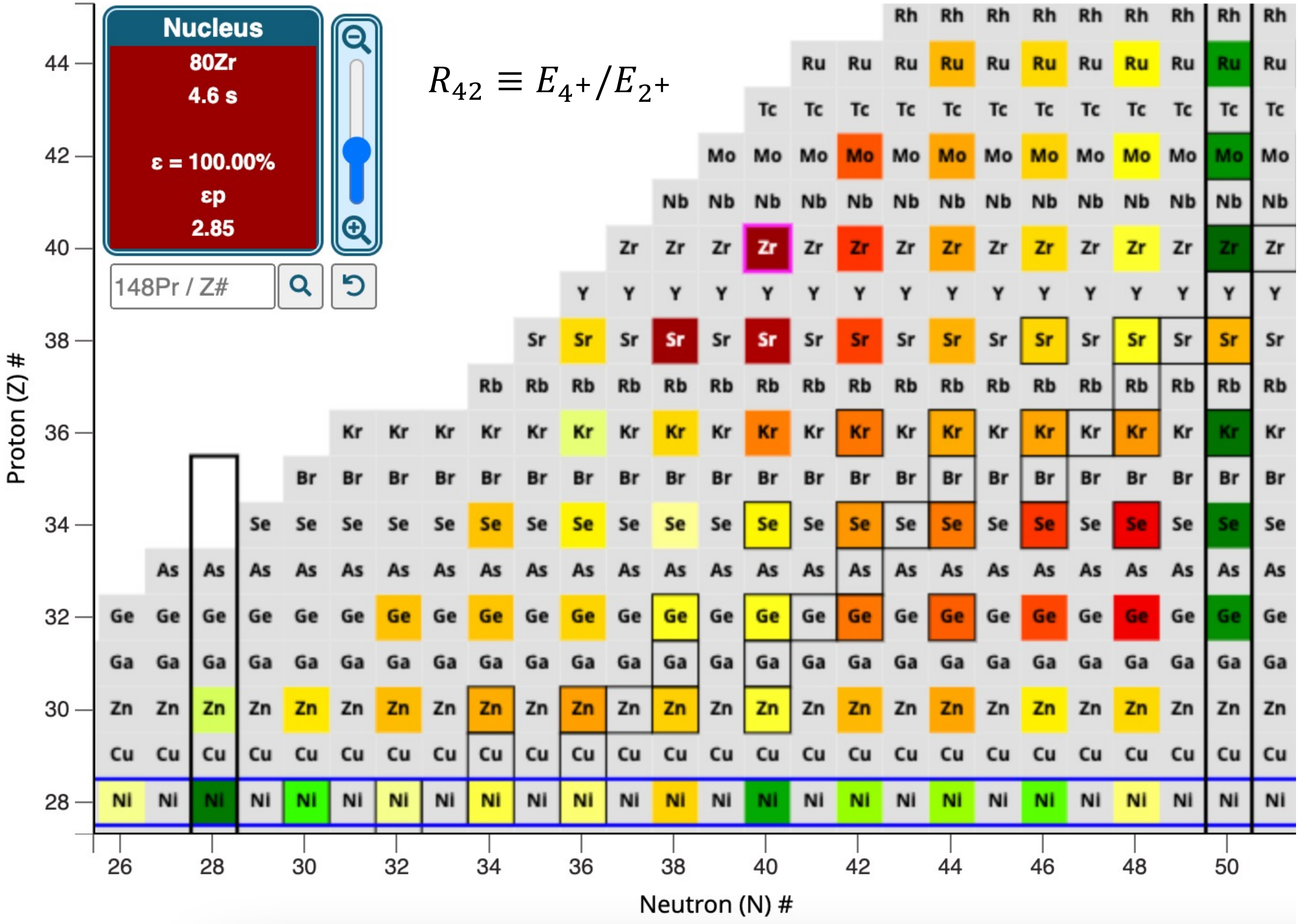


More detailed view



Zhonghao Sun et al., arXiv:2404.00058

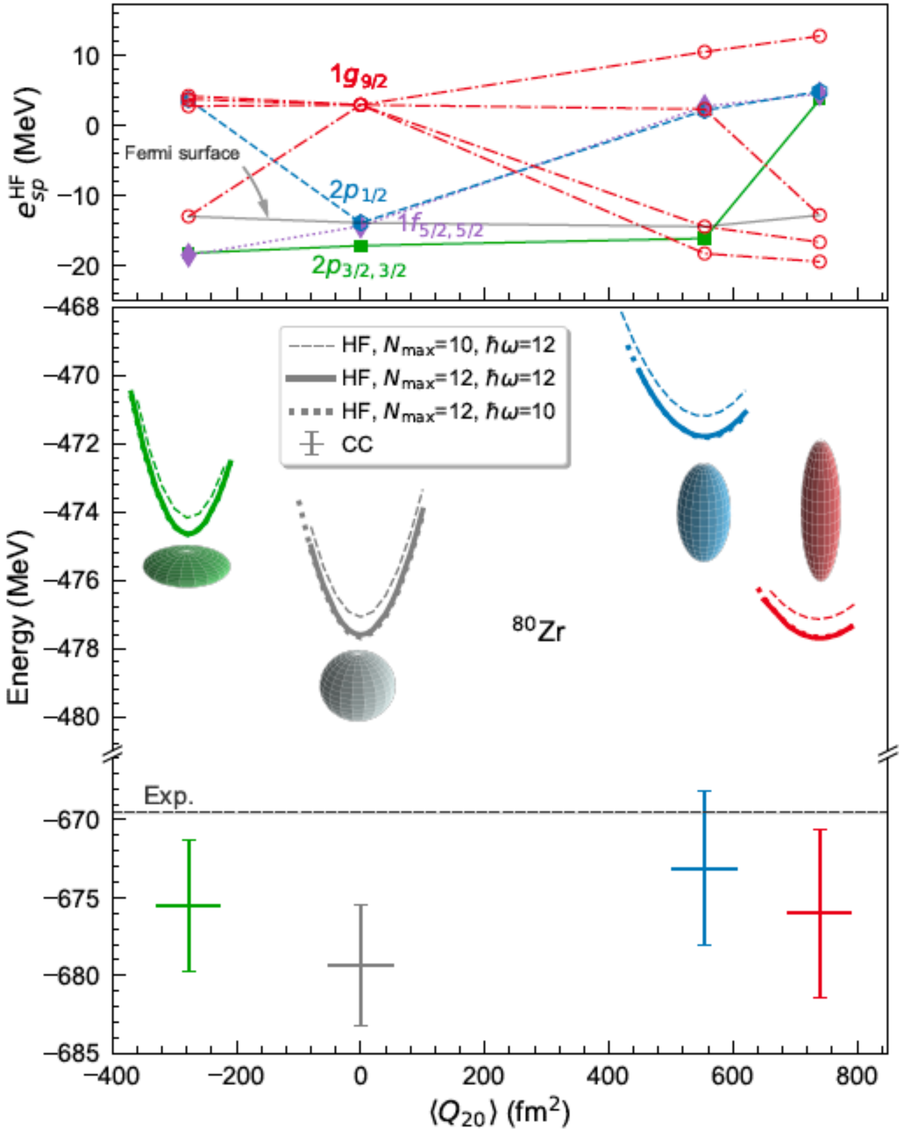
The region around ^{80}Zr



$$R_{42} \equiv E_{4^+}/E_{2^+}$$

Baishan Hu, Zhonghao Sun et al., arXiv:2405.05052

Shapes of ^{80}Zr



Quadrupole constrained HF computations

- several minima identified
- angular momentum projected

Shape coexistence identified

- coupled-cluster computations too uncertain to predict shape of ground state

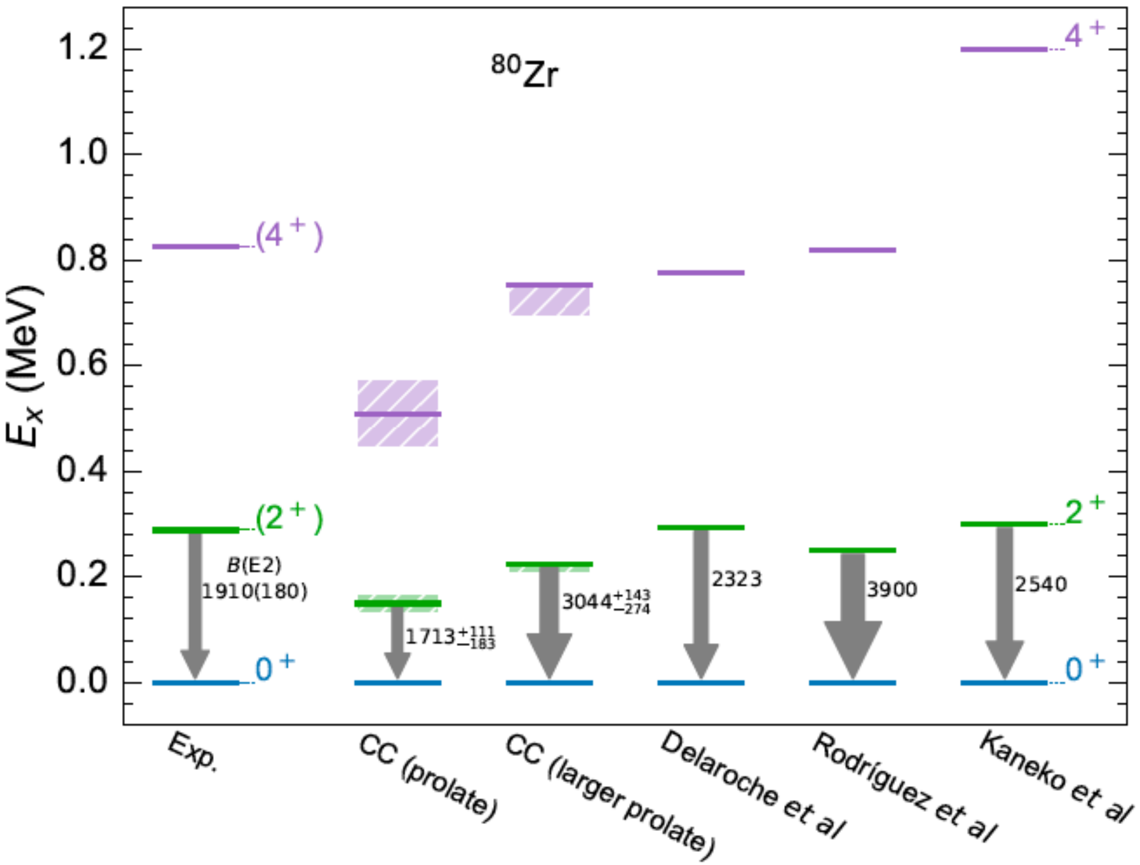
Used Miyagi (2023) for 3NFs in large model spaces

Fun fact: ^{80}Zr has higher energy than two ^{40}Ca nuclei

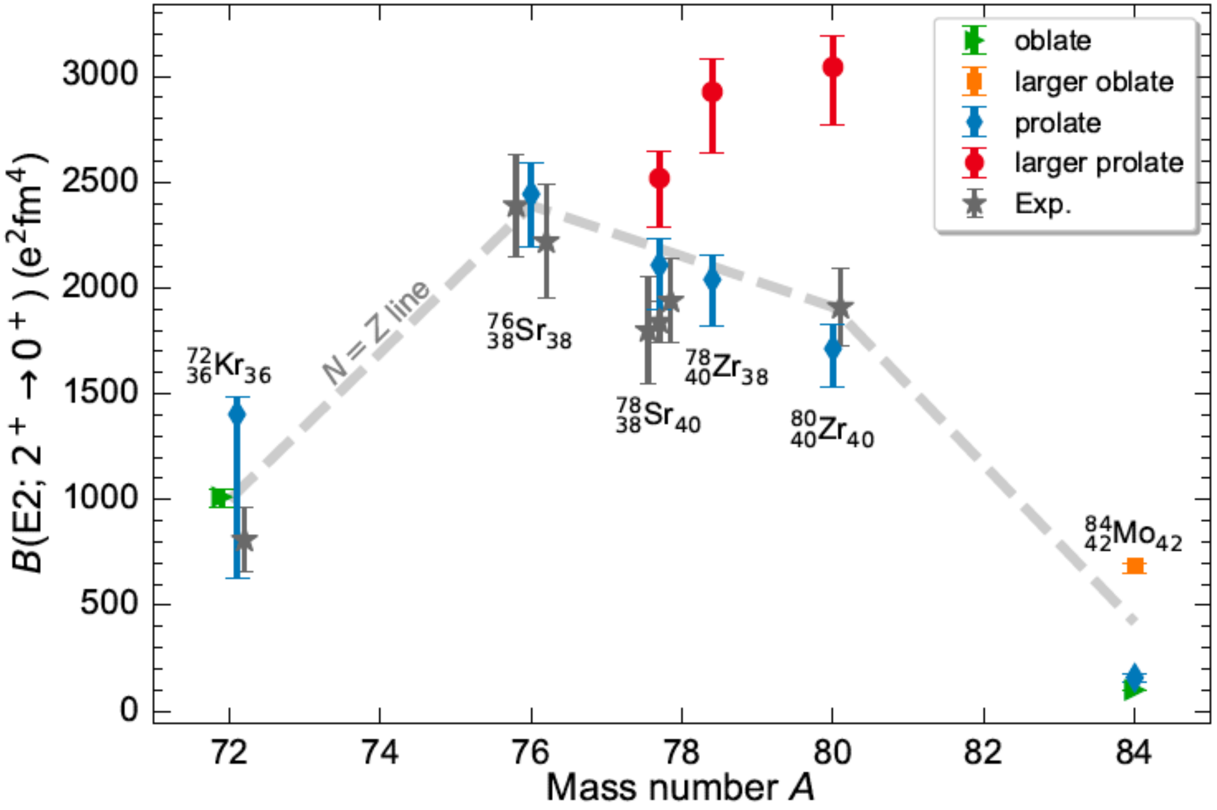
Baishan Hu, Zhonghao Sun et al., arXiv:2405.05052

The region around ^{80}Zr

Spectrum prefers larger prolate shape



$B(E2)$ prefers prolate band



Baishan Hu, Zhonghao Sun et al., arXiv:2405.05052

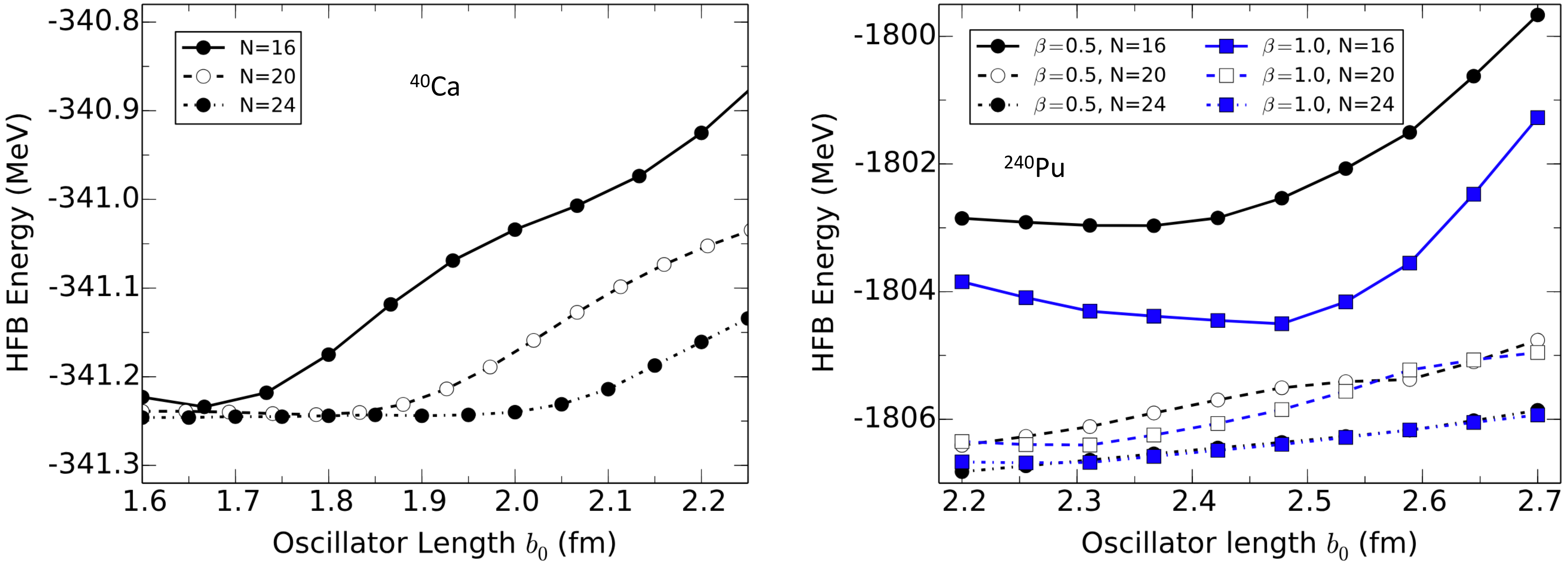
Ab initio comparable to mean field computations

Nucleus	Exp.	This work	Ref. [29]	Other
^{80}Zr	$1910(180)^a$	1713^{+111}_{-183} 3044^{+143}_{-274}	2323	3900^b 2540^f
^{78}Zr	not known	2040^{+118}_{-220} 2927^{+155}_{-288}	2504	
^{78}Sr	$1840(100)^a$	2108^{+121}_{-211} 2519^{+125}_{-228}	1989	2291^f
^{76}Sr	$2390(240)^a$	2444^{+145}_{-248}	2350	2175^f
^{72}Kr	$810(150)^c$ $999(129)^e$	1012^{+36}_{-50} 1403^{+84}_{-775}	819	763^d 1097^f

[29] = Delaroche et al, PRC (2010)
b = Rodriguez & Egido, Phys Lett B (2011)
d = Bender, Bonche, Heenen, PRC (2006)
f = Kaneko, Shimizu, Mizusaki, Phys Lett B (2021)

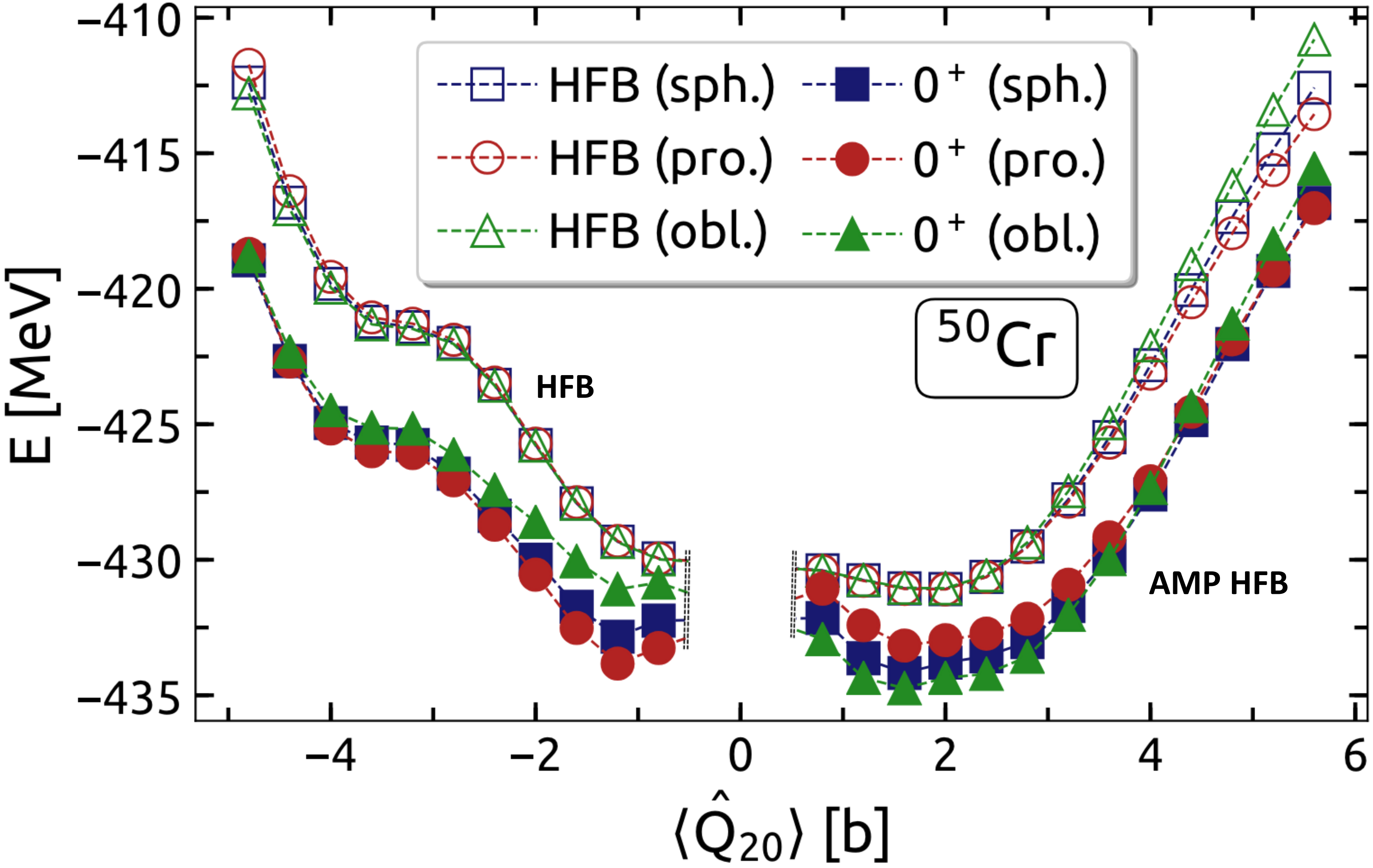
Baishan Hu, Zhonghao Sun et al., arXiv:2405.05052

Convergence of mean-field computations



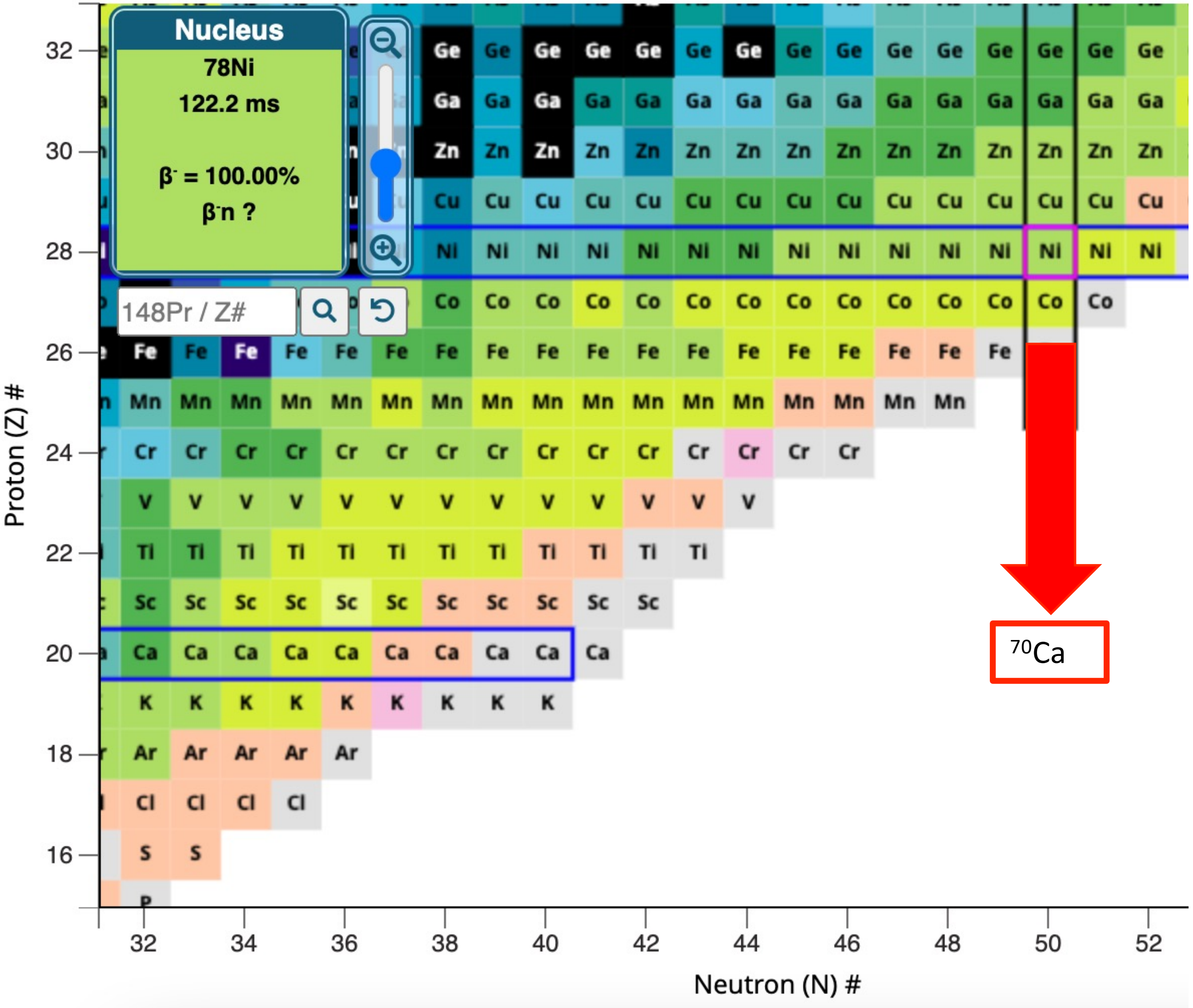
Schunck, McDonnell, Sarich, Wild, Higdon, J Phys G (2015)

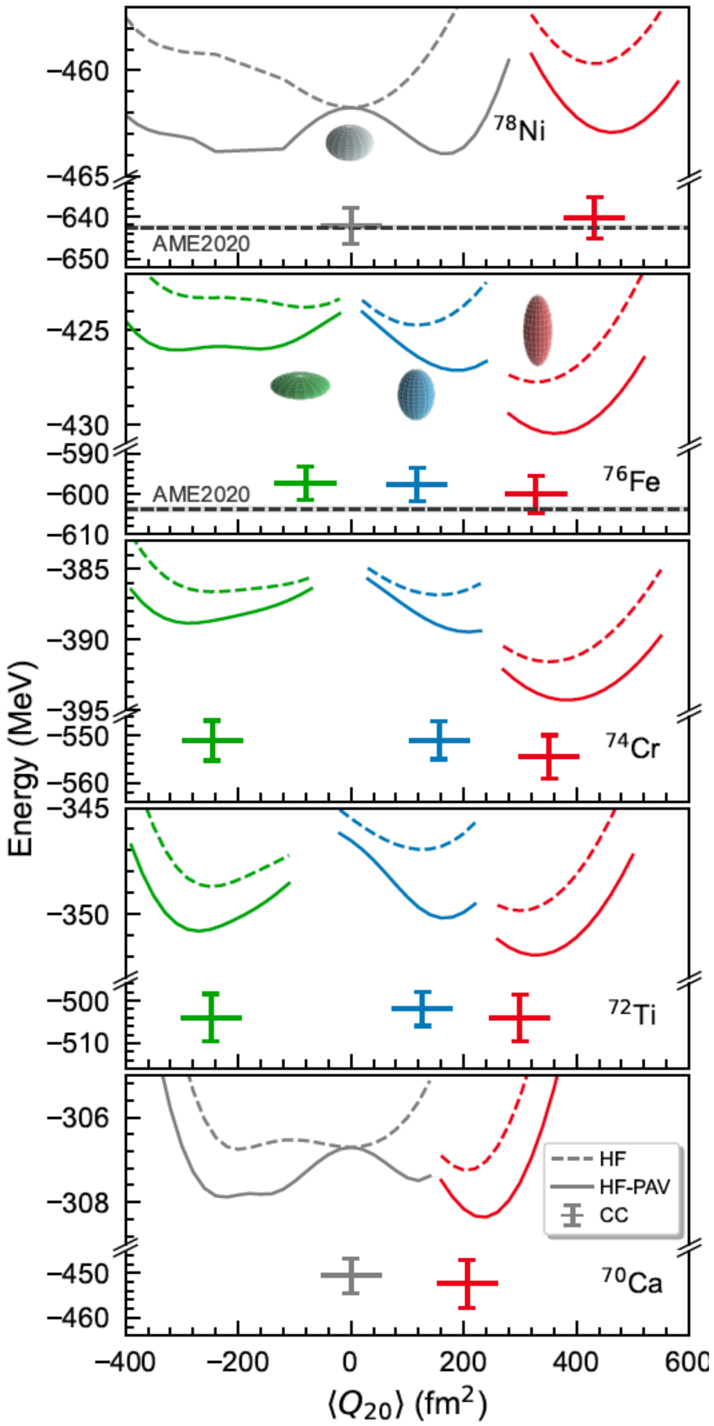
Convergence of mean-field computations



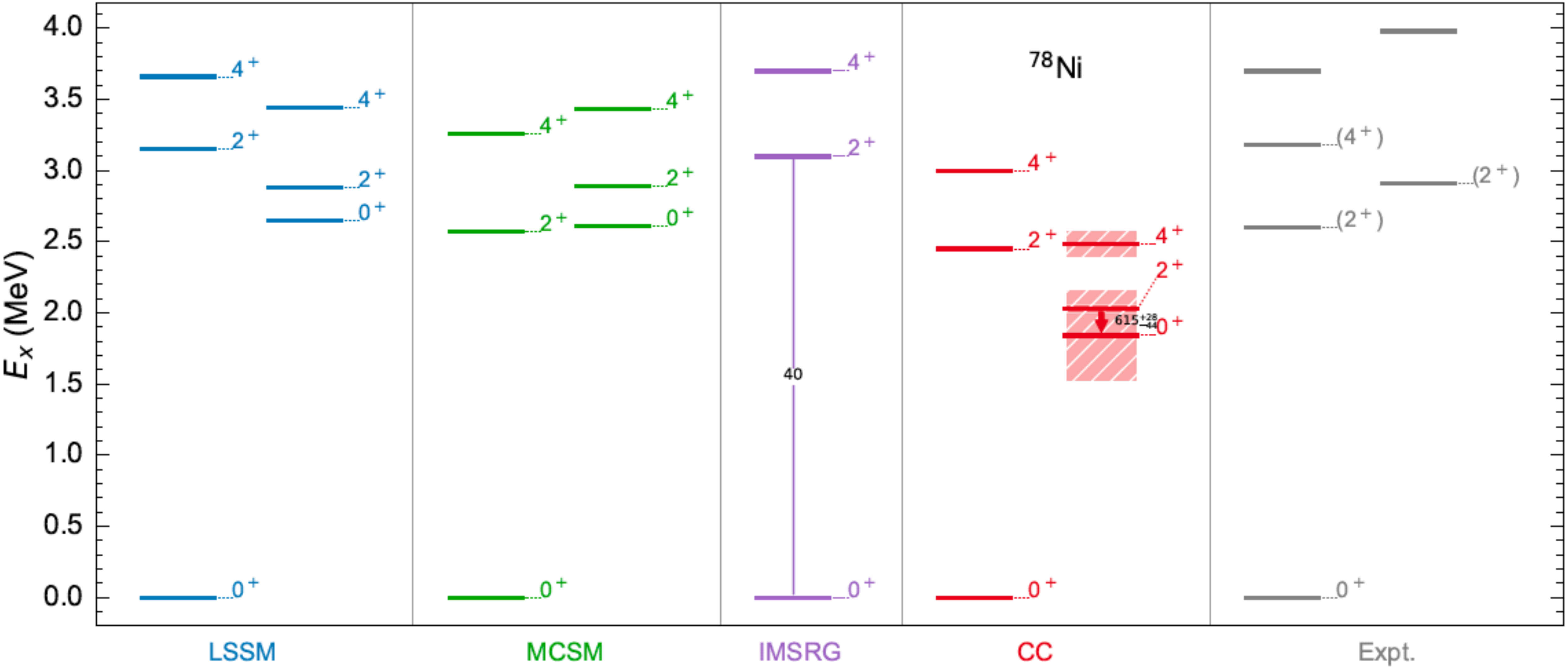
Marevic, Schunck, Ney, Navarro Pérez, Verriere, O'Neal, Comp. Phys. Comm. (2022)

South of ^{78}Ni





Structure of ^{78}Ni



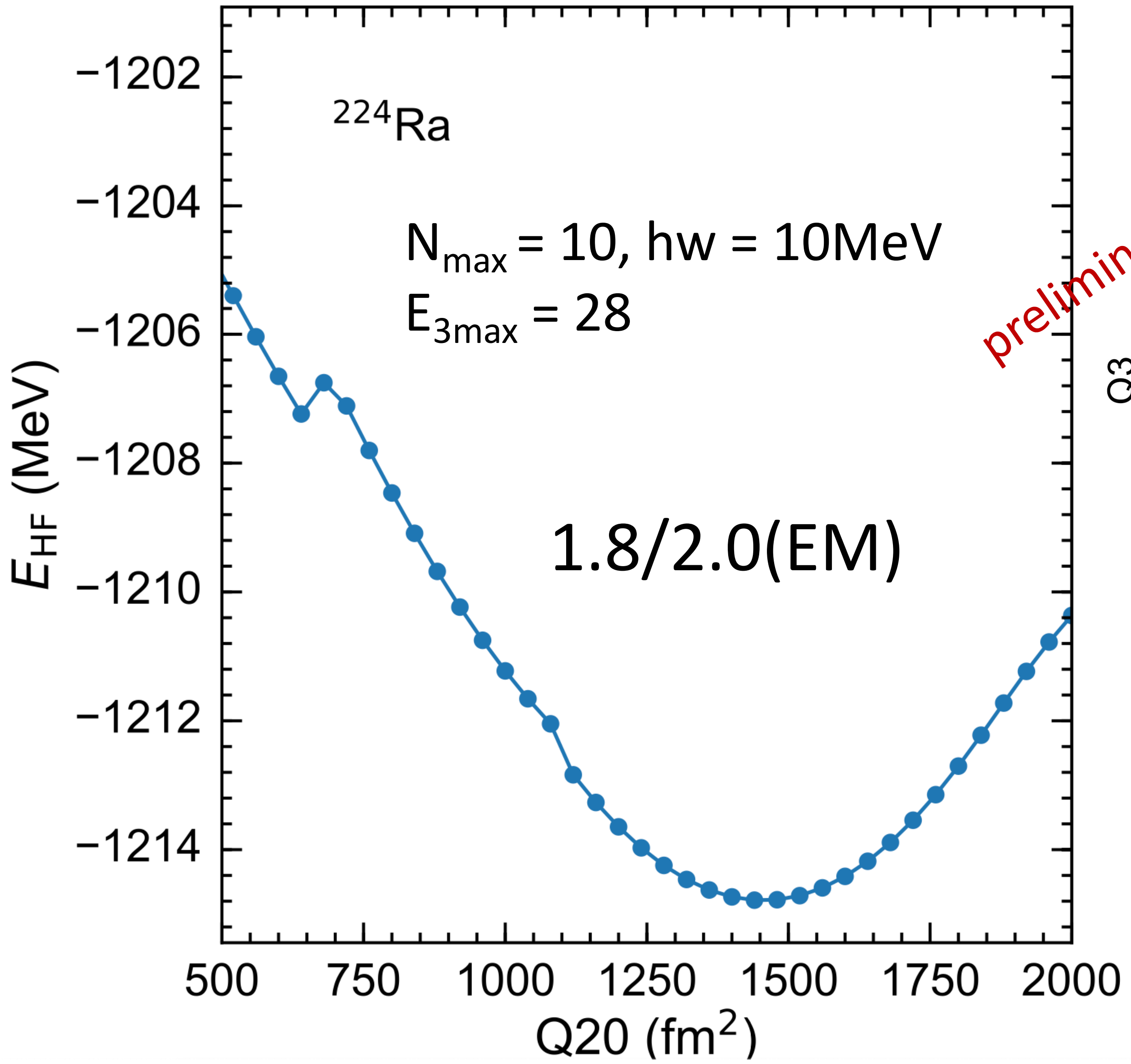
Nowacki, Poves, Caurier, Bounthong (2016)

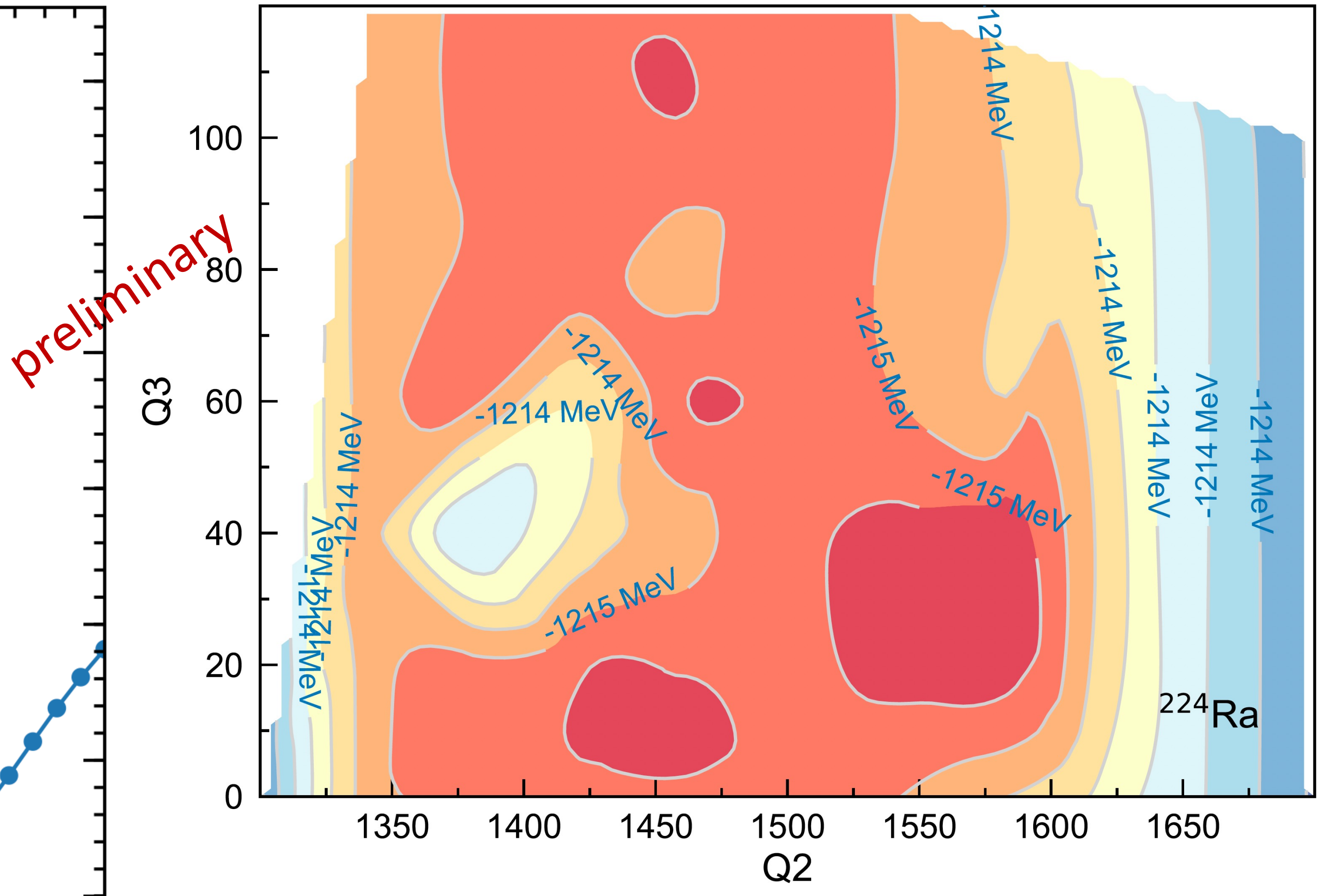
Taniuchi et al. (2019)

Tichai, Kapás, Miyagi, Werner, Legeza, Schwenk, Zarand (2024)

Taniuchi et al. (2019)

Towards coupled cluster computations of Schiff moments in radium nuclei

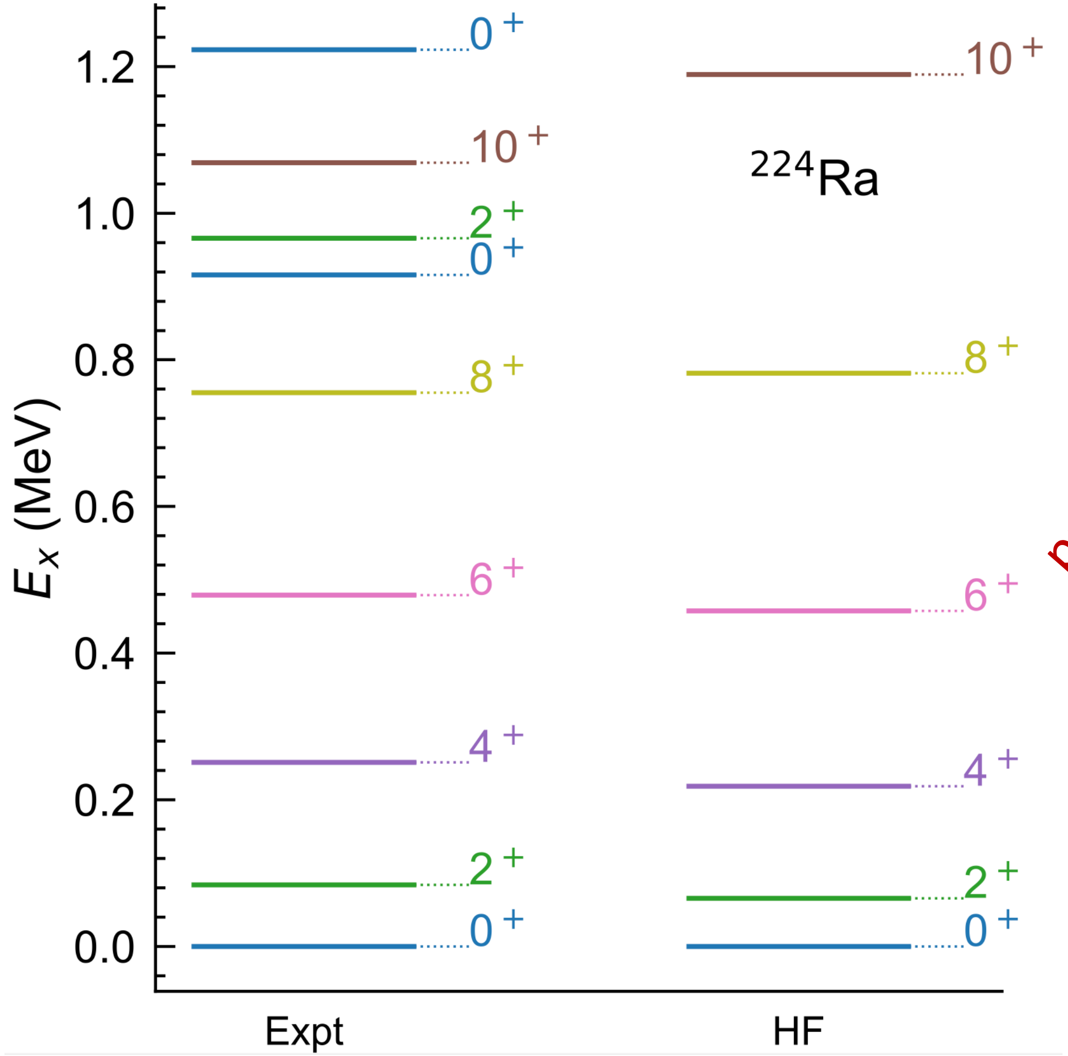


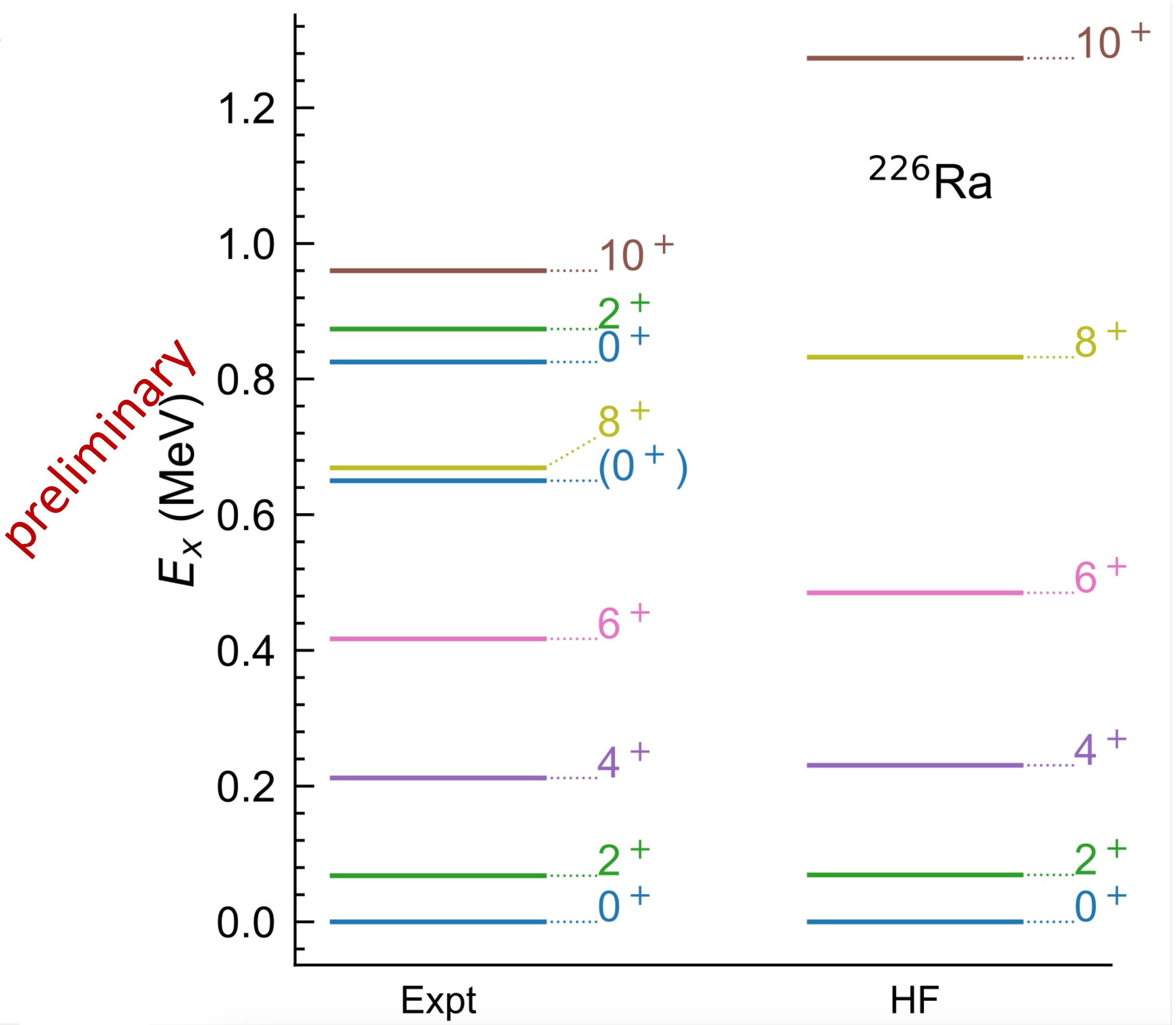


Quadrupole (Q2) and octupole (Q3) constrained Hartree-Fock calculations of ^{224}Ra with chiral forces

Baishan Hu, Zhonghao Sun, G. Hagen, TP, … work in progress

Towards coupled cluster computations of Schiff moments in radium nuclei





Baishan Hu, Zhonghao Sun, G. Hagen, TP, … work in progress

Summary

Breaking and restoring symmetries

Physical insights at mean-field level (deformation, superfluidity,...)

Exploits separation of scale between universal collective and specific UV physics

Conceptually simple & computationally affordable

- Shape coexistence in ^{30}Ne
- Related deformation to microscopic forces
- Much improved B(E2) values
- ^{3x}Ne, ^{3x}Mg, ^{80}Zr, ^{22x}Ra

Thank you!