Collectivity in neutron-rich neon isotopes

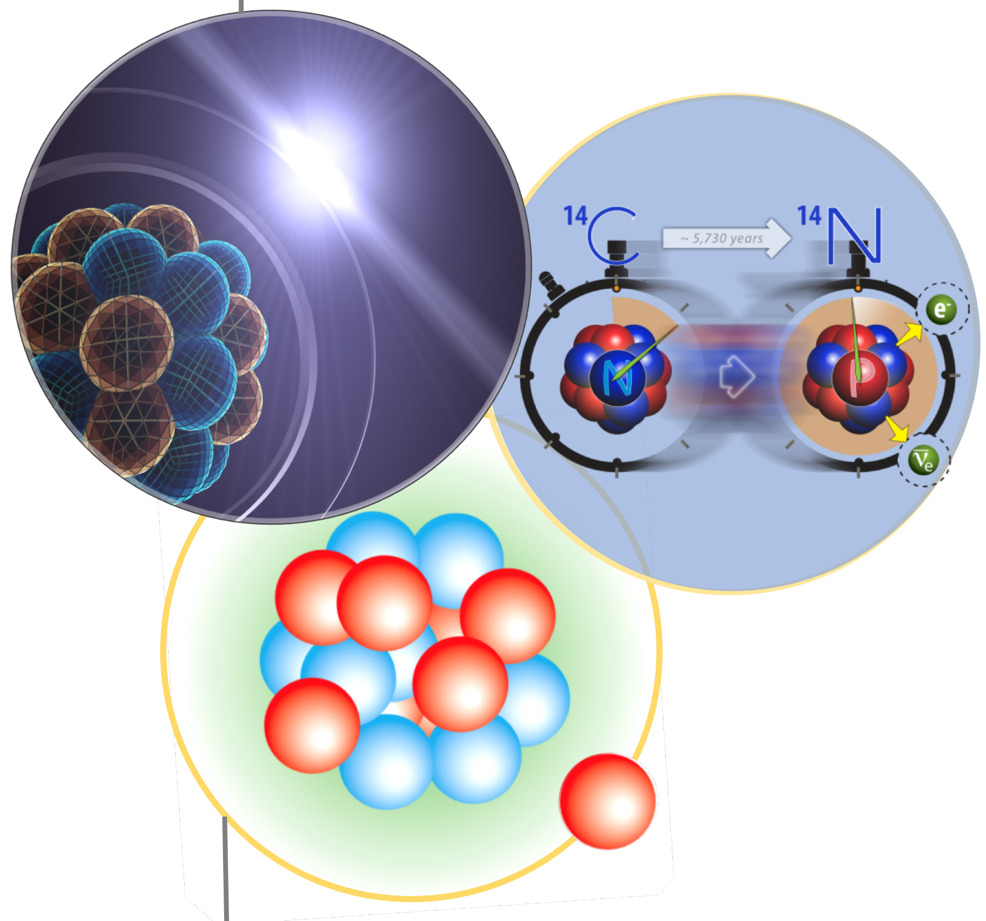
Gaute Hagen
Oak Ridge National Laboratory

Workshop on Progress in Ab-initio Nuclear Theory

TRIUMF, March 1st, 2024

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative



OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

TRIUMF Theory

Perspectives of the Ab Initio No-Core Shell Model

February 23-25, 2012

TRIUMF, Vancouver, BC, Canada

Home
Program
Participants
Travel Information

Program

Talks will be held in the NRC Building Room 1310 on Feb 23-24 and in the TRIUMF MOB Conference Room on Feb 25

Thursday, February 23, NRC Building Room 1310
09:00-09:15 Reiner Kruecken, Head of the TRIUMF Science Division, Welcome and Introduction
09:15-10:00 Ruprecht Machleidt, Three-nucleon forces at N3LO and beyond
10:00-10:30 Angelo Calci, Similarity Renormalization Group for Chiral NN+3N Interactions: Physics & Technology
10:30-11:00 Coffee

In memory of friend and colleague Rup

Evolution of Shell Structure in Neutron-Rich Calcium Isotopes

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, and T. Papenbrock
Phys. Rev. Lett. **109**, 032502 – Published 17 July 2012

Continuum Effects and Three-Nucleon Forces in Neutron-Rich Oxygen Isotopes

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, and T. Papenbrock
Phys. Rev. Lett. **108**, 242501 – Published 15 June 2012

Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, and S. M. Wild
Phys. Rev. Lett. **110**, 192502 – Published 7 May 2013

Collaborators

@ ORNL / UTK: **Baishan Hu**, G. R. Jansen, **Z. H. Sun**, T. Papenbrock

@ CEA/Saclay: T. Duguet

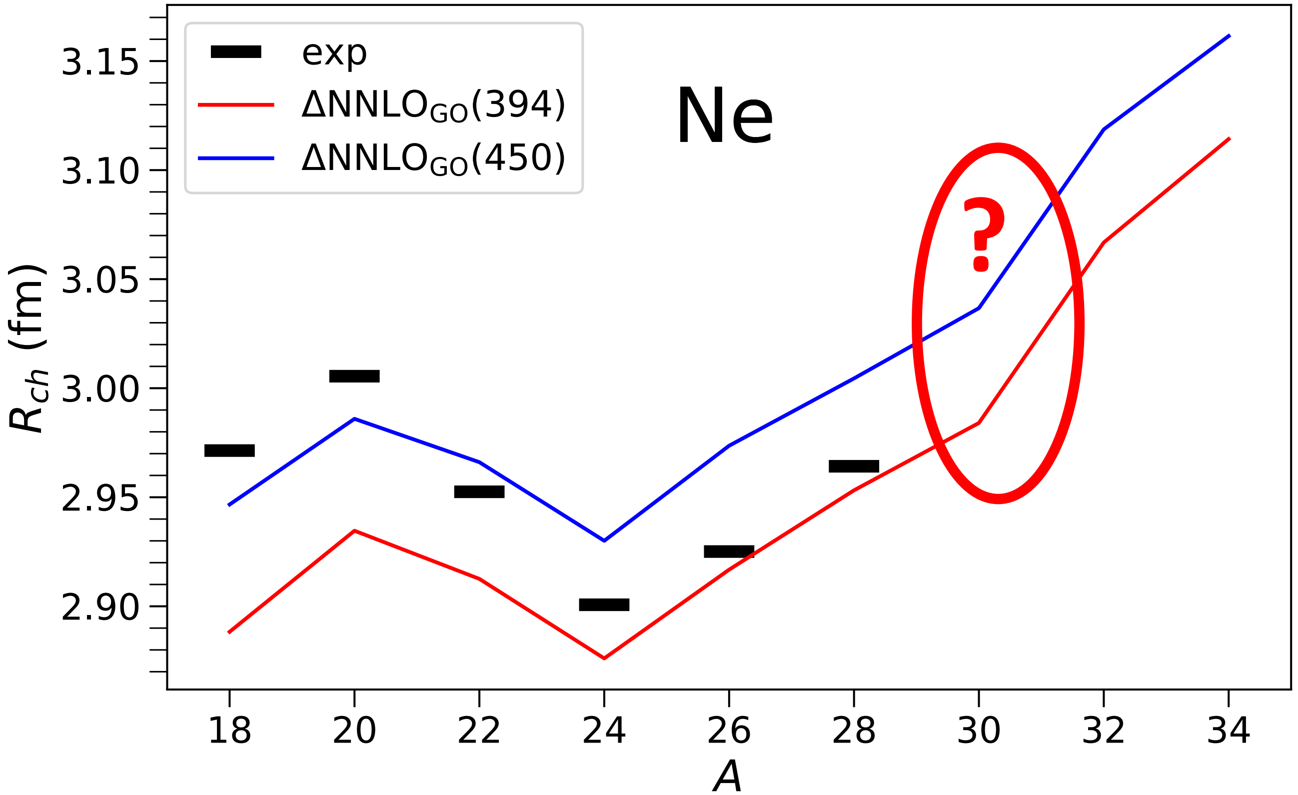
@ Chalmers: A. Ekström, C. Forssén

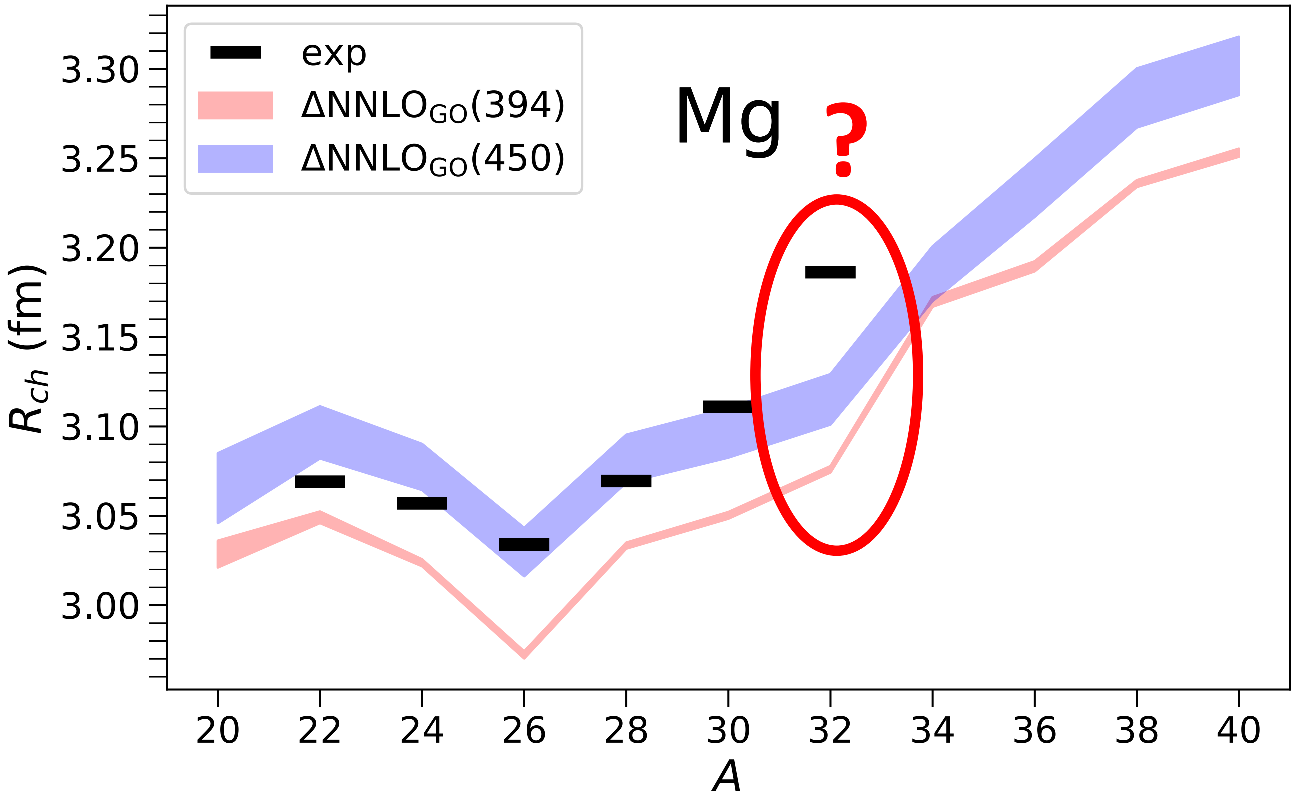
@ WUSTL: **S. Novario**

@ TU Darmstadt: **A. Tichai**

What's going at N = 20?

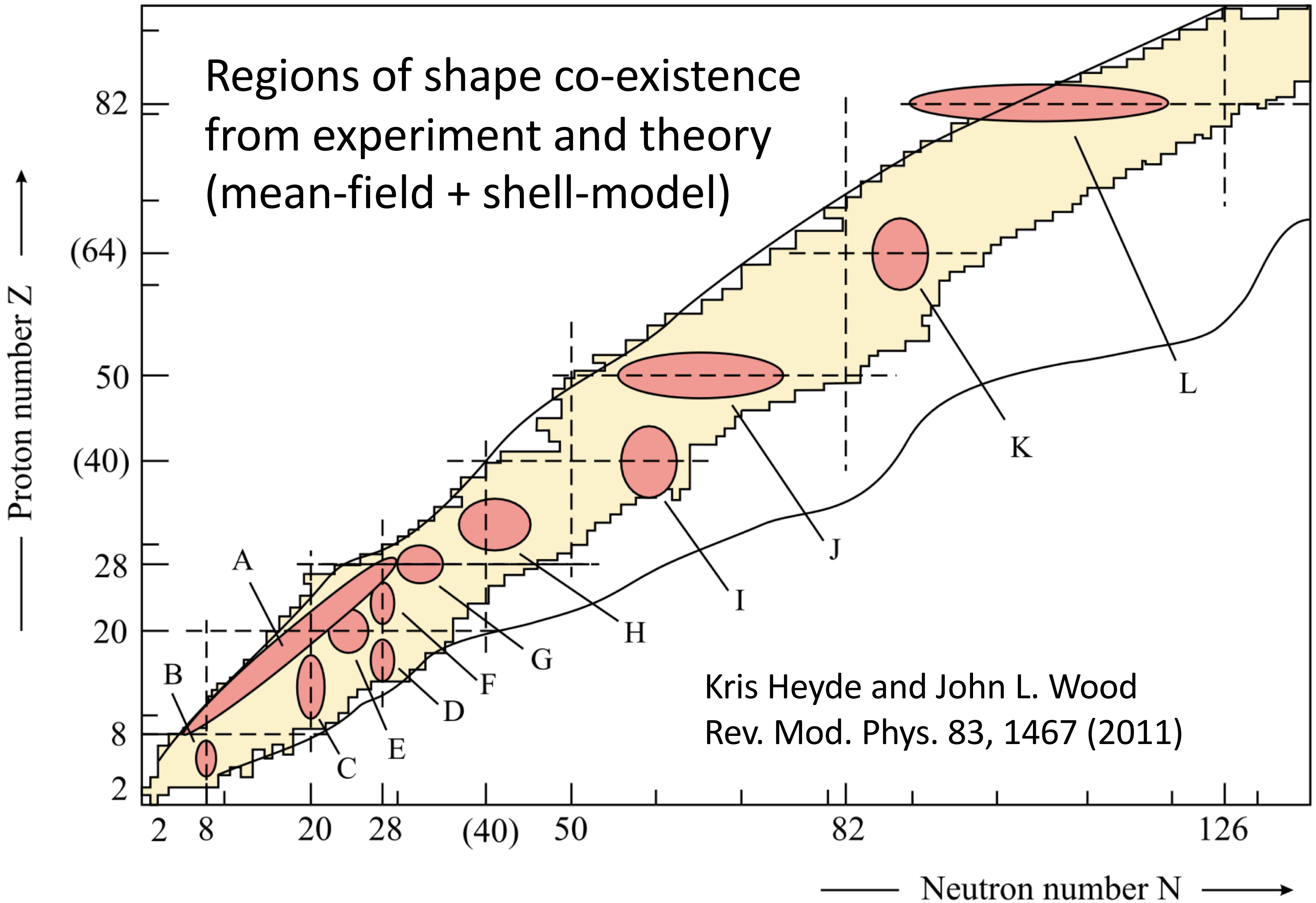
Interaction/method deficiency or something else?



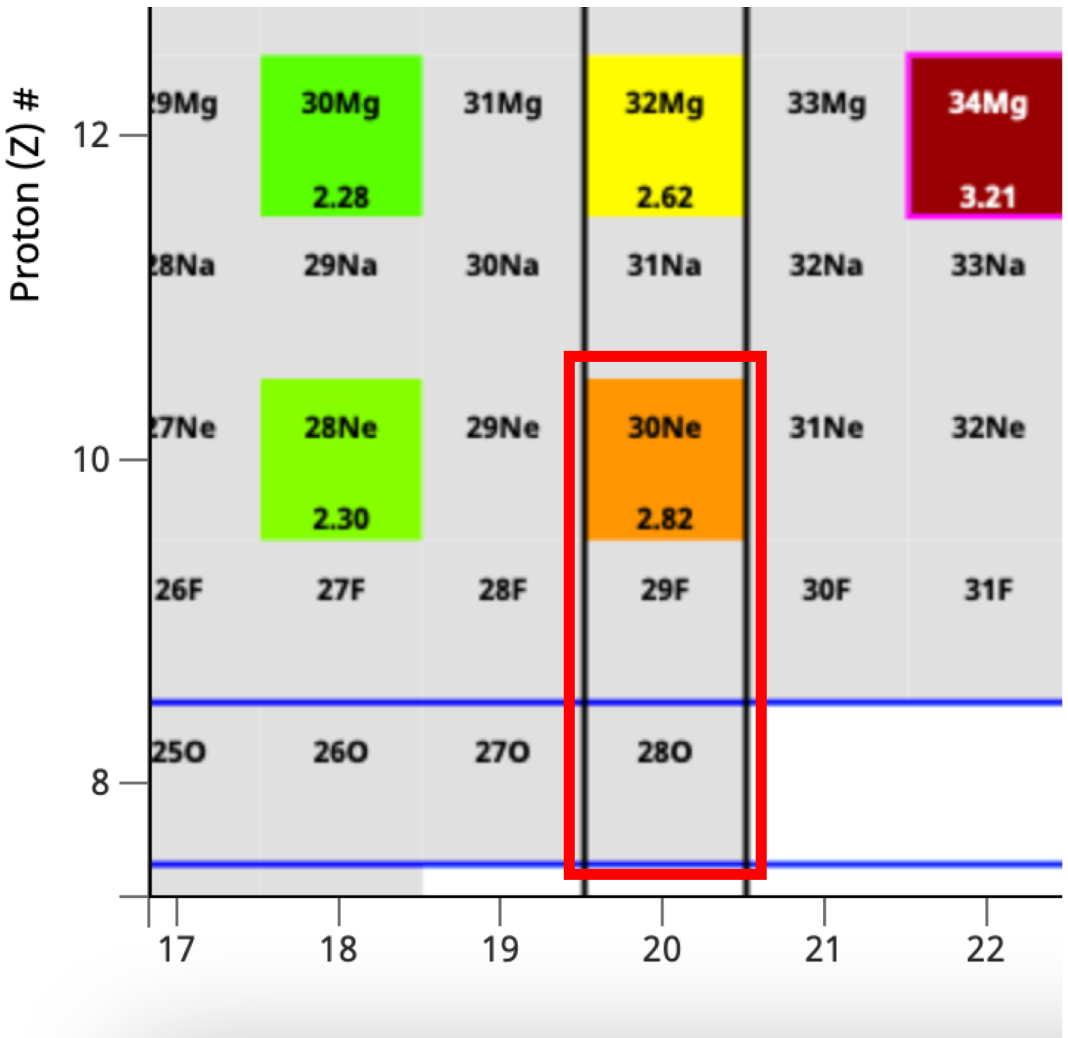


S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

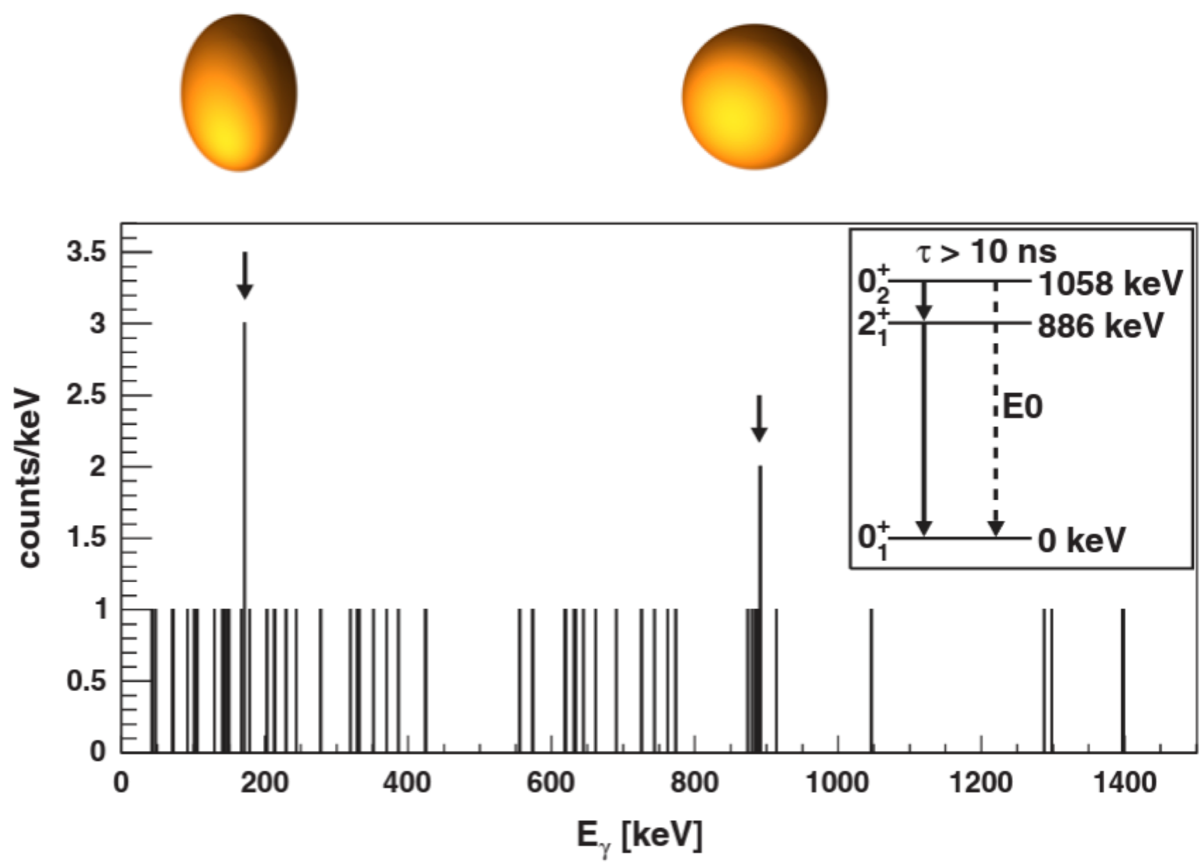
Onset of deformation and shape co-existence in nuclei



Onset of deformation and shape co-existence along N = 20

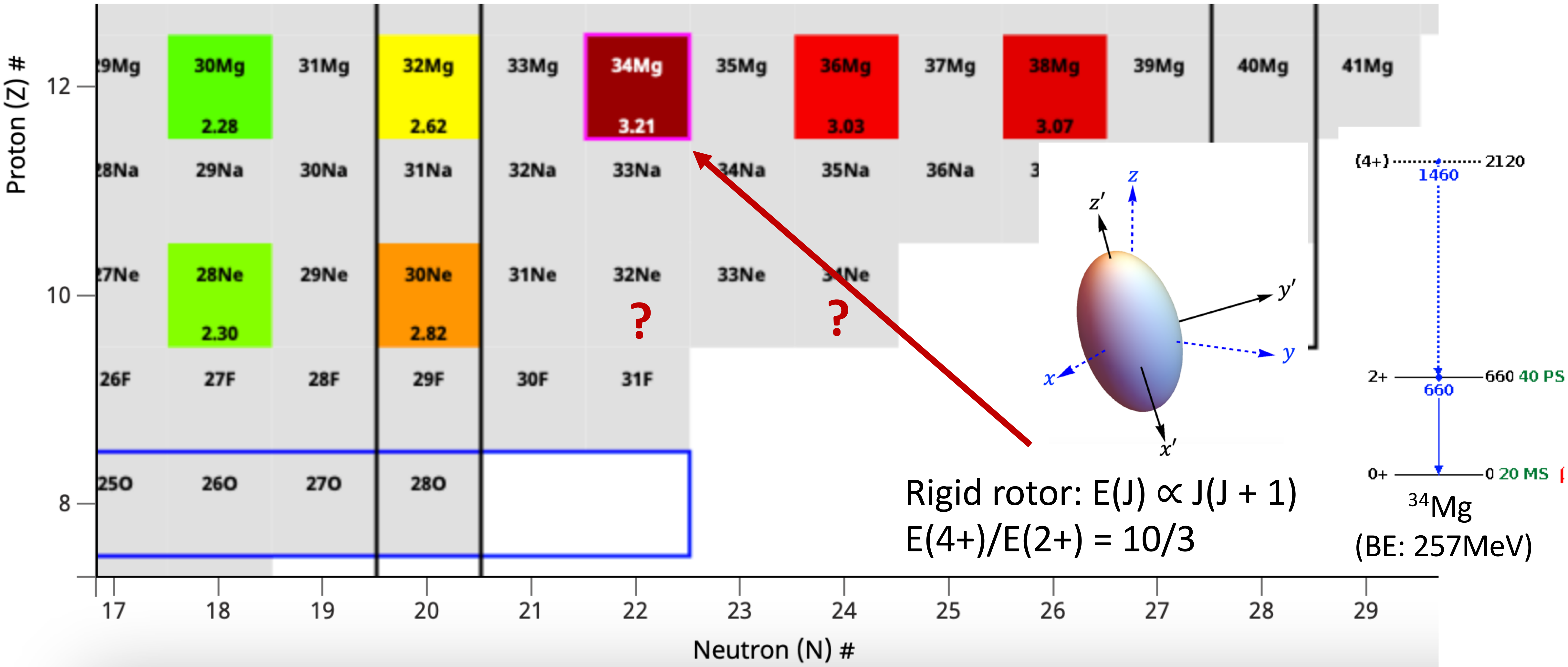


Shape co-existence in ^{32}Mg



K. Wimmer et al, PRL (2010)

Towards island of inversion with ab initio methods



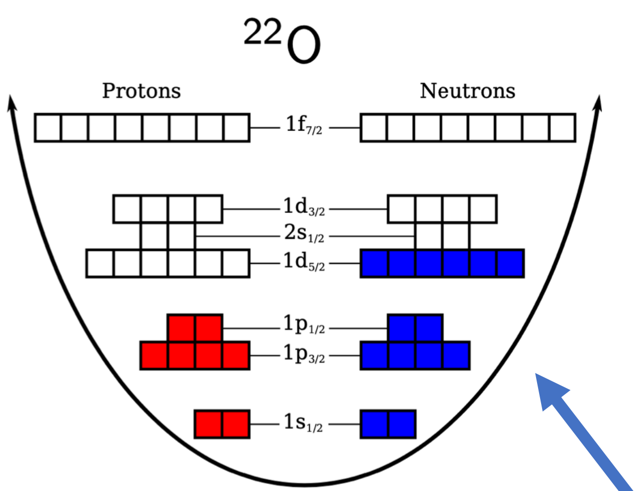
G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai Phys. Rev. C 105, 064311 (2022)

S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

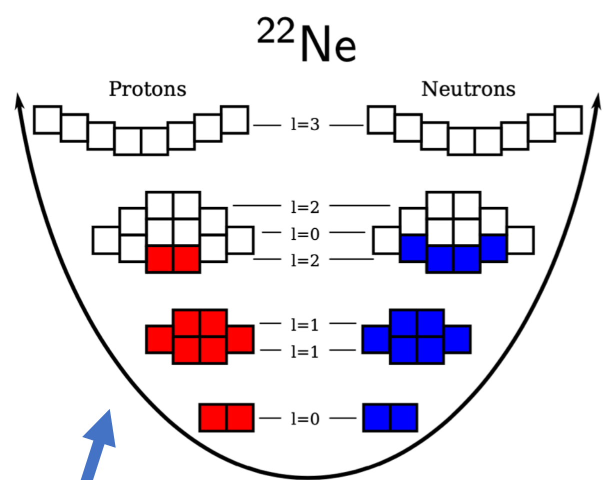
Coupled-cluster computations of deformed nuclei

The key lies in choosing the correct starting point

Wave-function based methods starts from a mean-field reference state



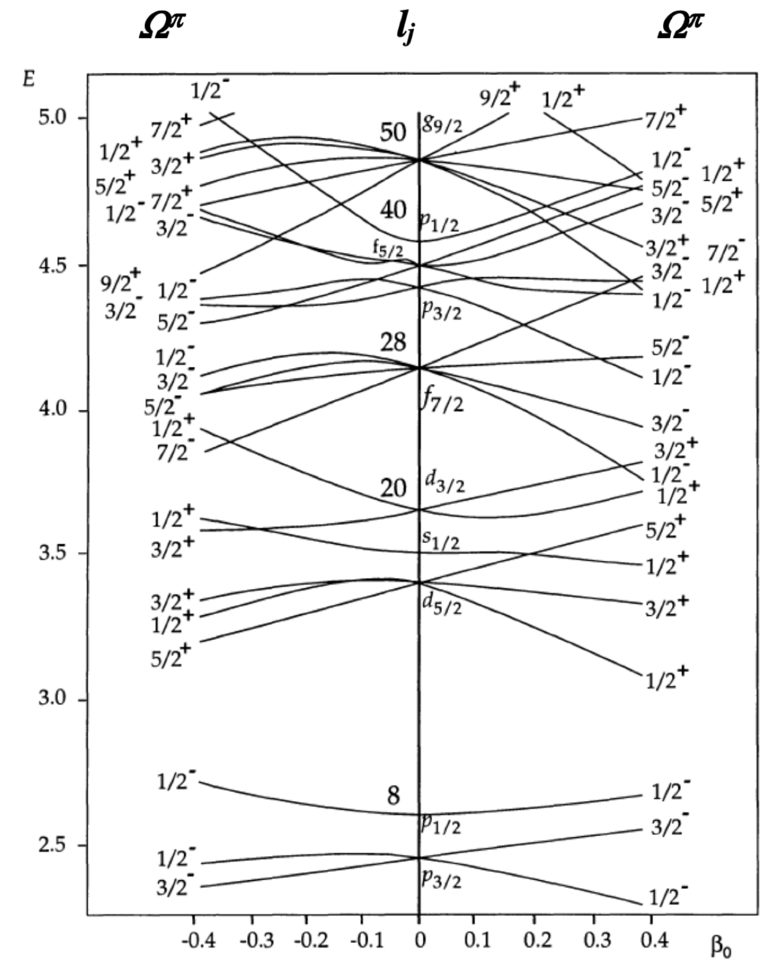
Spherical

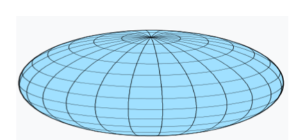


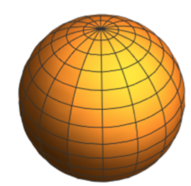
Deformed

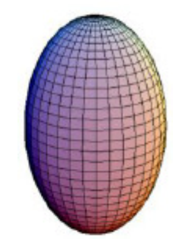
$$|\Psi\rangle = \Omega|\Phi\rangle$$

Wave-operator (includes many-body correlations)









Coupled-cluster computations of deformed nuclei

1. Compute Hartree-Fock reference state
   - Nontrivial vacuum state informs us about emergent breaking of symmetries
   - Yields normal-ordered two-body Hamiltonian
2. Include dynamical (extensive) correlations via coupled-cluster theory
   - (or via IMSRG, or Gorkov methods, or Green's functions)
   - Cost increases polynomial with mass number
3. Perform symmetry projections
   - Non-extensive contributions to the energy
   - Often relevant for transition matrix elements

The total energy of a nucleus

Dynamic correlation (large contribution and requires size-extensive methods)

Static correlation (can use non size-extensive methods)

$$E = E_{\mathrm{ref}} + \overbrace{\Delta E_{\mathrm{CC}}} + \overbrace{\delta E}$$

Symmetry restored coupled-cluster theory

Projection after variation (PAV): $$E^{(J)} = \frac{\langle\widetilde{\Psi}|P_J H|\Psi\rangle}{\langle\widetilde{\Psi}|P_J|\Psi\rangle}$$

Image credit: Wikimedia Commons

Right coupled-cluster state: $$|\Psi\rangle = e^T|\Phi_0\rangle$$

Left state is parametrized differently:

$$\langle\widetilde{\Psi}| = \langle\Phi_0|(1+\Lambda)e^{-T}$$

Bi-variational

For axial symmetry around the z-axis the rotation operator is:

$$P_J = \frac{1}{2}\int_0^\pi d\beta \sin(\beta) d^J_{00}(\beta) R(\beta)$$

$$R(\beta) \equiv e^{i\beta J_y}$$

Symmetry restored coupled-cluster theory

The kernels can be evaluated by using Thouless theorem:

$$\langle\Phi_0|R(\beta) = \langle\Phi_0|R(\beta)|\Phi_0\rangle\langle\Phi_0|e^{V_1(\beta)}$$

$$\mathcal{H}(\beta) = \langle\Phi|\overline{R}(\beta)|\Phi\rangle\langle\Phi|Z(\beta)\widetilde{H}(\beta)e^{V(\beta)}e^{T_2}|\Phi\rangle$$

$$\mathcal{N}(\beta) = \langle\Phi|\overline{R}(\beta)|\Phi\rangle\langle\Phi|Z(\beta)e^{V(\beta)}e^{T_2}|\Phi\rangle$$

Similarity transformed rotation operator and Hamiltonian:

$$\overline{R}(\beta) = e^{-T_1}R(\beta)e^{T_1}$$

$$\widetilde{H}(\beta) = e^{V_1(\beta)}\overline{H}e^{-V_1(\beta)}$$

$$e^{V(\beta)}e^{T_2}|\Phi\rangle = e^{W_0(\beta)+W_1(\beta)+W_2(\beta)+\dots}|\Phi\rangle$$

- Does not truncate
- How to evaluate the disentangled amplitudes?

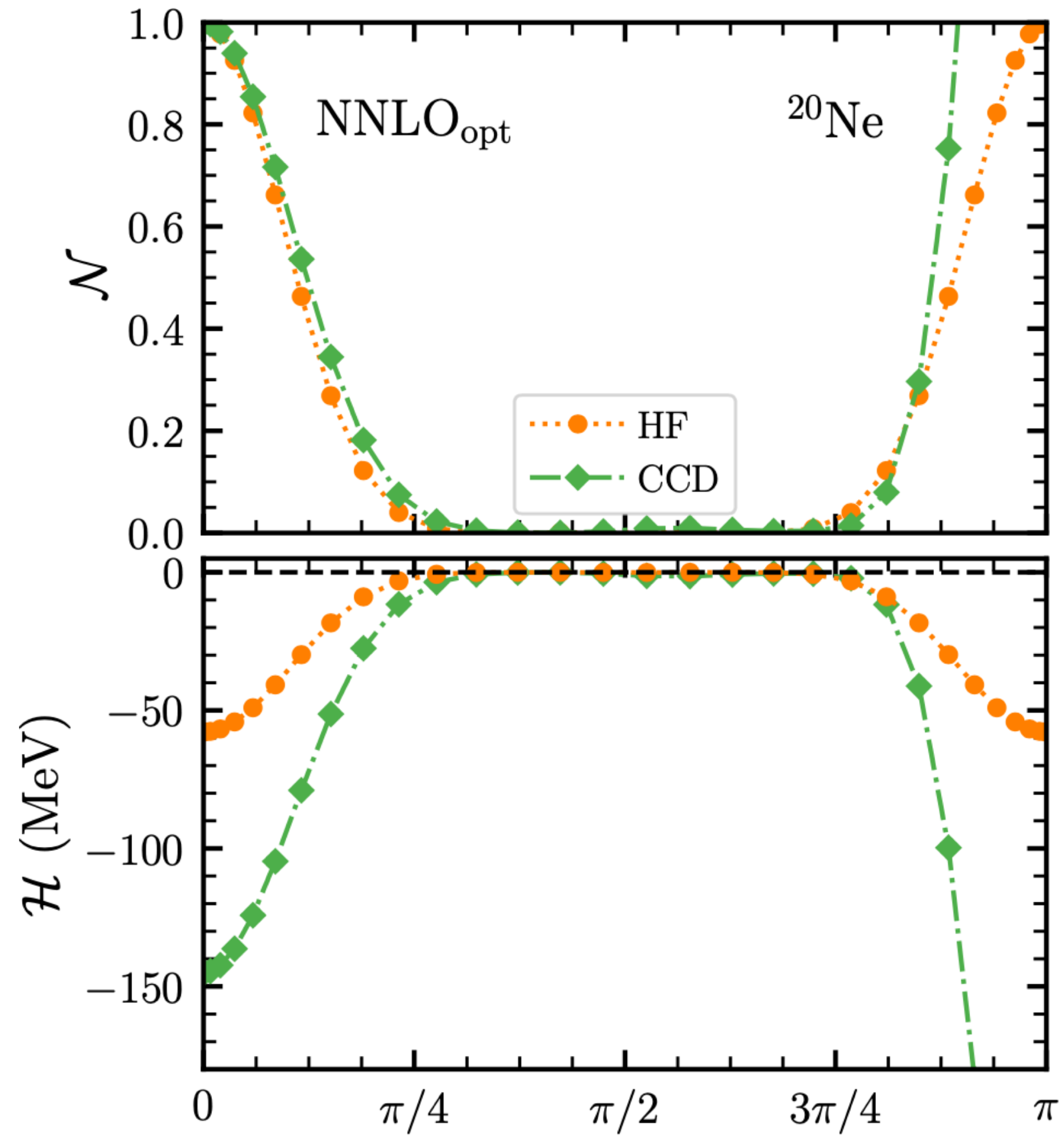
[Qiu et al, J. Chem. Phys. 147, 064111 (2017)]

Solving for the disentangled amplitudes [Qiu et al]

Approximate: $$e^{V(\beta)}e^{T_2}|\Phi\rangle \approx e^{W_0(\beta)+W_1(\beta)+W_2(\beta)}|\Phi\rangle$$

Taking the derivative with respect to β leads to a set of ODEs with initial conditions:
$W_0(\beta = 0) = W_1(\beta = 0) = 0, W_2(\beta = 0) = T_2$
[Qiu et al, J. Chem. Phys. 147, 064111 (2017)]

- Approximate restoration of symmetries
- Can lead to stiffness as $dV(\beta)/d(\beta)$ might be large for $\langle\Phi|R(\beta)|\Phi\rangle \approx 0$.
- The truncation at W_2 might lead to loss of accuracy at larger angles
- Kernels are not symmetric around $\beta = \frac{\pi}{2}$

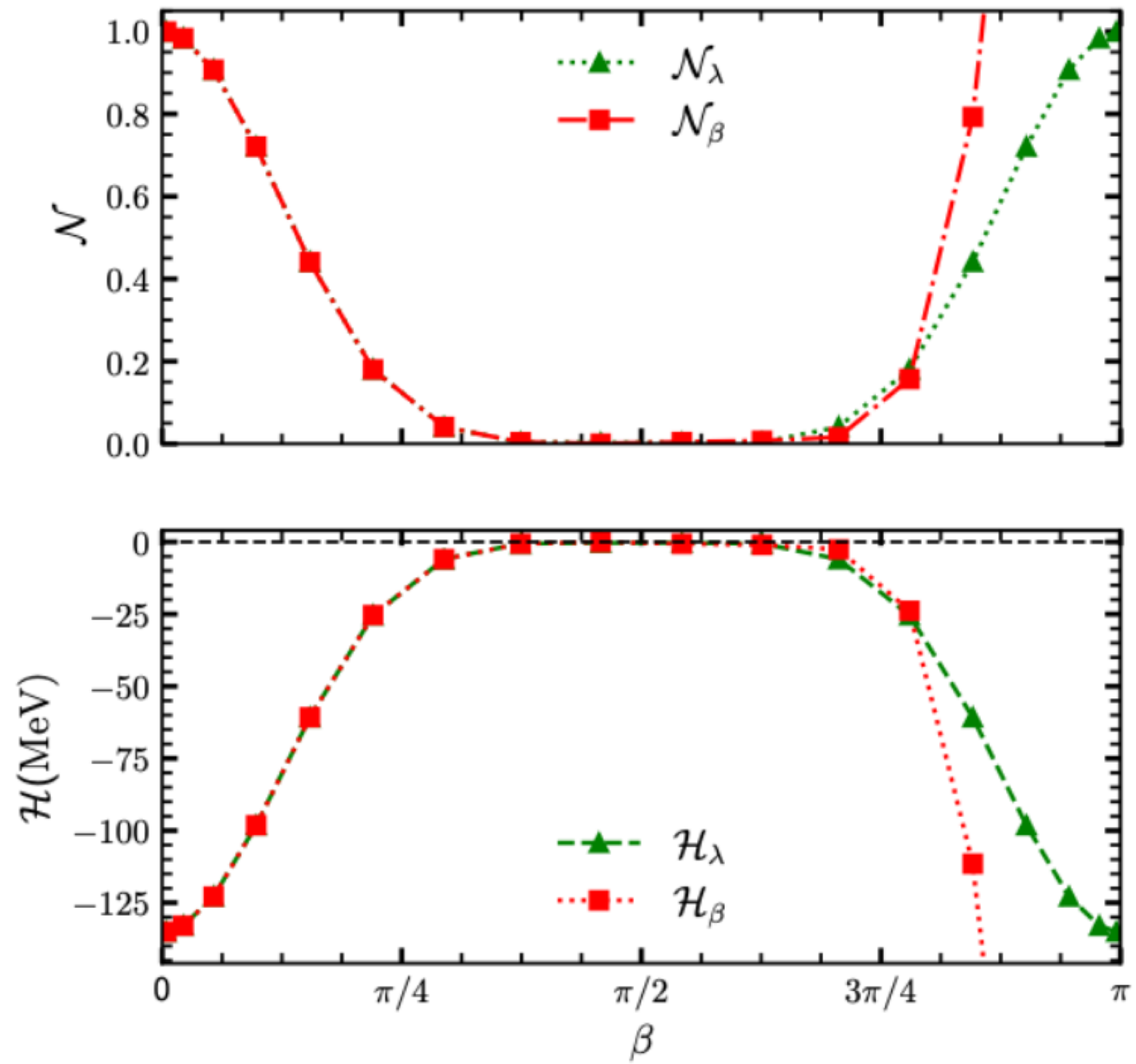


New approach to solve for disentangled amplitudes

We write: $$e^{\lambda V} e^{T_2} |\Phi\rangle \approx e^{W_0(\lambda)+W_1(\lambda)+W_2(\lambda)} |\Phi\rangle$$

Taking the derivative with respect to λ for fixed β leads to a new set of ODEs with initial conditions: $W_n(\lambda = 0) = T_n$

- Approximate restoration of symmetries
- Significantly improves stability of ODEs
- Kernels are fully symmetric around $\beta = \frac{\pi}{2}$



Zhonghao Sun, A. Ekstrom, C. Forssen,
G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Electromagnetic transitions

$$B(E2,\downarrow) \equiv |\langle 0^+||Q_2||2^+\rangle|^2$$

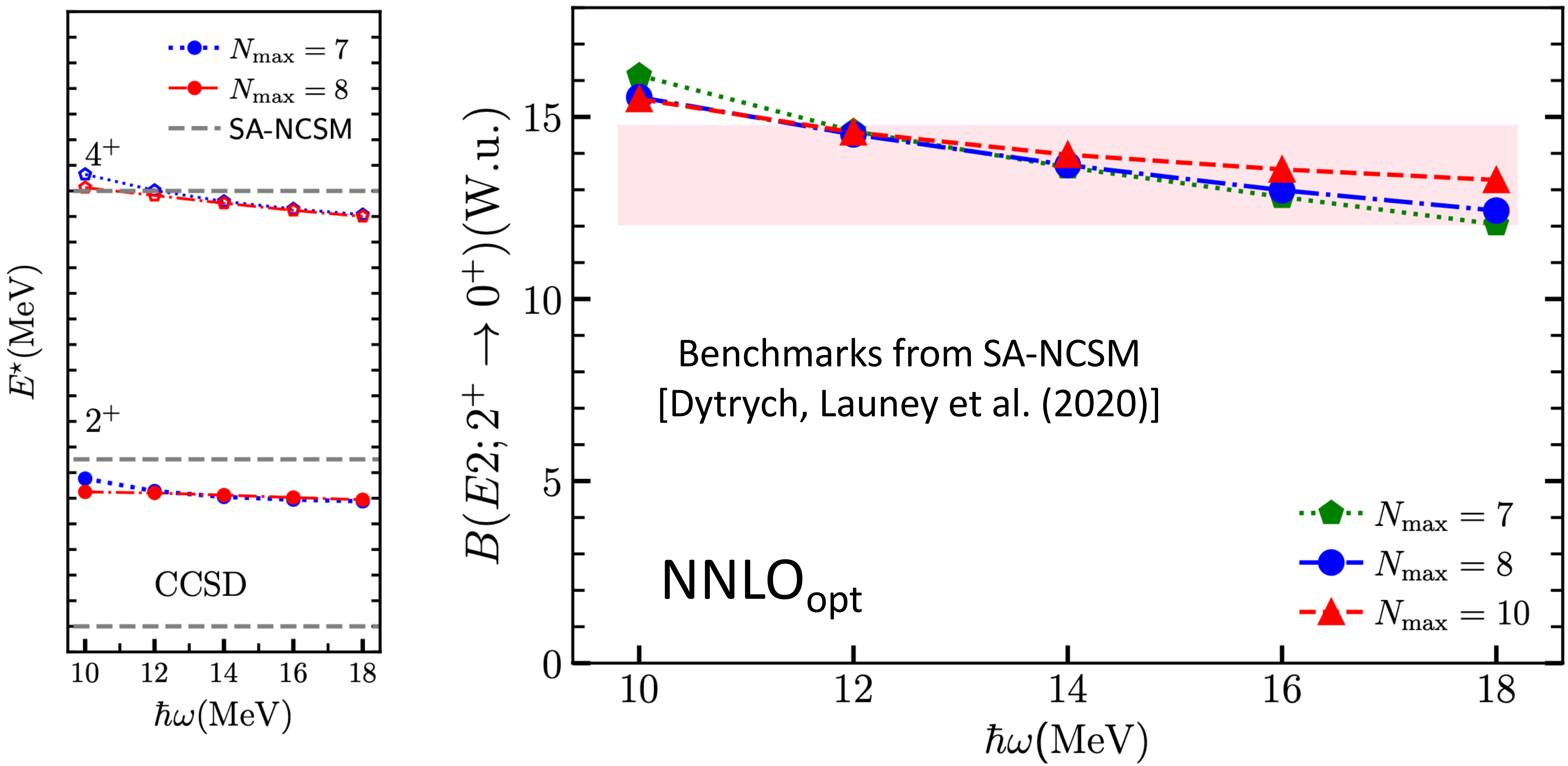
$$B(E2,\downarrow) = \frac{\langle\widetilde{\Psi}|P_0 Q_{20} P_2|\Psi\rangle\langle\widetilde{\Psi}|P_2 Q_{20} P_0|\Psi\rangle}{\langle\widetilde{\Psi}|P_0|\Psi\rangle\langle\widetilde{\Psi}|P_2|\Psi\rangle}$$

Recall the left and right coupled-cluster states:

$$\langle\widetilde{\Psi}| \equiv \langle\Phi_0|(1+\Lambda)e^{-T} \qquad\qquad |\Psi\rangle \equiv e^{T}|\Phi_0\rangle$$

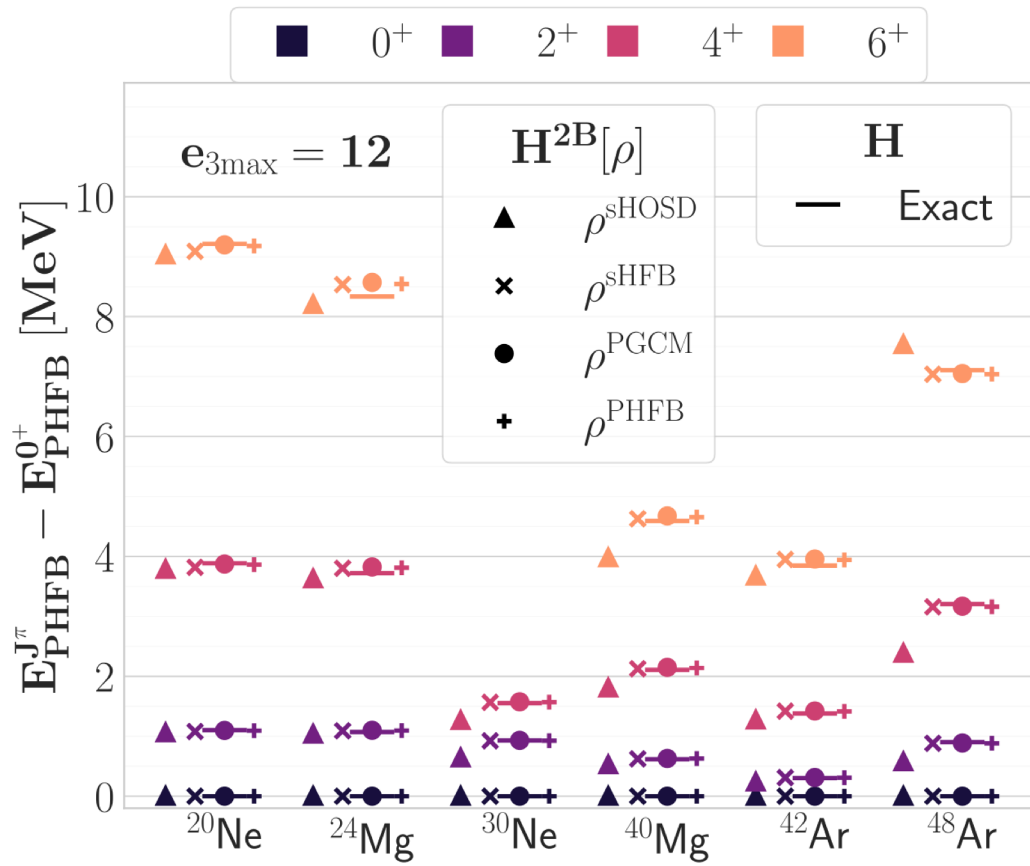
Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Benchmarking projected coupled-cluster in ^{20}Ne

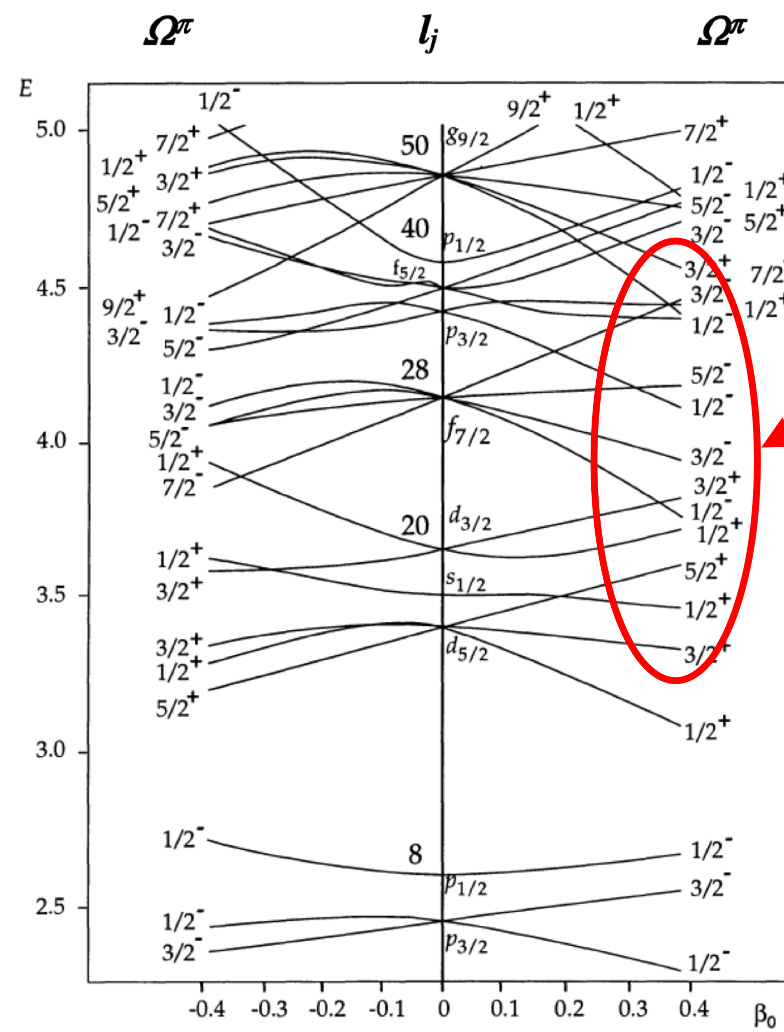


Inclusion of three-body forces

- The normal ordered 2-body approximation breaks rotational symmetry when normal-ordered with respect to a broken symmetry reference state
- Perform spherical HF with fractional filling to normal-order three-nucleon force
- Use normal-ordered Hamiltonian in the 2-body approximation in a second HF calculation of deformed nuclei

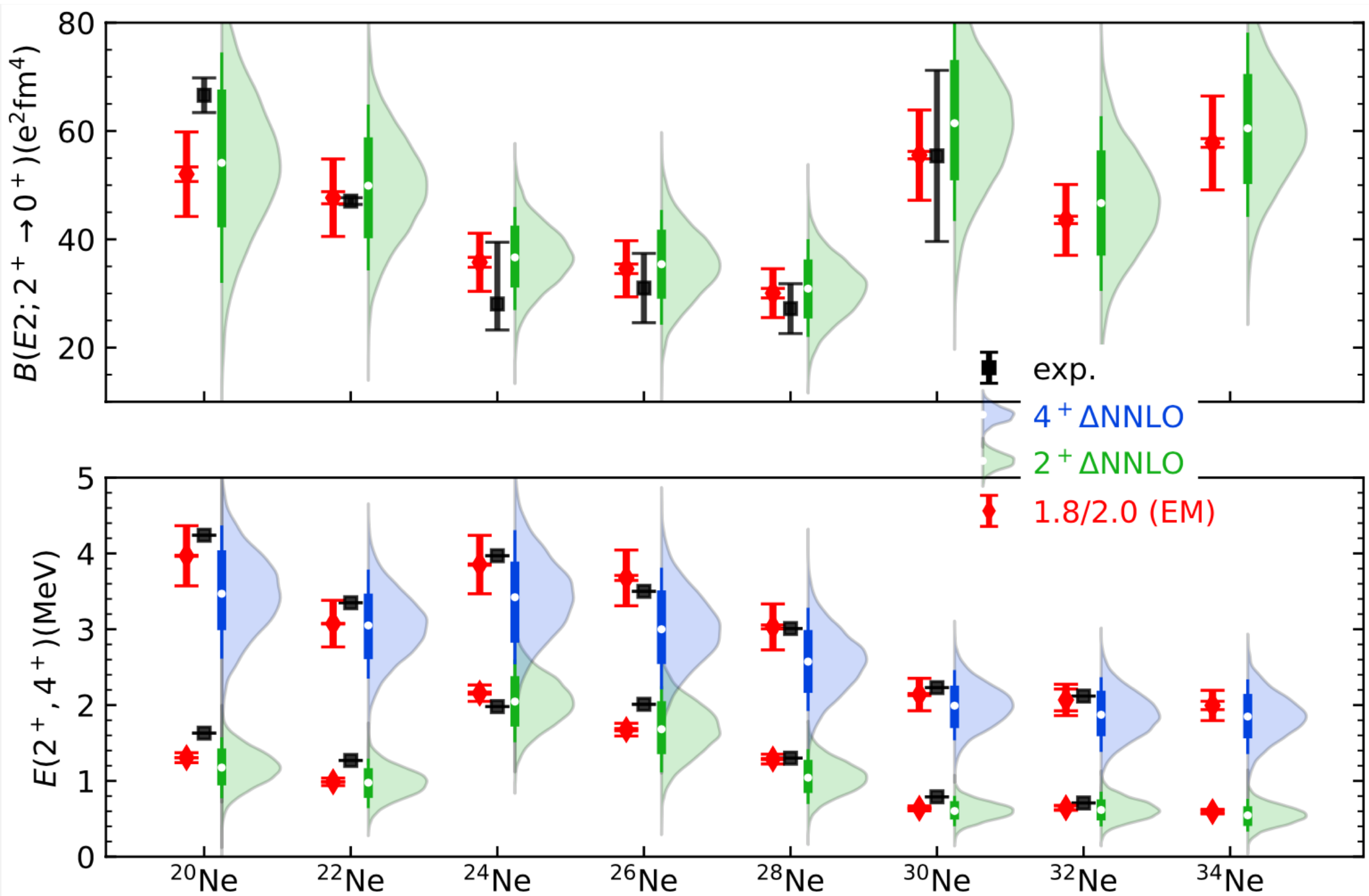


Mikael Frosini et al, Eur. Phys. J. A 57 (2021)



What is the correct spherical filling in very deformed nuclei?

Collectivity in neon isotopes



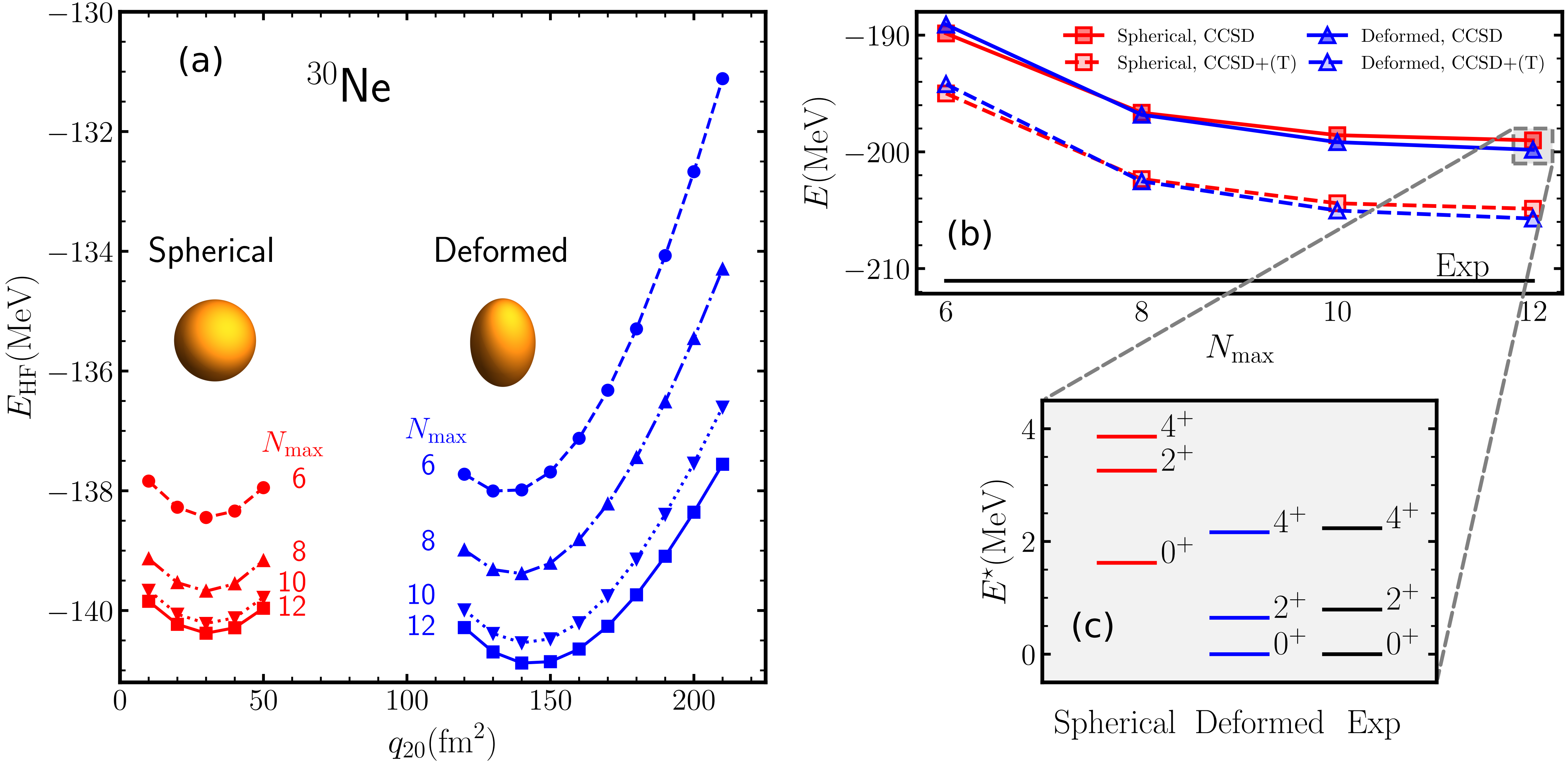
Rotational structure of neutron-rich neon isotopes in good agreement with data

Spectra of $^{30\text{-}34}$Ne follow that of a rigid rotor $E(J) \propto J(J + 1)$

Small energies reflect a large moment of inertia and a strong deformation

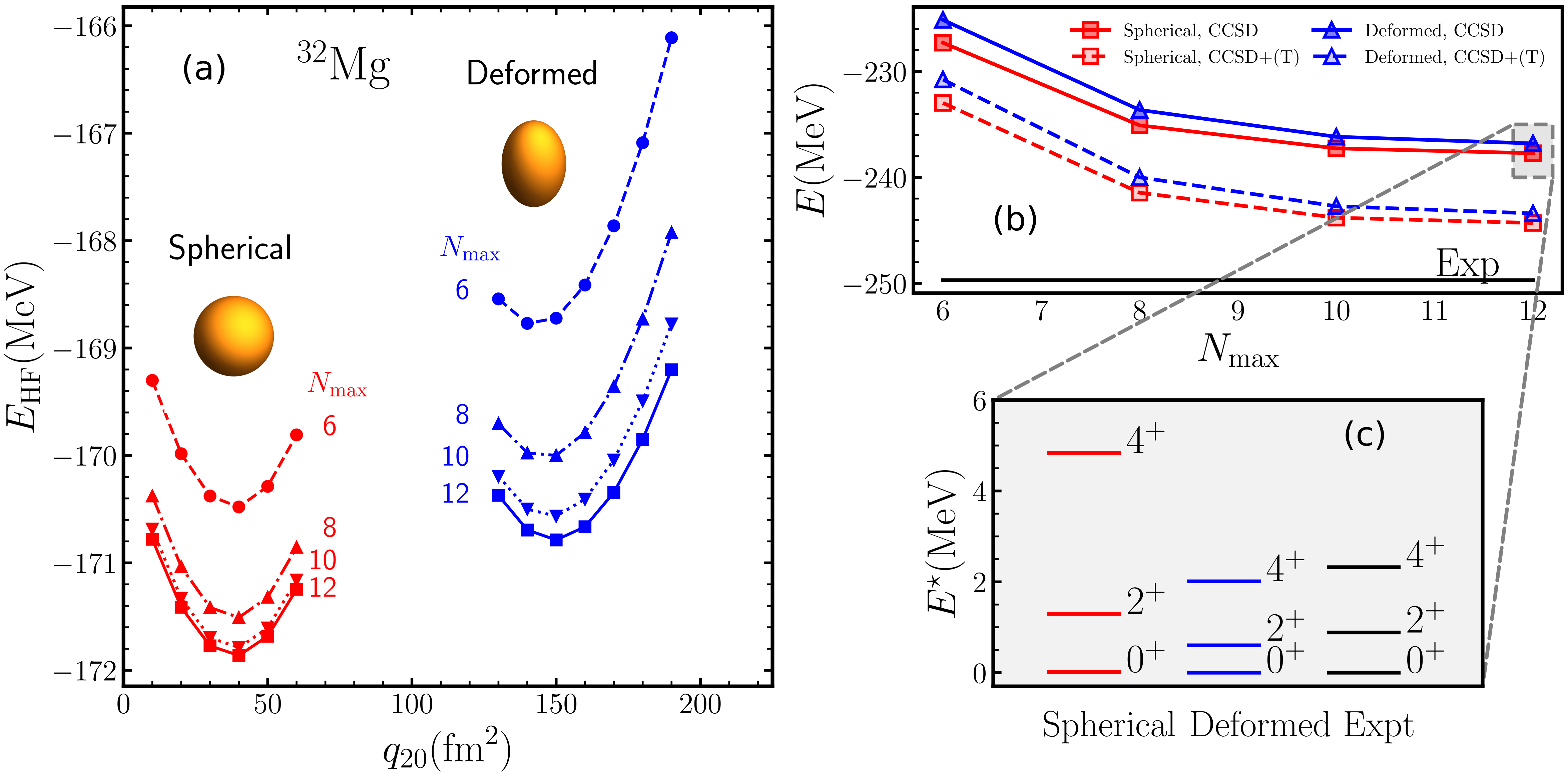
Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Shape co-existence in ^{30}Ne



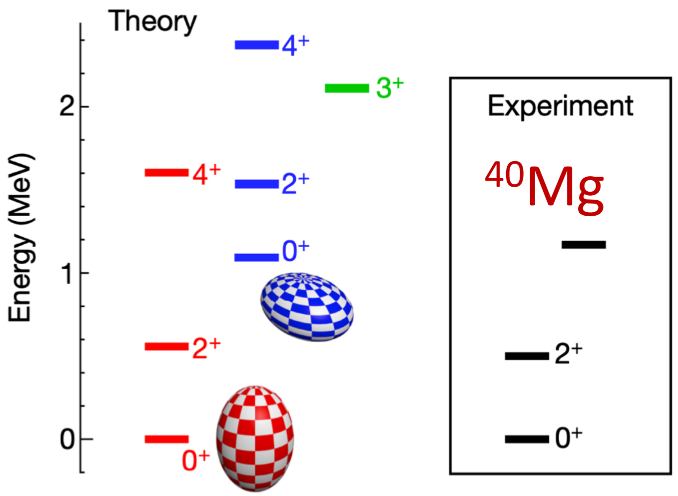
Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Shape co-existence in ^{32}Mg

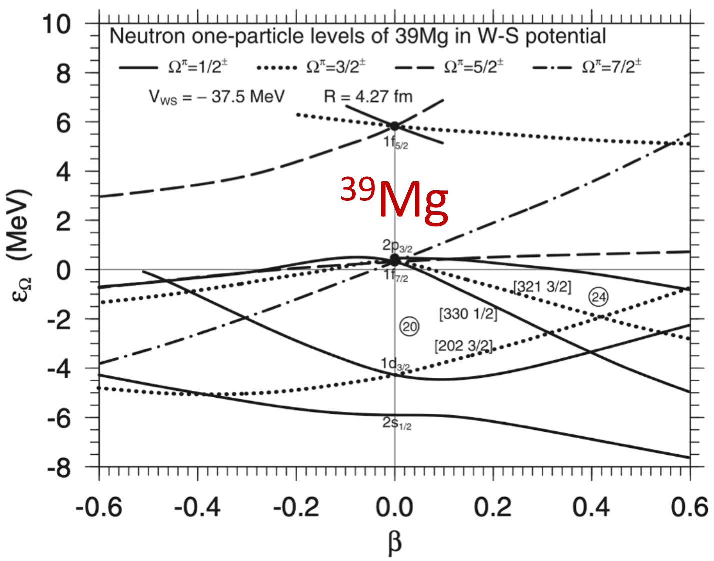


Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2023)

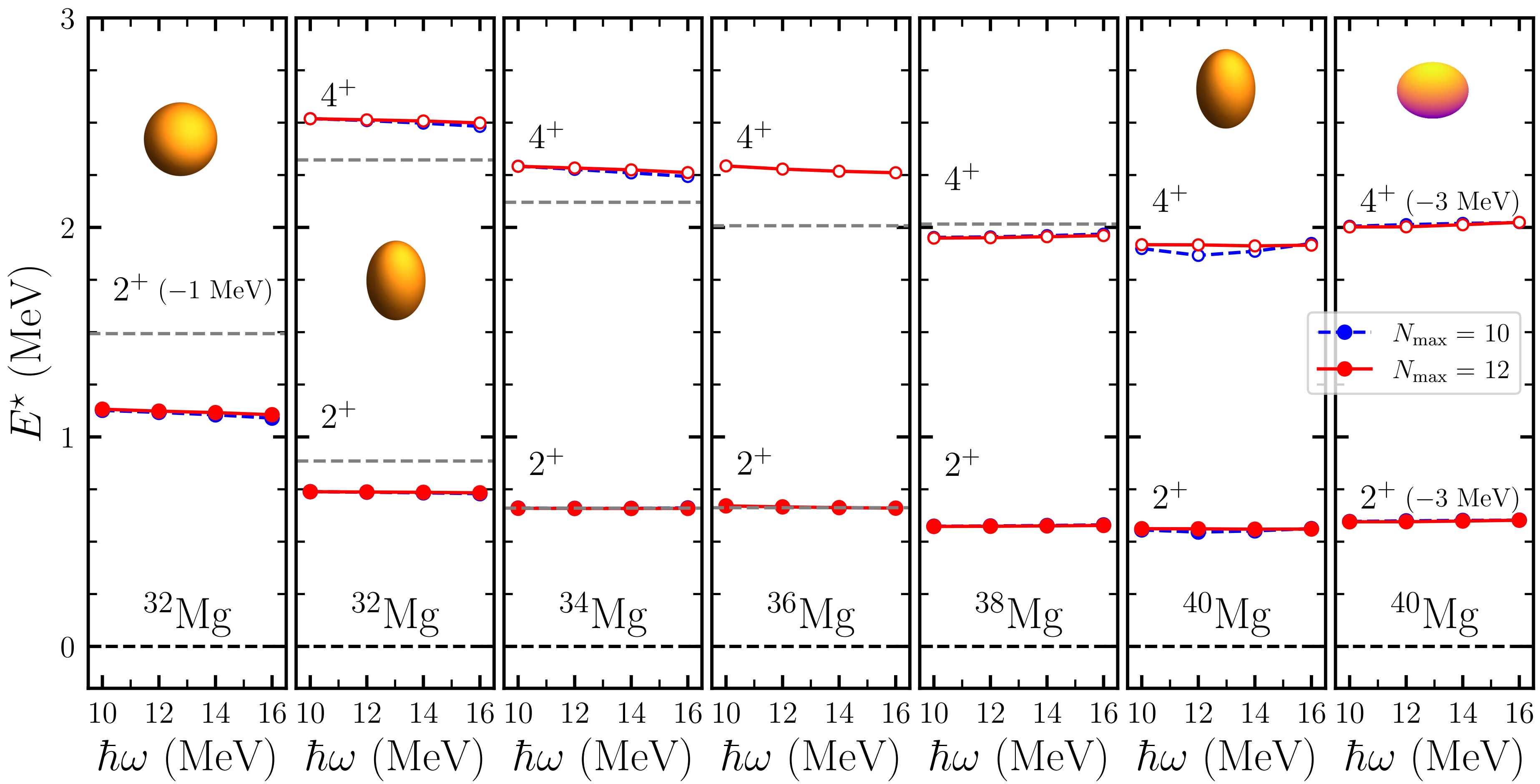
Deformation in neutron-rich magnesium



Crawford et al. PRL 122, 052501 (2019)
Tsunuda et al, Nature 587, 66 (2020)



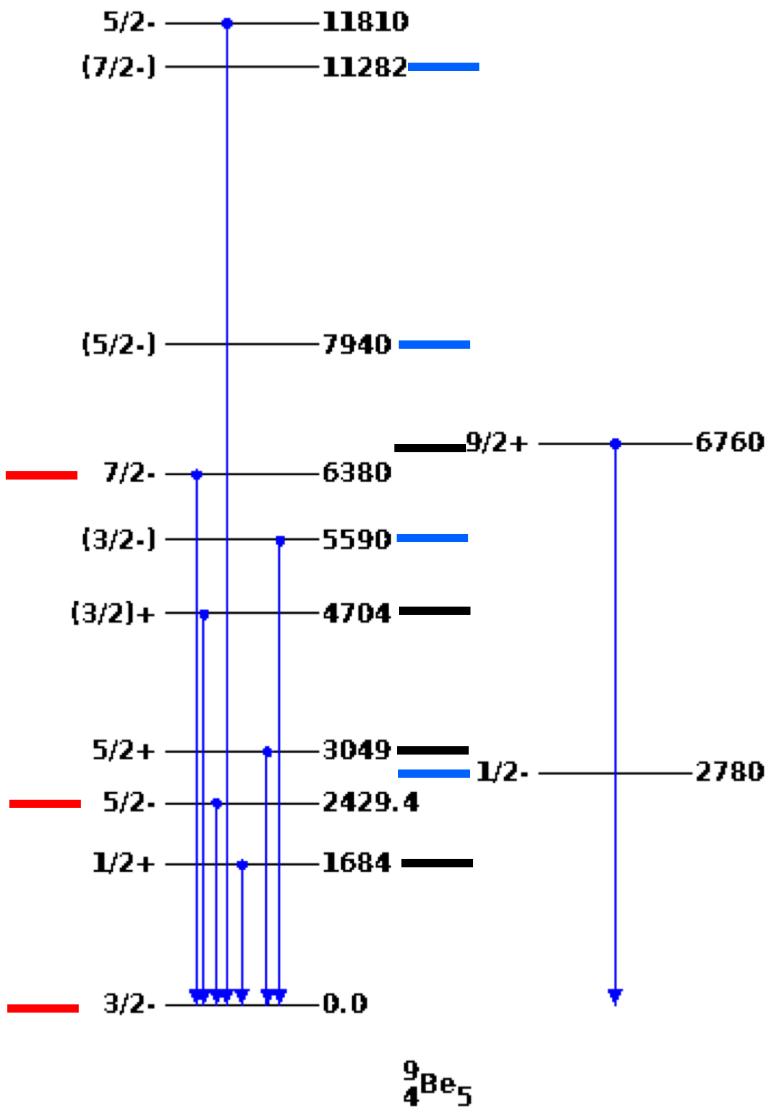
Ikuko Hamamoto, Phys. Rev. C **93**, 054328 (2016)

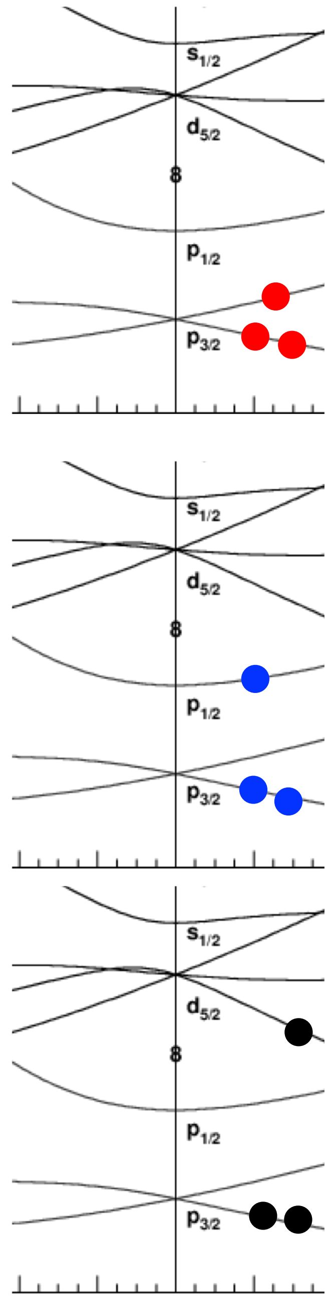


- Rotational structure in good agreement with experiment
- Indications of shape co-existence in ^{40}Mg
- Find oblate band in ^{40}Mg 2-3MeV above the prolate band

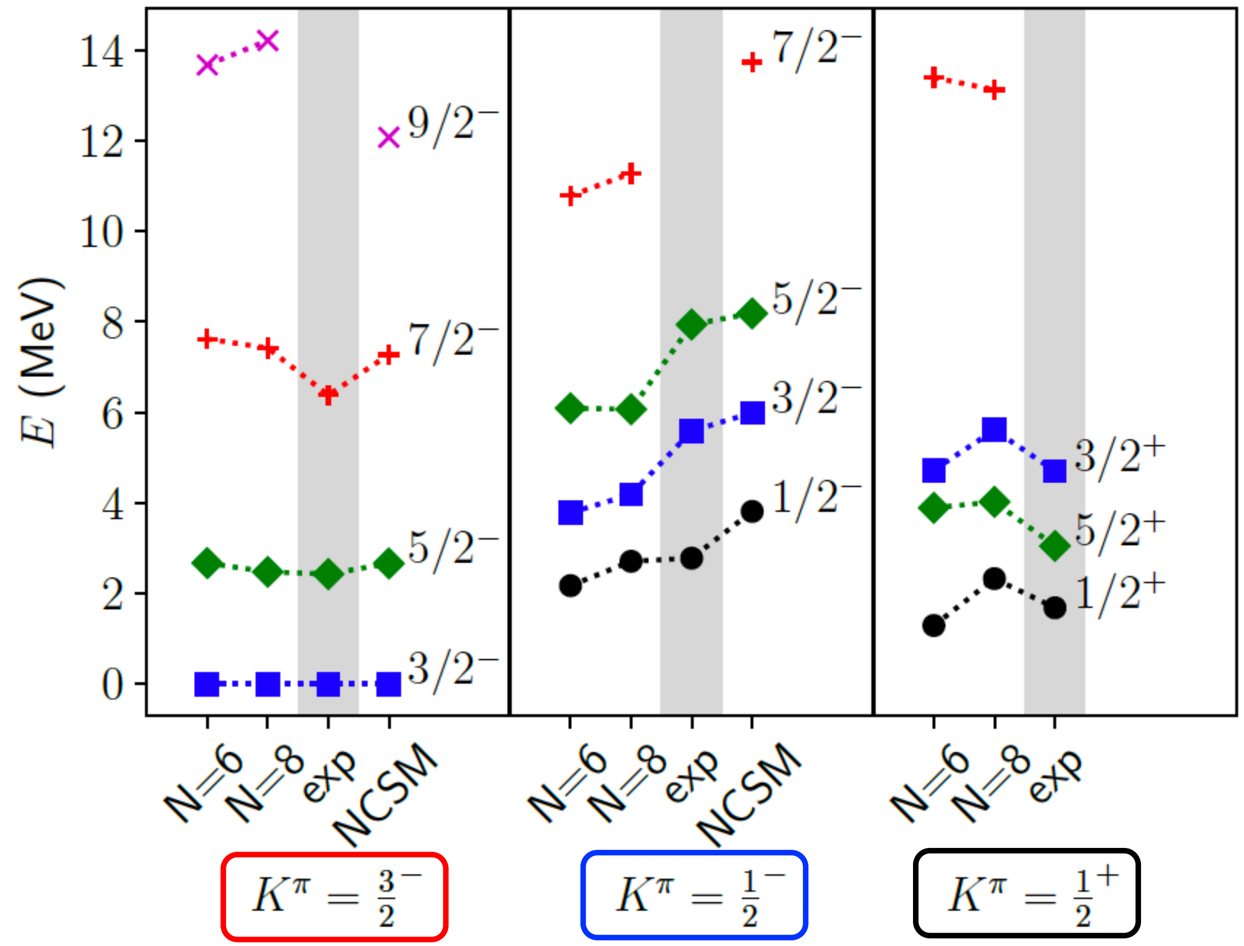
Making sense of spectra in odd-mass nuclei

Looks complicated;
shown data lacks understanding





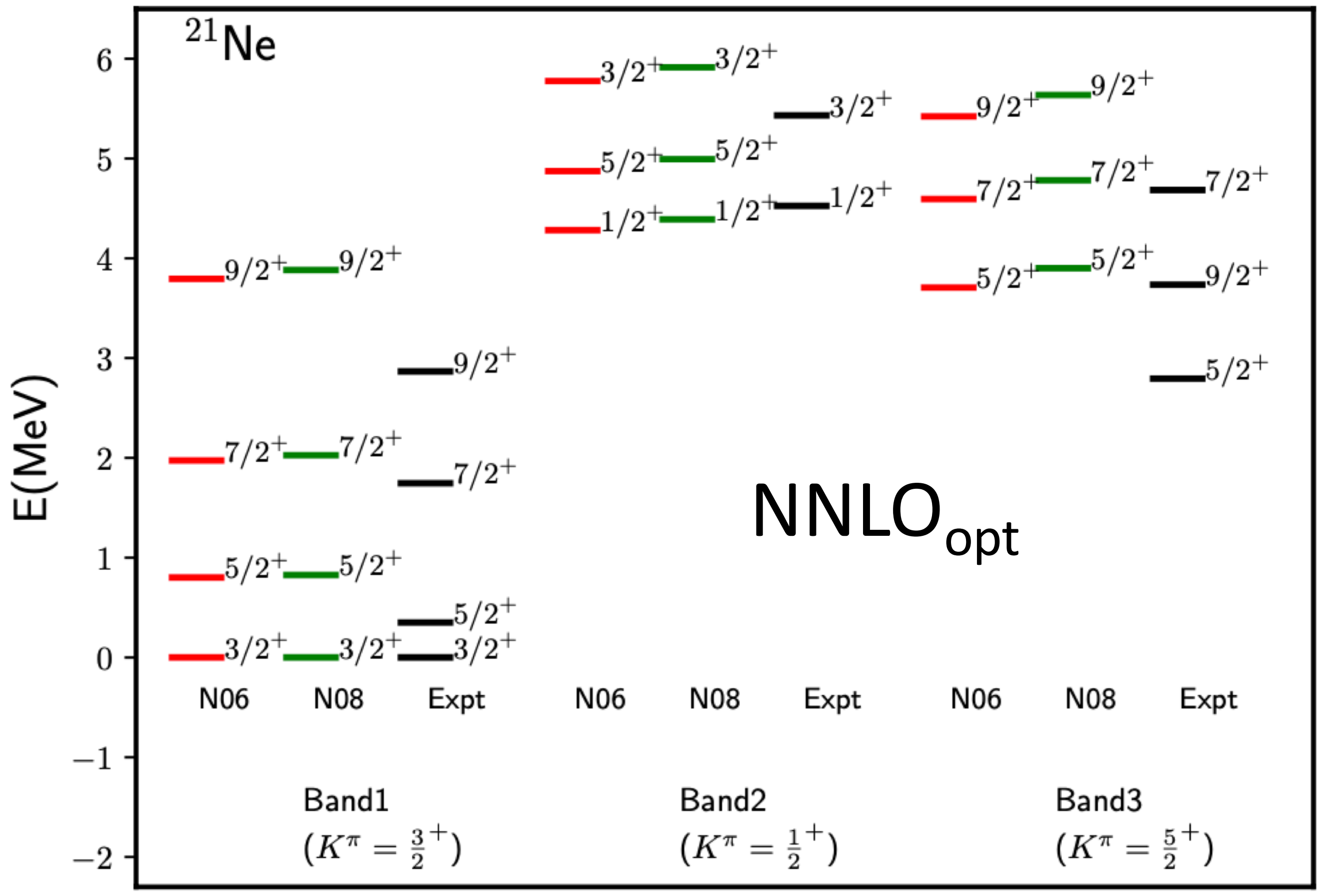
Zhonghao Sun et al., in preparation
Hartree-Fock computations yield deformed reference
Coupled-cluster + projection yields bands



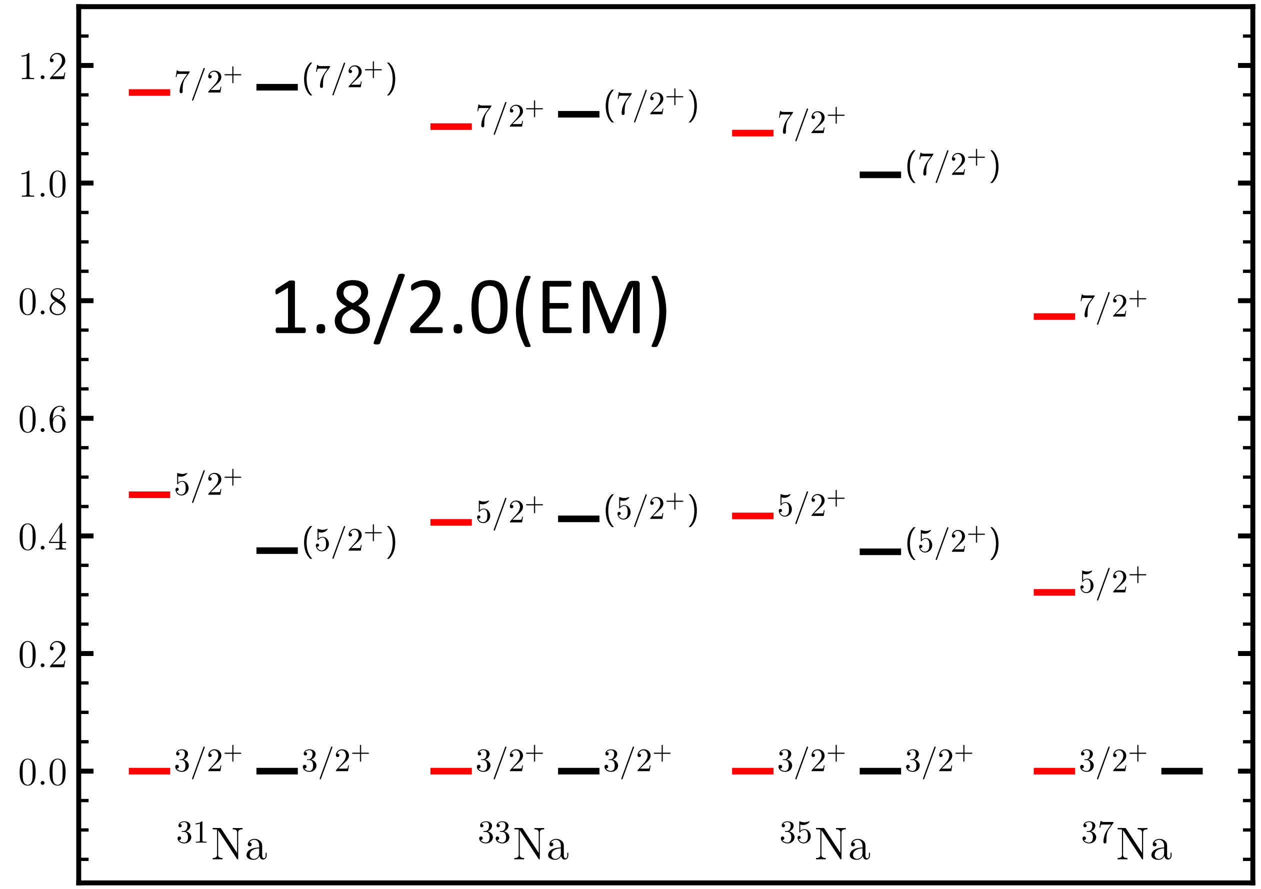
NCSM from Caprio, Maris, Vary & Smith,
Int. J. Mod. Phys. E 24, 1541002 (2015)

Rotational bands in odd-mass nuclei

Protons are paired
Neutron occupy (j = d5/2, j_z=1/2, 3/2 and 5/2)

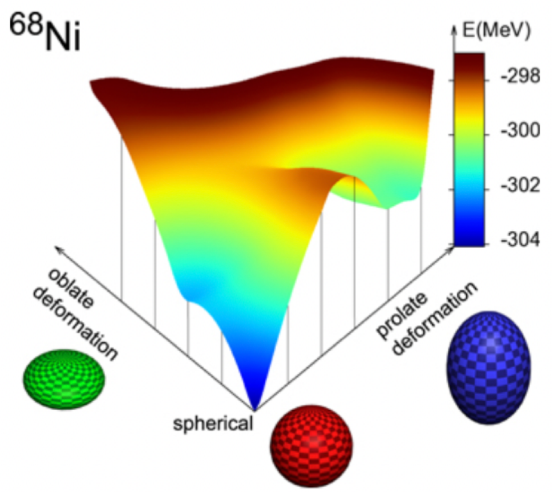


Proton occupy (j = d5/2, j_z=3/2)
Neutrons are paired.



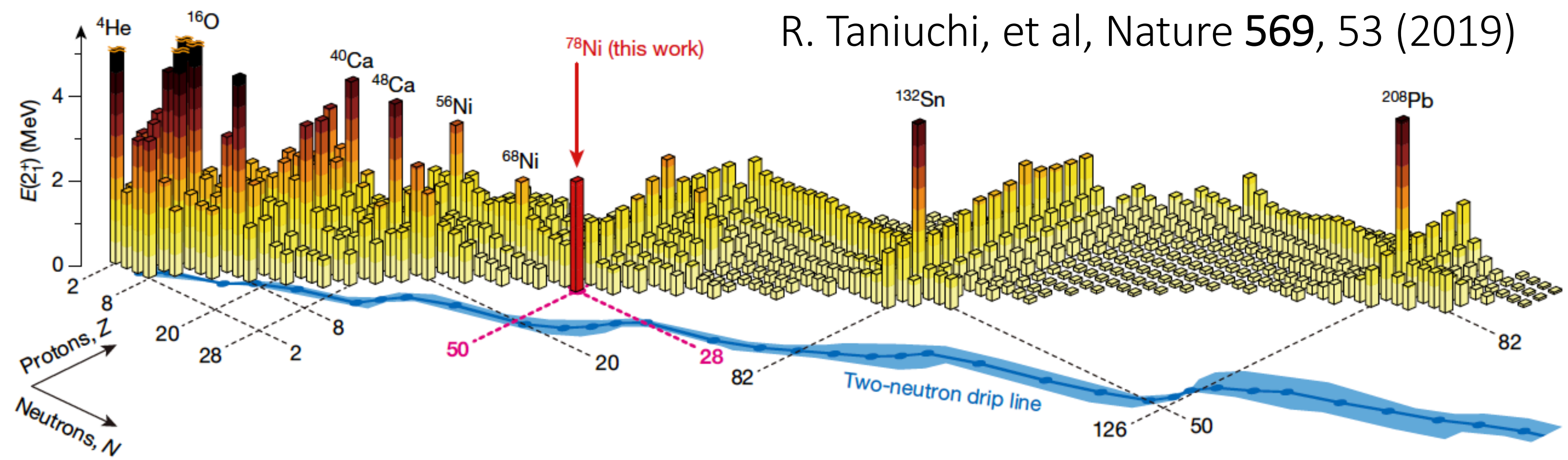
Zhonghao Sun et al., in preparation (2024)

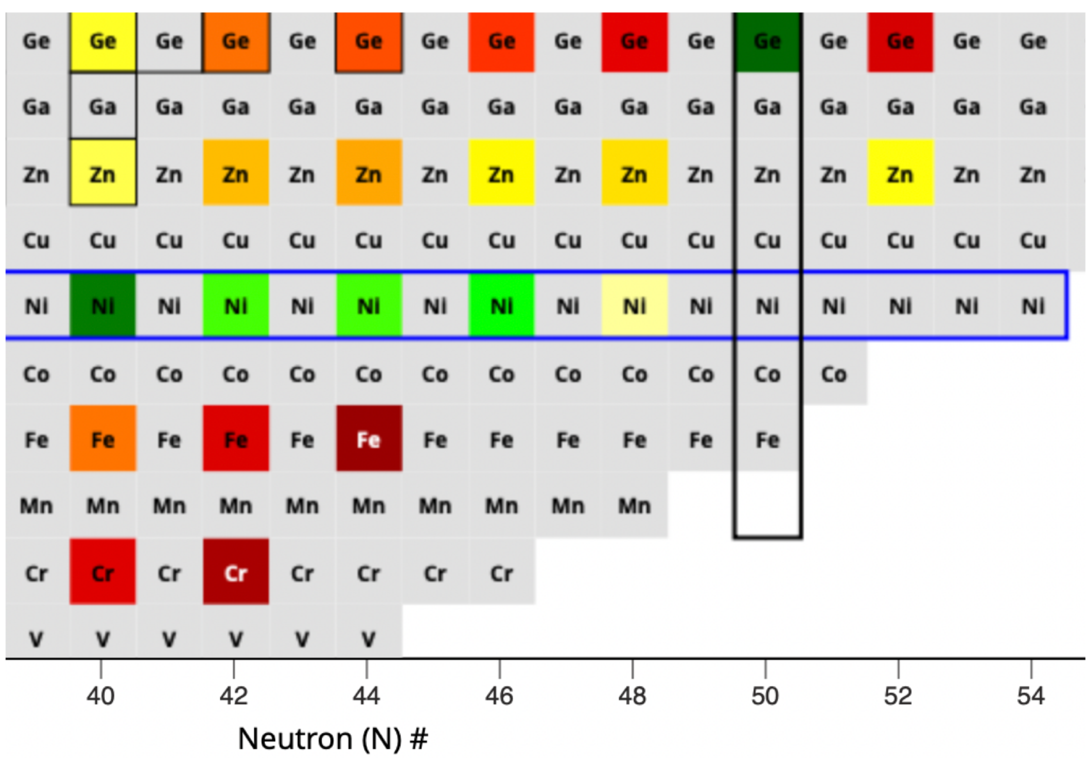
Onset of deformation around ^{78}Ni



T Otsuka and Y Tsunoda *J. Phys. G* **43** 024009 (2016)

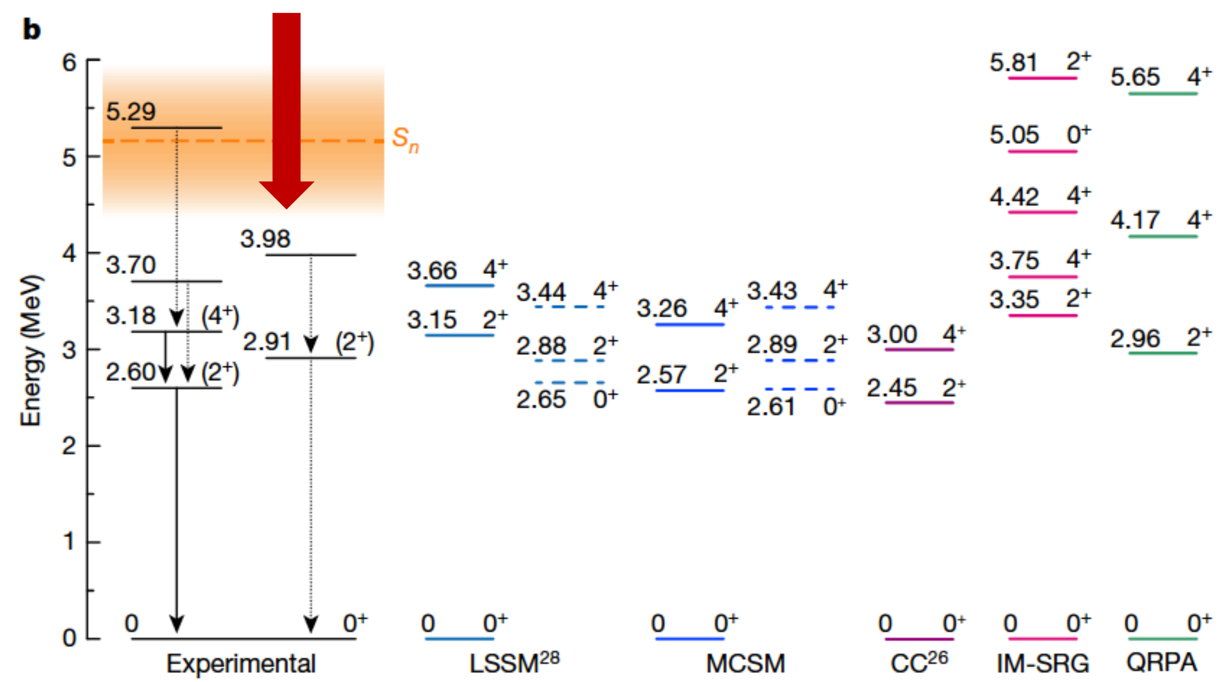
R. Taniuchi, et al, Nature **569**, 53 (2019)





Deformed band?

Where is the band head?



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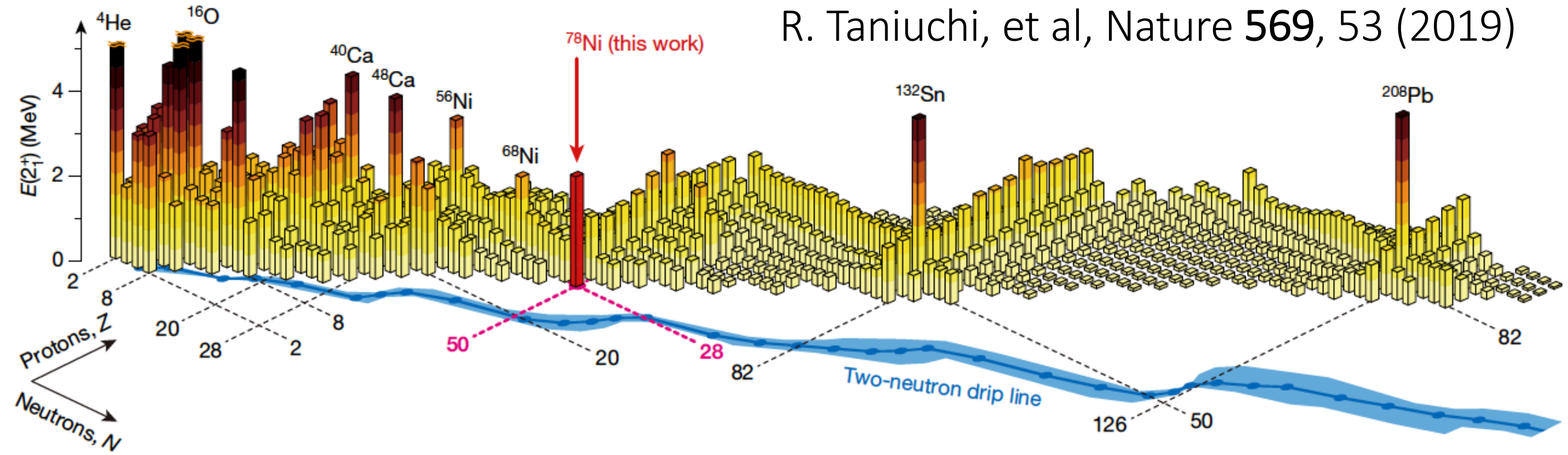
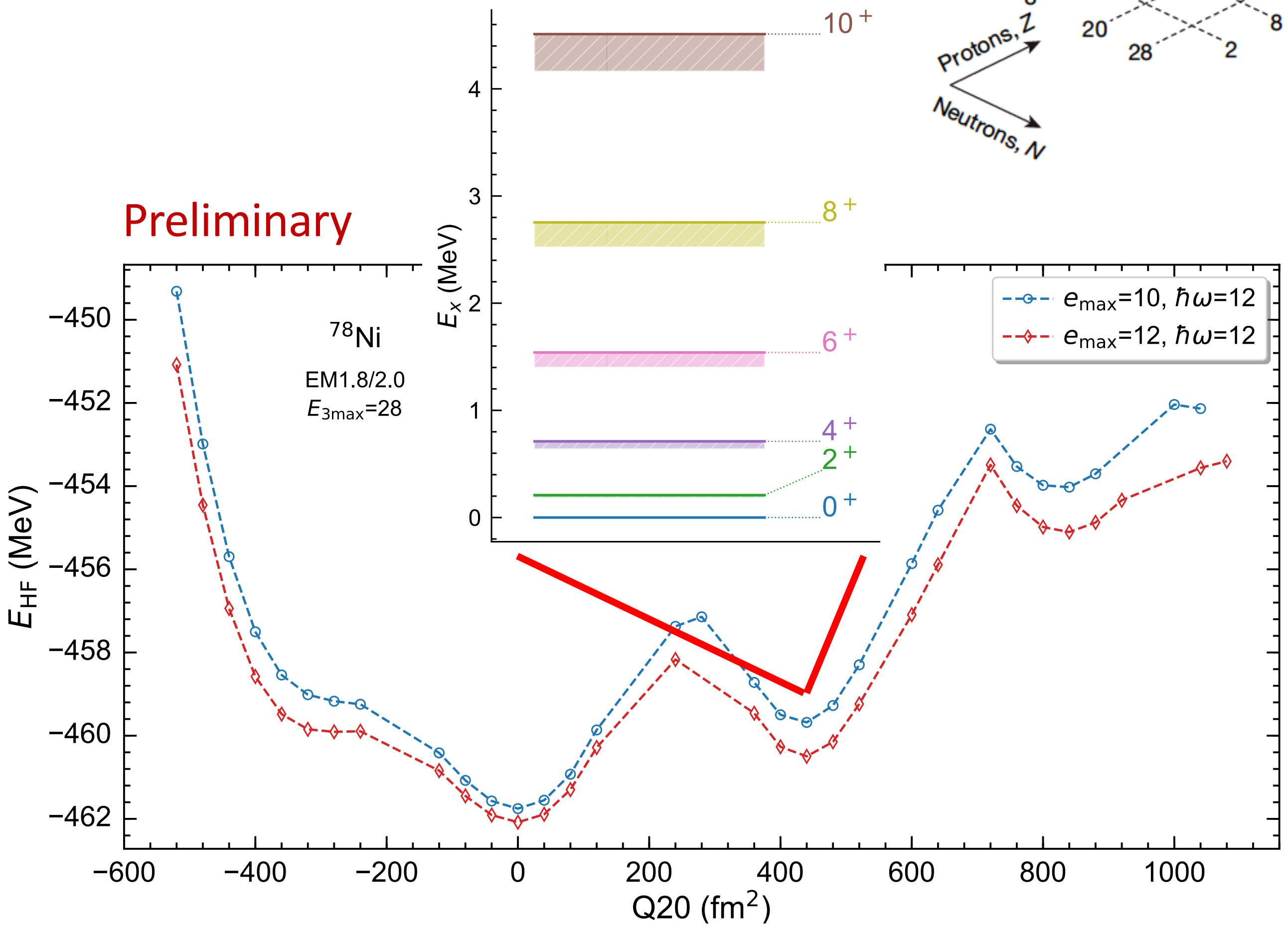
R. Taniuchi, et al, Nature **569**, 53 (2019)



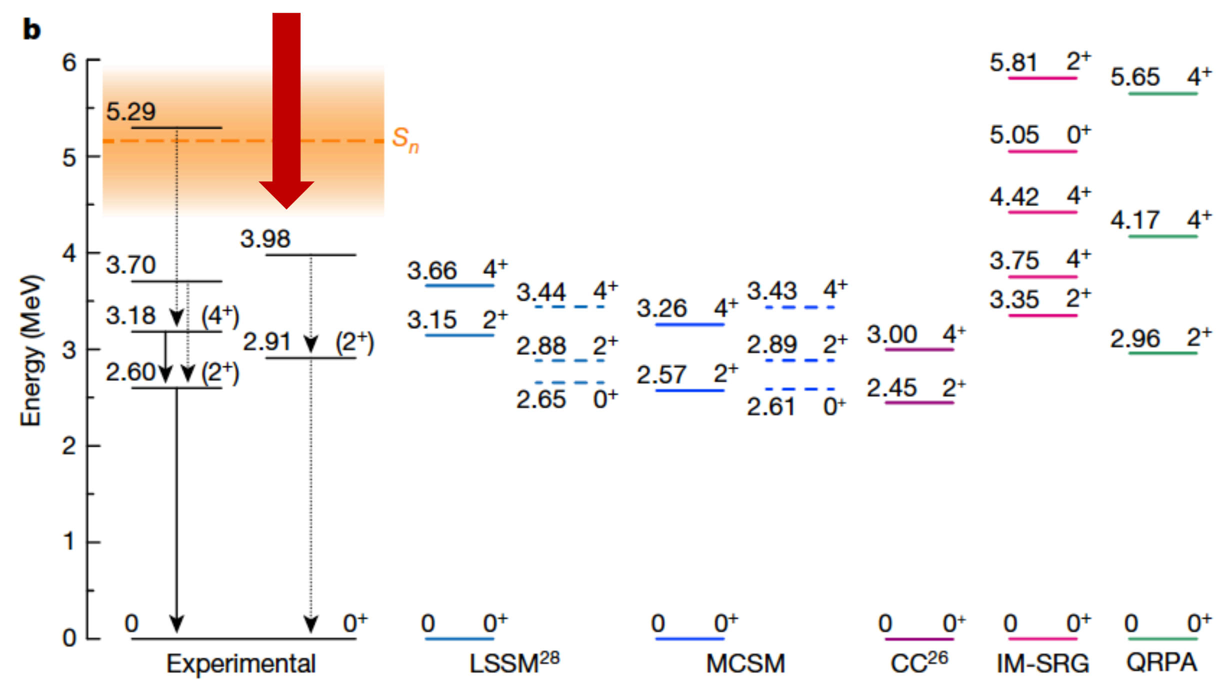
Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock. in preparation (2024)

Preliminary

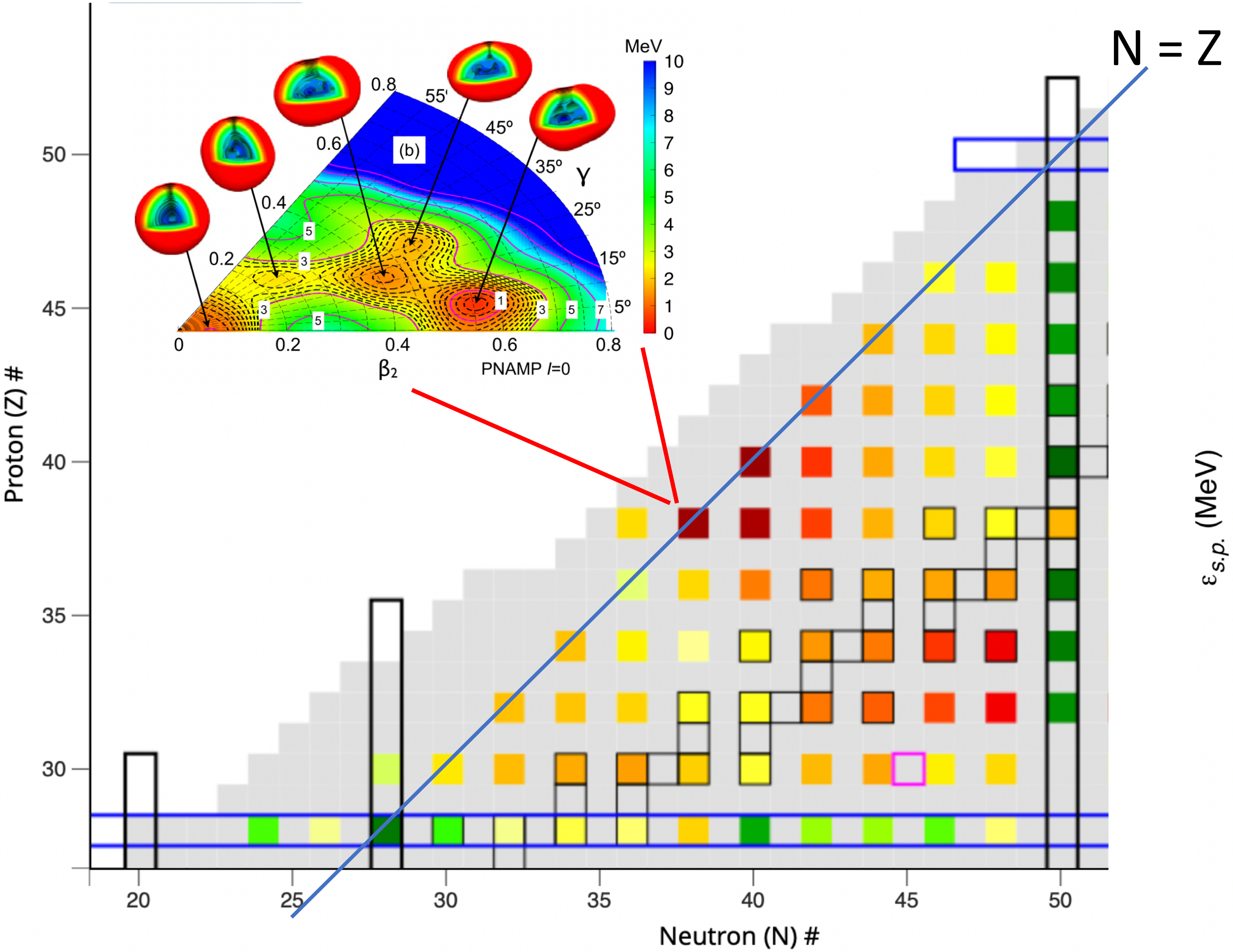


Deformed band?

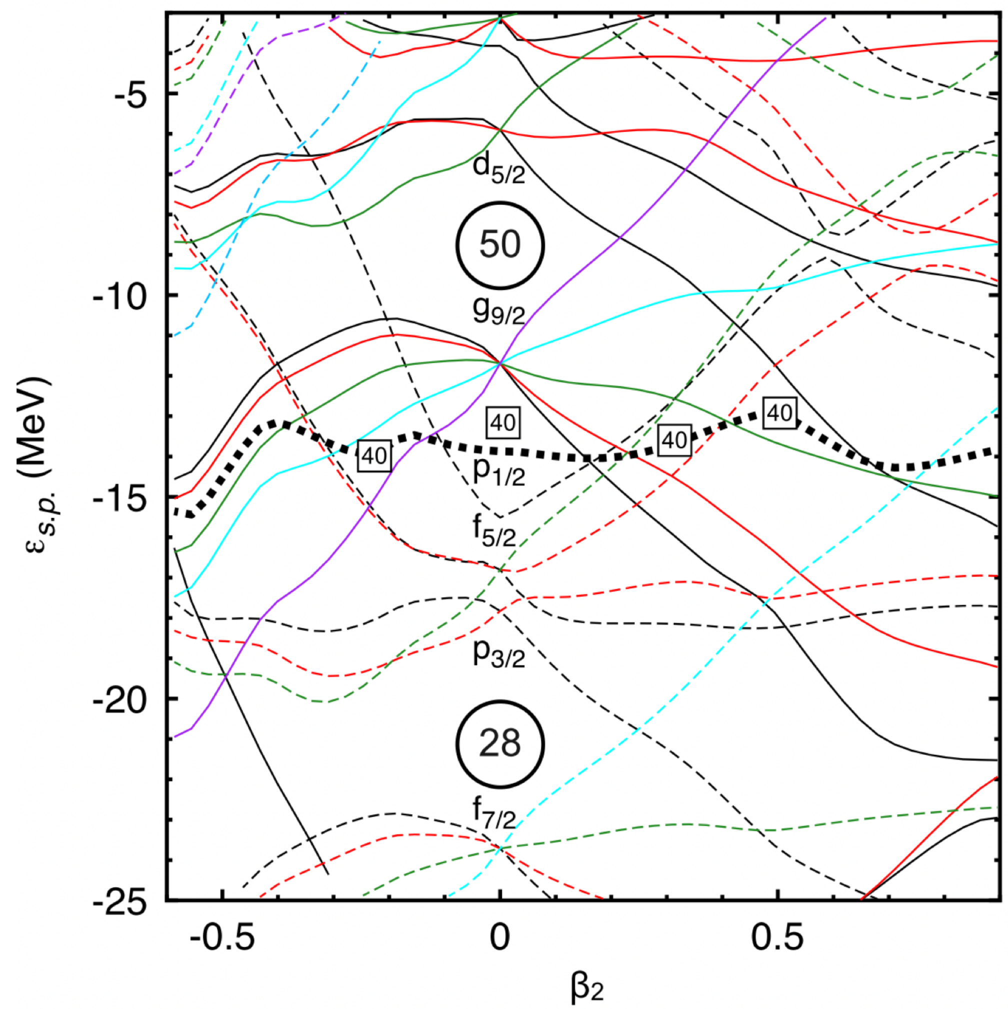
Where is the band head?



Coupled-cluster computations of strongly deformed nuclei around ^{80}Zr



Tomás R. Rodríguez, J. Luis Egido, Phys. Lett. B 705 255 (2011)



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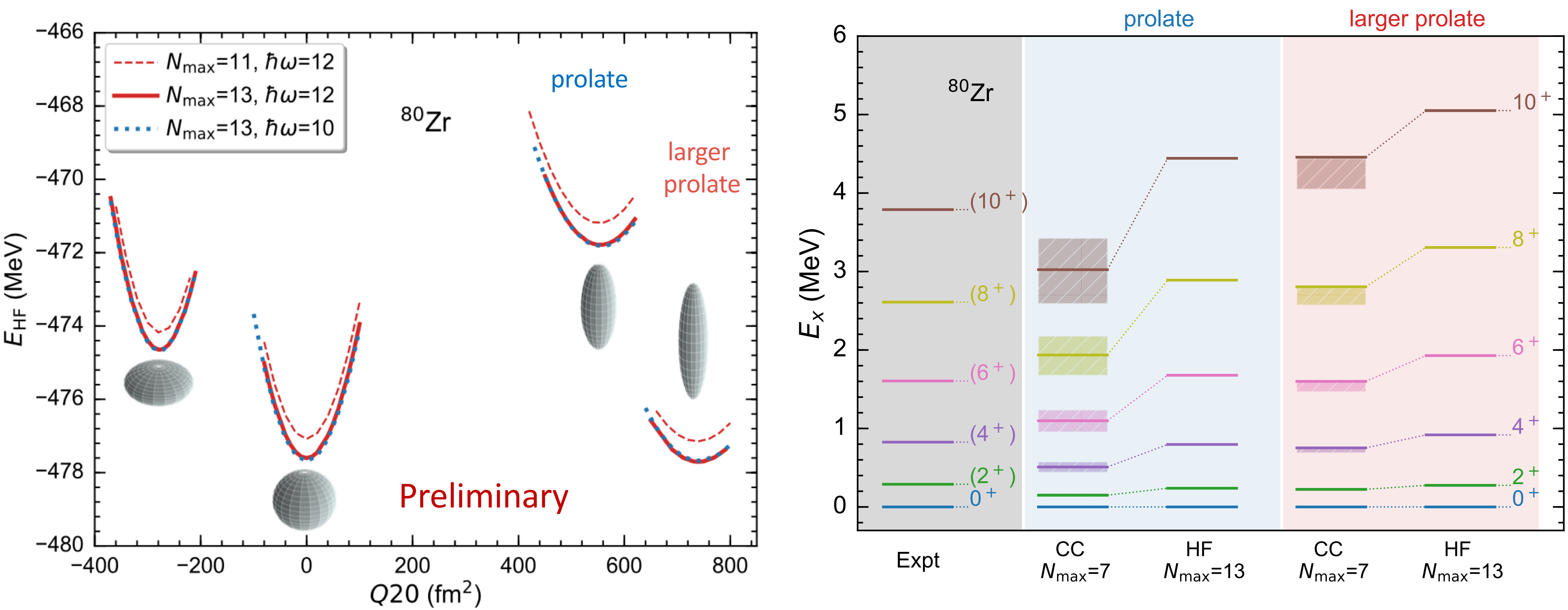
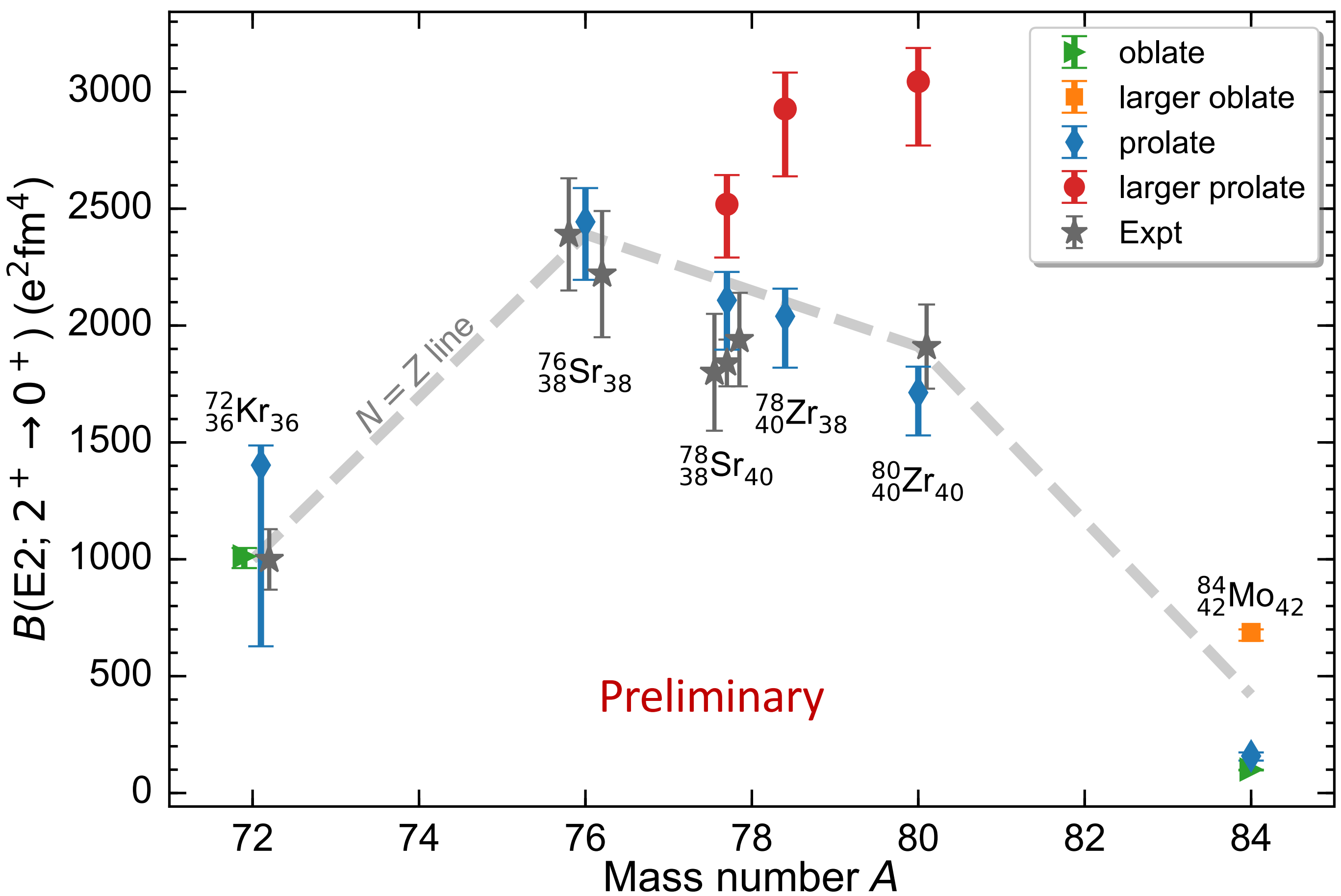


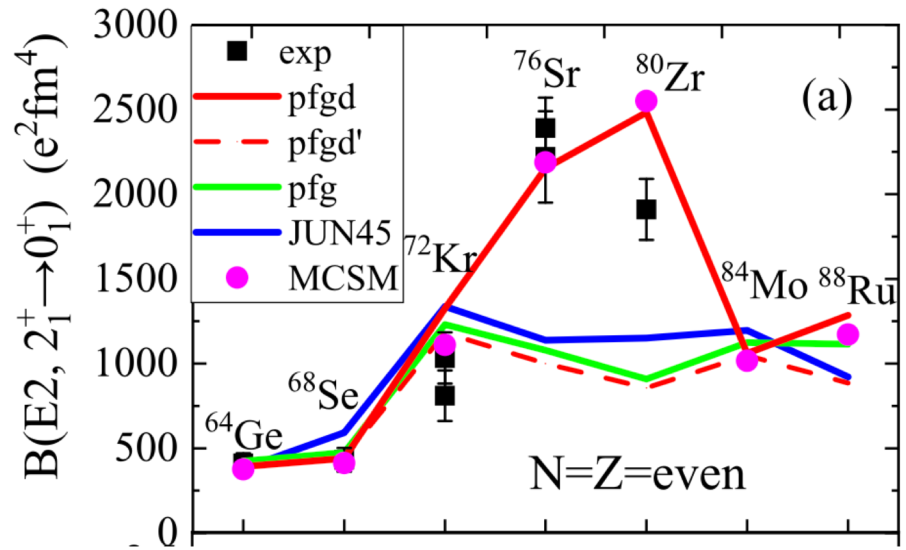
Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock. in preparation (2024)

Coupled-cluster computations of strongly deformed nuclei around ^{80}Zr

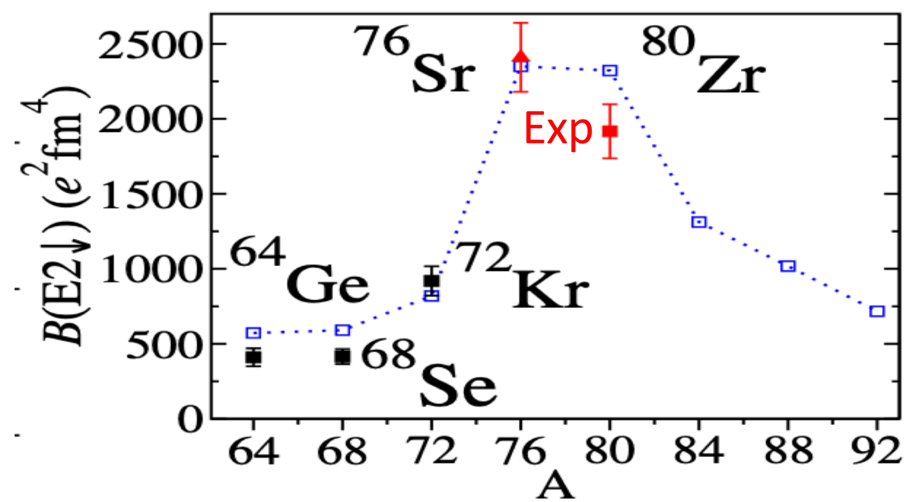


Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock.
in preparation (2024)

Shell model K. Kaneko, et al, Phys Lett B **817**, 136286 (2021)



Mean field R.D.O. Llewellyn, et al, Phys Rev Lett **124**, 152501 (2020)



Summary

- Neutron-rich neon isotopes are strongly deformed: ^{34}Ne as rotational as ^{32}Ne and ^{34}Mg
- Electromagnetic transitions follow experimental trends
- Signatures of shape co-existence along N = 20 towards ^{28}O
- Nuclei around ^{80}Zr are strongly deformed with rich prolate and oblate structure
- Predict low-lying rotational states in ^{78}Ni consistent with data and shell-model predictions

Thank you for your attention!