Ab initio computations of strongly deformed nuclei near ^{80}Zr

B. S. Hu, Z. H. Sun, G. Hagen, and T. Papenbrock
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Changfeng Jiao
Shool of Physics and Astronomy
Sun Yat-Sen University

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Introduction

- Atomic nuclei in the vicinity of the neutron deficient nucleus ^{80}Zr have a rich and interesting structure: strongly deformed, exhibit shape coexistence and mixing, and pose a difficult task to nuclear models.
  - energy ratio $R_{4/2}$ and reduced *E*2 transition probability B(*E*2)
- Shape transition and coexistence and deformation in the heavy $N \approx Z$ region have been studied using:
  - mean-field methods
  - large-scale shell model
- Unsolved issues:
  - Mean-field methods overpredict the B(*E*2) in ^{80}Zr
  - Several calculations yield a spherical (and not a deformed) ground state.
  - The recent high-precision mass measurement of ^{80}Zr revealed a large deformed shell gap which nuclear models find difficult to explain
- It interesting to see how *ab initio* methods fare in this region.

Introduction

This paper study the structure and electric quadrupole transitions of the nuclei ^{72}Kr, ^{76,78}Sr, ^{78,80}Zr, and ^{84}Mo based on chiral nucleon-nucleon and three-nucleon forces.

"to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities."

In this paper, the calculations start from axially deformed Hartree-Fock states, and one calculates the energy using single reference coupled cluster theory. The broken rotational symmetry is then restored through angular momentum projection.

The Model

Start from the intrinsic Hamiltonian

$$H = T - T_{\text{c.m.}} + V_{NN} + V_{3N},$$

For the two-nucleon (NN) interaction V_{NN} and three-nucleon (3N) interaction V_{3N} they use the chiral interaction 1.8/2.0(EM), which yields accurate ground-state energies and spectra of light, medium, and heavy mass nuclei.

The *NN* interaction is calculated in the harmonic-oscillator basis with spacing $\hbar\omega$ and single-particle energies up to $N_{\max}\hbar\omega$; the 3*N* interaction is truncated to excitation energies of three nucleons up to $E_{3\max} = 28\hbar\omega$.

One uses the NO2B approximation modified for deformed nuclei.

The Model

The calculations start from the symmetry-unrestricted product state

$$|\Phi\rangle \equiv \prod_{i=1}^{A} c_i^\dagger |0\rangle$$

This state breaks angular momentum but its projection J_z, parity, isospin projection, and mass number A are conserved, and that they deal with even-even nuclei.

Then, the reference is also invariant under time reversal , invariant under rotations by an angle π around any axis that is perpendicular to the symmetry axis (denoted as *R*-parity), and fulfills $J_z|\Phi\rangle = 0$

One performed axially symmetric Hartree-Fock computations using the Hamiltonian

$$H' = H - \lambda Q_{20} \quad \text{where} \quad Q_{20} = \sqrt{\frac{16\pi}{5}} \sum_{i=1}^{A} r_i^2 Y_{20}(\theta_i, \phi_i)$$

The corresponding product state is the Hartree-Fock restricted-variation-after-projection (HF-RVAP) reference.

The Model

One need to account for short-range (dynamical) and long-range (static) correlations. The former is included via couple-cluster with singles and doubles (CCSD) computations, and the latter via symmetry restoration.

The Hamiltonian is

$$H = \sum_{pq} \varepsilon_{pq} c_p^\dagger c_q + \frac{1}{4} \sum_{pqrs} v_{pqrs} c_p^\dagger c_q^\dagger c_s c_r$$

Normal order the Hamiltonian with respect to the vacuum state and write

$$H = E_{\text{ref}} + H_N$$

where the vacuum energy is

$$E_{\text{ref}} = \langle \Phi | H | \Phi \rangle = \sum_{i=1}^{A} \varepsilon_{ii} + \frac{1}{2} \sum_{i,j=1}^{A} v_{ijij}$$

The normal ordered Hamiltonian is

$$H_N = \sum_{pq} f_{pq} \left\{ c_p^\dagger c_q \right\} + \frac{1}{4} \sum_{pqrs} v_{pqrs} \left\{ c_p^\dagger c_q^\dagger c_s c_r \right\}$$

The Fock matrix elements are $f_{pq} = \varepsilon_{pq} + \sum_{i=1}^{A} v_{piqi}$.

The Model

Traditional couple-cluster method

Couple-cluster theory parameterizes the ground state as

$$|\Psi\rangle \equiv e^{T}|\Phi\rangle \ .$$

The cluster operator

$$T \equiv T_1 + T_2 + ... + T_A$$

consists of *np-nh* excitation operators

$$T_n = \frac{1}{(n!)^2} \sum_{\substack{a_1 \ldots a_n \\ i_1 \ldots i_n}} t_{i_1 \ldots i_n}^{a_1 \ldots a_n} c_{a_1}^{\dagger} \cdots c_{a_n}^{\dagger} c_{i_n} \cdots c_{i_1} \ .$$

where $t_{i_1 \ldots i_n}^{a_1 \ldots a_n}$ is the cluster amplitudes.

The Model

Traditional couple-cluster method

Inserting this wave function ansatz into the Shroedinger equation yields

$$H\mathrm{e}^{T}|\Phi\rangle = E\mathrm{e}^{T}|\Phi\rangle$$

$$0 = \langle\mu|(H-E)\mathrm{e}^{T}|\Phi\rangle, \quad \text{where } |\mu\rangle \text{ is an excited determinant.}$$

One multiplies both sides by exp(−T) to get a similarity-transformed Schroedinger equation

$$\mathrm{e}^{-T}H\mathrm{e}^{T}|\Phi\rangle = \bar{H}\Phi|\rangle = E|\Phi\rangle$$

Now the energy and amplitudes define T are obtained from

$$E = \langle\Phi|\bar{H}|\Phi\rangle,$$
$$0 = \langle\mu|\bar{H}|\Phi\rangle.$$

Since $\bar{H}$ is non-Hermitian, its left-hand eigenstate is not the adjoint of its right-hand eigenstate.

The Model

Traditional couple-cluster method

One can parameterize the left-hand eigenstate as

$$\langle L| = \langle \Phi|(1+\Lambda),$$

The de-excitation operator Λ describe the different *ph* de-excitation levels

$$\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3 + \cdots + \Lambda_A$$

$$\Lambda_n = \frac{1}{(n!)^2} \sum_{\substack{i_1 \ldots i_n \\ a_1 \ldots a_n}} \lambda^{i_1 \ldots i_n}_{a_1 \ldots a_n} c^\dagger_{i_1} \cdots c^\dagger_{i_n} c_{a_n} \cdots c_{a_1}$$

We can solve for Λ by demanding that

$$\langle \Phi|(1+\Lambda)\bar{H} = E\langle \Phi|(1+\Lambda).$$

The Model

Traditional couple-cluster method

Or, solving Shroedinger equation can be equivalent to bi-variation

$$\mathcal{E} = \langle \Phi | (1+\Lambda)\bar{H} | \Phi \rangle = \frac{\langle \Phi | (1+\Lambda)\bar{H} | \Phi \rangle}{\langle \Phi | 1+\Lambda | \Phi \rangle},$$

$$0 = \frac{\partial \mathcal{E}}{\partial \Lambda_\mu}, \quad 0 = \frac{\partial \mathcal{E}}{\partial T_\mu},$$ individual amplitudes in the operator Λ and T

This is the coupled-cluster energy functional.

In practical calculations, Λ and T must be truncated. for example, the simplest theory is coupled cluster doubles (CCD). The numerically inexpensive couple-cluster singles and doubles (CCSD) approximation yields about 90% correlation energy for closed-shell nuclei.

$$T \approx T_1 + T_2$$ **(CCSD)**

The Model

Traditional couple-cluster method

In CCSD, the cluster amplitudes are computed by solving the couple-cluster equations (or the bi-variation)

$$\langle \Phi_i^a | e^{-T} H_N e^T | \Phi \rangle = 0 \ ,$$
$$\langle \Phi_{ij}^{ab} | e^{-T} H_N e^T | \Phi \rangle = 0 \ .$$

Here $|\Phi_{i_1 \cdots i_n}^{a_1 \cdots a_n}\rangle \equiv c_{a_1}^\dagger \cdots c_{a_n}^\dagger c_{i_n} \cdots c_{i_1} |\Phi\rangle$

The energy associated with the dynamical CCSD correlation is

$$\Delta E_{\mathrm{CCSD}} = \langle \Phi | e^{-T} H_N e^T | \Phi \rangle \ .$$

As $\langle \Phi | e^{-T} = \langle \Phi |$ and $\langle \Phi | \Psi \rangle = 1$

We can rewrite the total energy as

$$E = E_{\mathrm{ref}} + \Delta E_{\mathrm{CCSD}} = \frac{\langle \Phi | H | \Psi \rangle}{\langle \Phi | \Psi \rangle} \ .$$

The Model

Angular-momentum projection in CCSD approximation

and the AMP operator (axially) is

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

The projected coupled-cluster energy and amplitudes

$$E = \frac{\langle \Phi | P_J H \mathrm{e}^T | \Phi \rangle}{\langle \Phi | P_J \mathrm{e}^T | \Phi \rangle},$$

$$0 = \langle \mu | P_J (H - E) \mathrm{e}^T | \Phi \rangle,$$

or

$$E = \frac{\langle \Phi | \bar{P}_J \bar{H} | \Phi \rangle}{\langle \Phi | \bar{P} | \Phi \rangle}$$

$$0 = \langle \mu | \bar{P}_J (\bar{H} - E) | \Phi \rangle$$

Or the bi-variational coupled-cluster energy functional

$$E^{(J)} = \frac{\langle \widetilde{\Psi} | P_J H | \Psi \rangle}{\langle \widetilde{\Psi} | P_J | \Psi \rangle}.$$

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

$$0 = \frac{\partial E^{(J)}}{\partial T_\mu}, \quad 0 = \frac{\partial E^{(J)}}{\partial \Lambda_\mu}$$

The Model

Angular-momentum projection in CCSD approximation

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

with

$\mathcal{N}(\beta) \equiv \langle\Phi|R(\beta)|\Psi\rangle\,, \mathcal{H}(\beta) \equiv \langle\Phi|R(\beta)H|\Psi\rangle$ noted that $\mathcal{N}(\pi-\beta) = \mathcal{N}(\beta)\,,$ $\mathcal{H}(\pi-\beta) = \mathcal{H}(\beta)\,.$

To evaluate the kernels, one applies the Thouless theorem to act with the rotation operator on the symmetry-broken reference state

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

with

$$V(\beta) = \sum_{ia} V^i_a(\beta) c^\dagger_i c_a \,.$$

The Model

Angular-momentum projection in CCSD approximation

The kernels become (*V* depends on the Euler angle beta)

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

left with the evaluation of the reduced kernels

$$n(\beta) \equiv \langle\Phi|e^V e^T|\Phi\rangle\,,$$
$$h(\beta) \equiv \langle\Phi|e^V H e^T|\Phi\rangle\,.$$

Introduce the similarity transformation

$$\overline{H} \equiv e^V H e^{-V}$$

different from previous $\overline{H}$ for simplicity

yields

$$h(\beta) = \langle\Phi|\overline{H}e^V e^T|\Phi\rangle$$

The Model

Angular-momentum projection in CCSD approximation

The exact evaluation of $e^V e^T$ is exponentially expensive, so one introduces the disentangled cluster operator

$$W(\beta) = W_0 + W_1 + W_2 + \cdots + W_A$$

via $$e^V e^T |\Phi\rangle \equiv e^{W_0 + W_1 + W_2 + \cdots} |\Phi\rangle$$

where

$$W_k = \sum_n \frac{1}{(2n-k)!n!} \left(V^{2n-k} T_2^n\right)_{\mathrm{ce}}$$

$$= \frac{1}{(k!)^2} \sum W^{a_1 \ldots a_k}_{i_1 \ldots i_k} c^\dagger_{a_1} \ldots c^\dagger_{a_k} c_{i_k} c_{i_1}.$$

for $k \geq 1$, W_0 is a number given by

$$\mathrm{e}^{W_0} = \langle \Phi | \mathrm{e}^V \mathrm{e}^{T_2} | \Phi \rangle$$

The Model

Angular-momentum projection in CCSD approximation

The disentangled cluster operators W can be obtained by solving a set of ordinary differential equations (ODEs) with the Euler angle beta.

The derivative of *V* with respecto to beta is

$$\frac{\mathrm{d}}{\mathrm{d}\beta}V = \left(\mathrm{e}^{V}\left(-\mathrm{i}\hat{J}_y\right)\mathrm{e}^{-V}\right)_d \equiv X$$

The detailed ODEs can be found in Ref. [Y. Qiu *et. al.*, *Projected coupled cluster theory*, J. Chem. Phys. 147, 064111 (2017)]

with the initial ($\beta = 0$) values $W_0(0) = 0$, $W_1(0) = T_1$, and $W_2(0) = T_2$.

In this work, only the amplitudes W_0, W_1, and W_2 are kept.

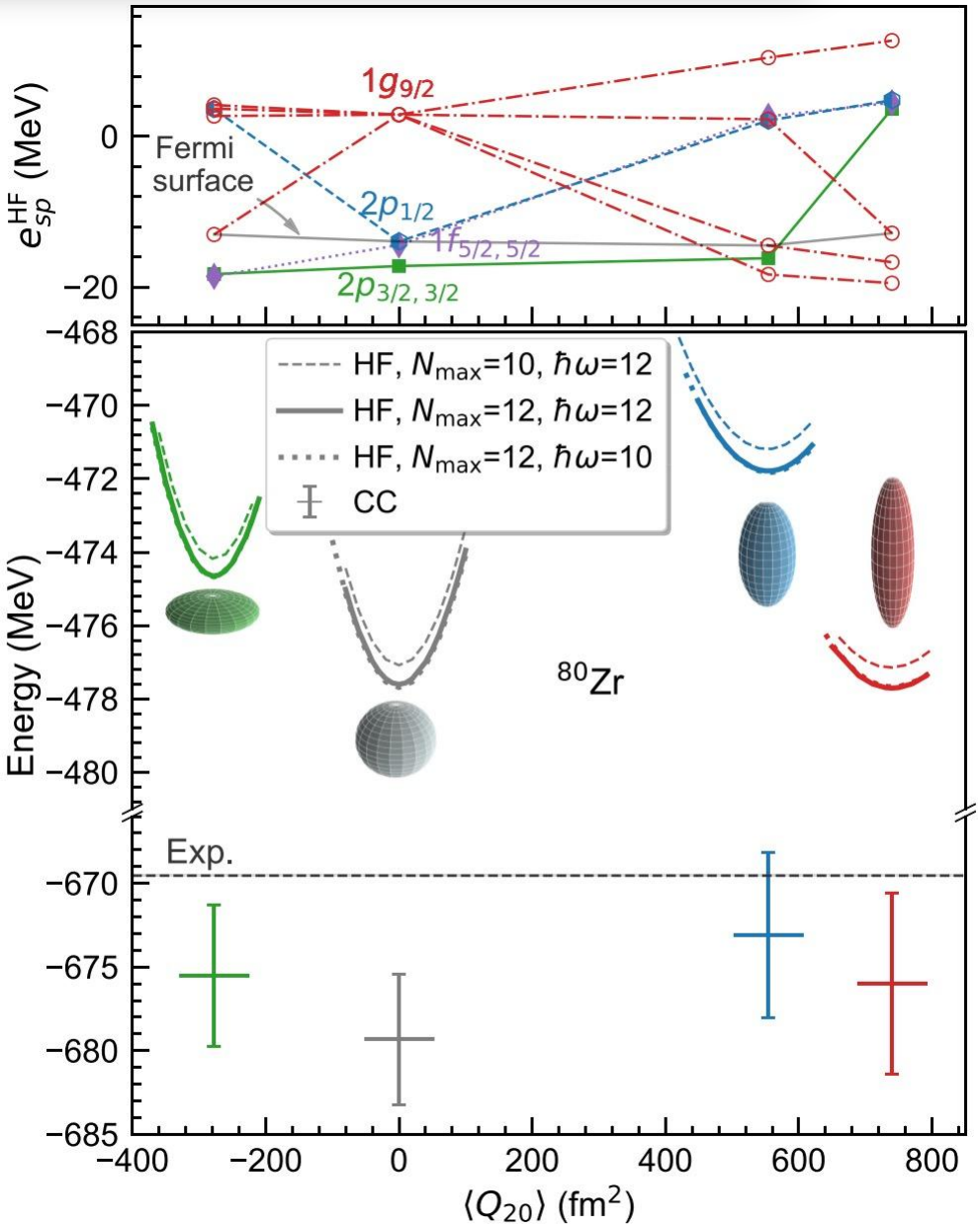
The detail of computing B(E2) can be found in Ref. [Z. H. Sun *et. al.*, *Multiscale physics of atomic nuclei from first principles*, arXiv:2404.00058.]

Results and discussions

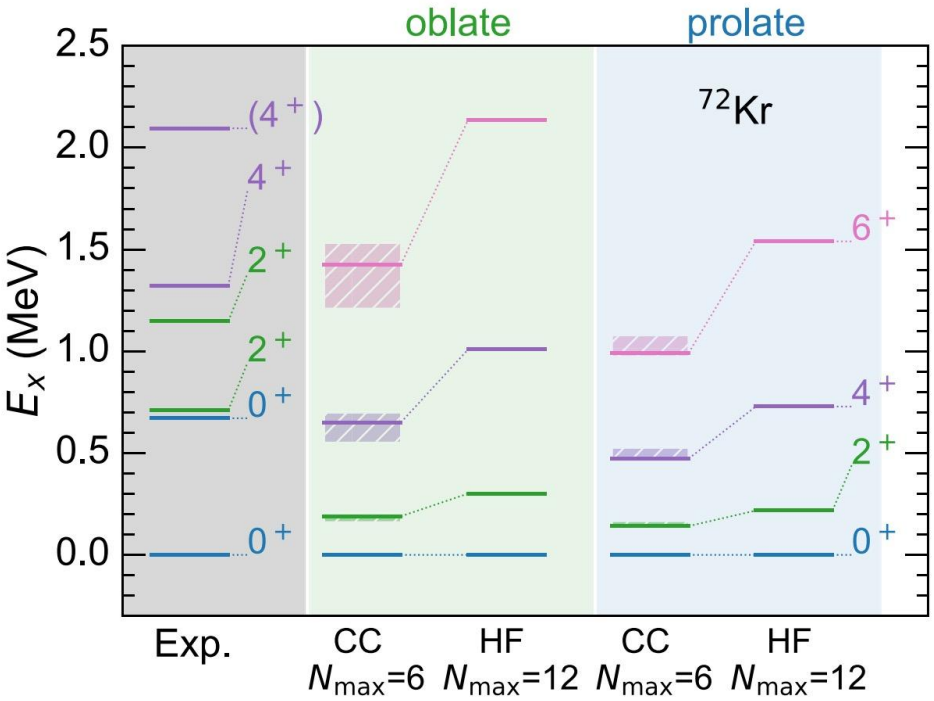
The middle part shows the unprojected Hartree-Fock energies of ^{80}Zr. The oblate, spherical, prolate, and larger prolate minimum have deformation parameters $\beta_2 \approx -0.17$, 0.0, 0.33 and 0.46, respectively.

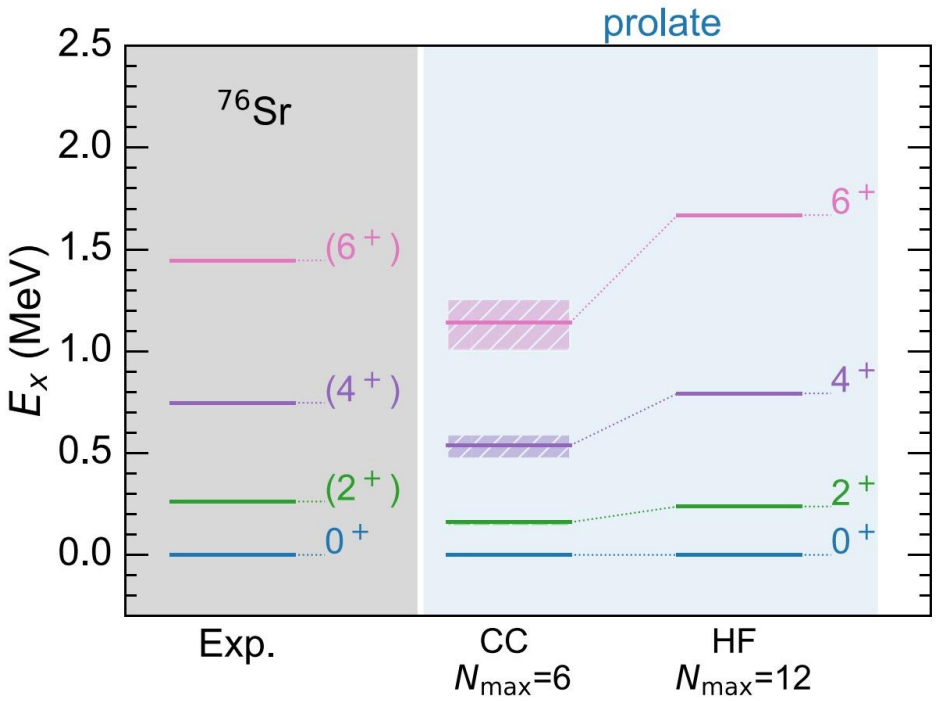
The lower part shows CC results obtained at each minimum that include estimated energy contributions from triples excitations and AMP.

The upper part shows how the different Hartree-Fock minima form a Nilsson diagram. The deformed minima are from the level crossing.



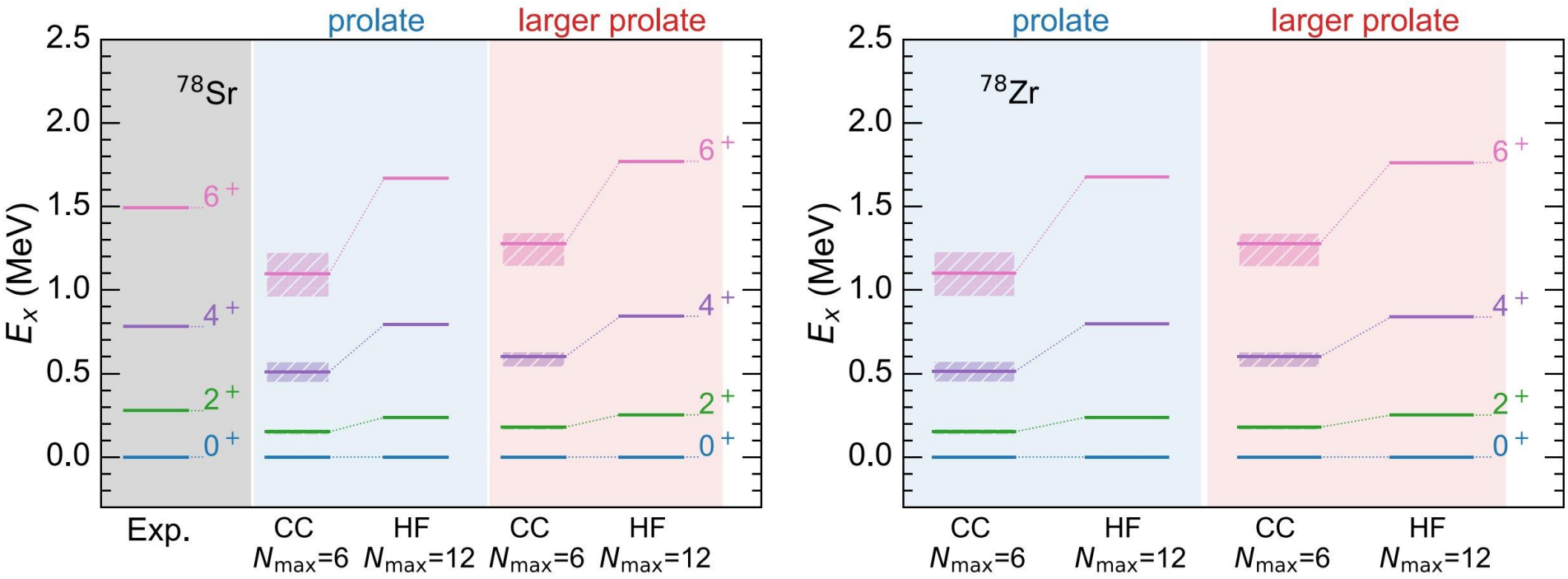
Results and discussions





The calculated rotational bands in ^{72}Kr and ^{76}Sr, and compares them to data. The angular-momentum projection in coupled cluster theory is expensive and restricted to $N_{max} = 6$ for spectra and $N_{max} = 8$ for the $B(E2)$'s. For ^{72}Kr, the computed spectrum suggests that the ground state and its rotational band are oblate deformed. *The pairs of oblate and prolate 0+ states and 2+ states are about 1 MeV and 0.8 MeV apart, respectively. This is probably too large a separation.*

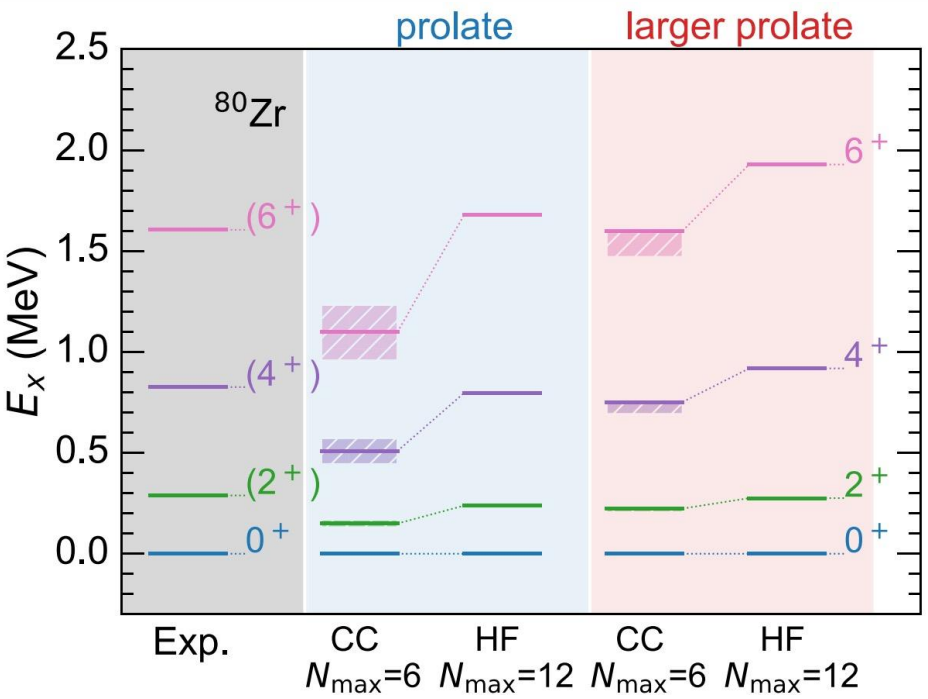
Results and discussions

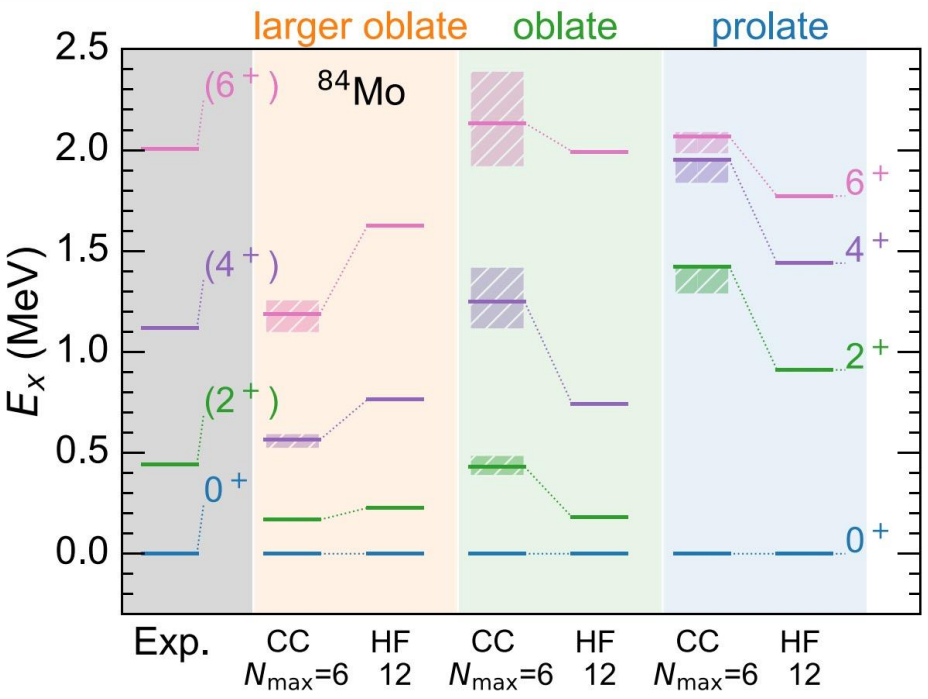


The mirror nuclei ^{78}Sr and ^{78}Zr both exhibit two deformed Hartree-Fock minima and similar rotational bands. Although the projected Hartree-Fock results are close to the results given by Delaroche et. al. [1] and the data in ^{78}Sr, the coupled-cluster spectra are too compressed.

[1] J. P. Delaroche et. al., Phys. Rev. C 81, 014303 (2010).

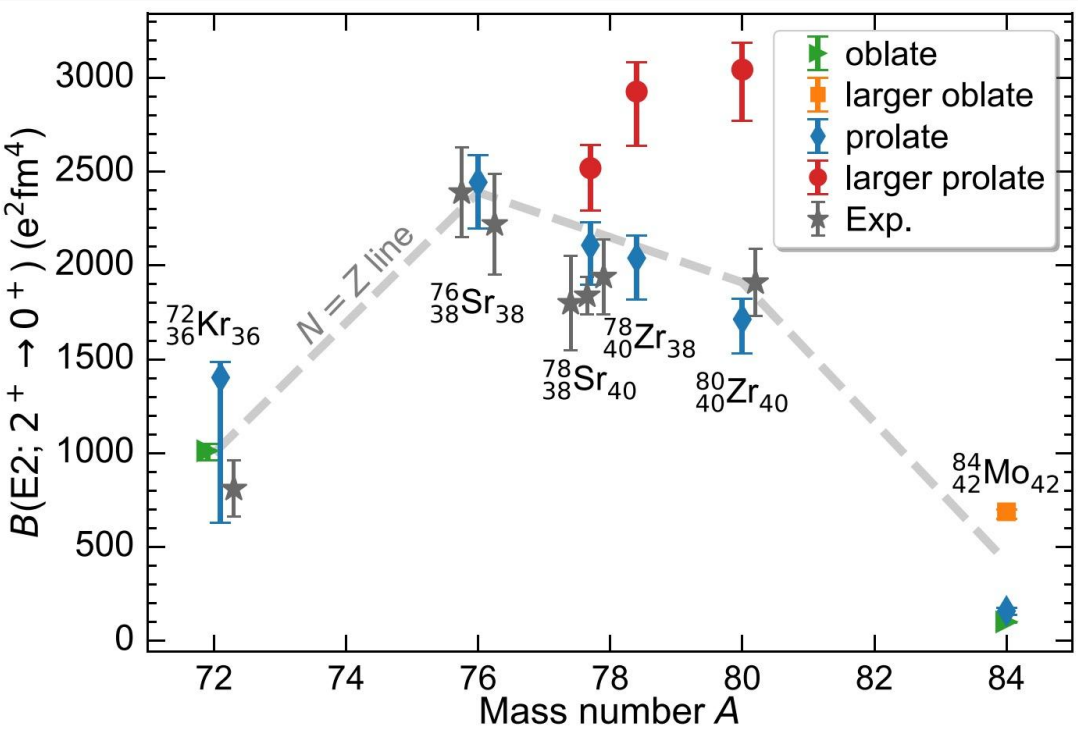
Results and discussions





In ^{80}Zr, the spectrum agrees with that found for the larger prolate minimum. For ^{84}Mo, Delaroche et al. found 2^+ and 4^+ states at 0.54 and 1.20 MeV, respectively, and this is close to data. The projected coupled-cluster results for the oblate deformation agree with these results.

Results and discussions



The coupled-cluster results of ^{72}Kr and ^{76}Sr agree with the data. The B(E2) of ^{78}Sr and ^{80}Zr suggest that the prolate state is the ground state. The larger-prolate configuration reproduces a relatively correct spectrum but too large B(E2). The B(E2) values of the mirror nuclei pair ^{78}Sr and ^{78}Zr agree within uncertainties for both deformations.

Results and discussions

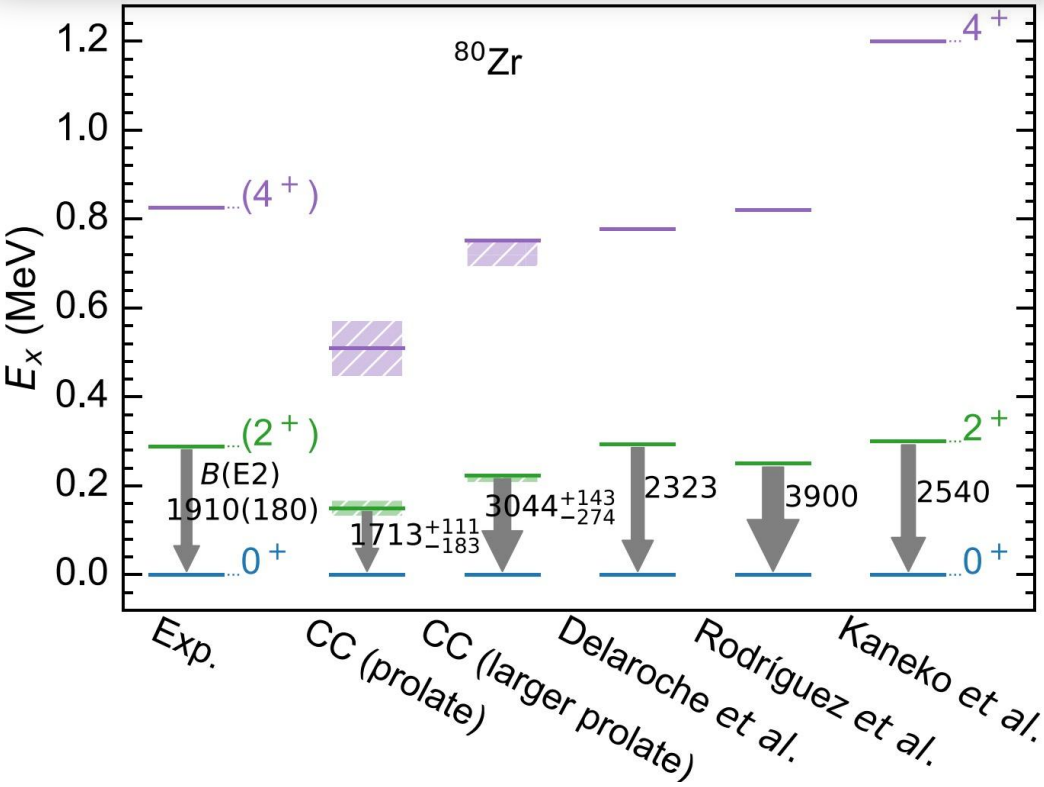


TABLE I. $B(E2; 2^+ \rightarrow 0^+)$ values (in units of e^2fm^4) from experiment, this work, Delaroche *et al.* [29], and other references for various nuclei. The values reported under "This work" are those presented in Fig. 3 and reflect the shapes and deformation as indicated there.

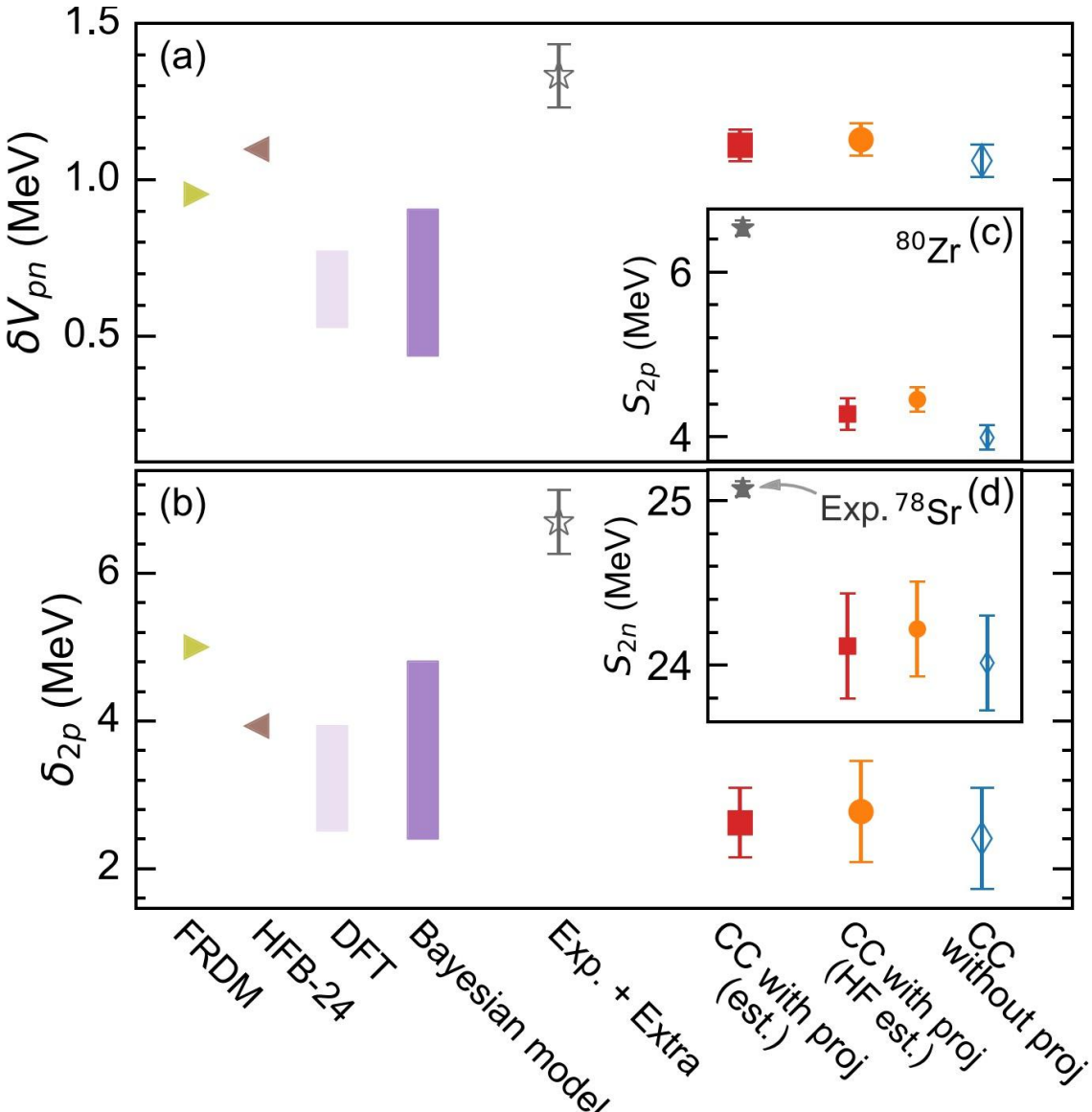
Nucleus	Exp.	This work	Ref. [29]	Other
^{80}Zr	1910(180)[a]	1713^{+111}_{-183}	2323	3900[b]
		3044^{+143}_{-274}		2540[f]
^{78}Zr	not known	2040^{+118}_{-220}	2504	
		2927^{+155}_{-288}		
^{78}Sr	1840(100)[a]	2108^{+121}_{-211}	1989	2291[f]
		2519^{+125}_{-228}		
^{76}Sr	2390(240)[a]	2444^{+145}_{-248}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

Here compares the data for ^{80}Zr with the results from this work and other models. ***Challenging!***

The main point is here that PCC calculations reach an accuracy that is comparable to other nuclear models.

Results and discussions

The mass anomaly near N = Z = 40.



Four-point mass difference

$$\delta V_{pn} = \tfrac{1}{4}[B(N,Z) - B(N-2,Z) - B(N,Z-2) + B(N-2,Z-2)]$$

Two-proton shell gap

$$\delta_{2p} = 2B(N,Z) - B(N,Z+2) - B(N,Z-2).$$

Theoretical approaches struggle to reproduce the four-point mass difference and the two-proton shell gap. The PCC results underestimated, which may due to missing correlations in the CCSD, the employed interaction, and the normal-ordered two-body approximation of the 3*N* interaction.

Summary

- Investigated the low-lying collective states and B(E2) values in the heavy $N = Z$ region using the ab initio coupled cluster calculations based on axially symmetric reference states followed by angular-momentum projection.
- While coexistence between various oblate and prolate shapes was found, the calculations were not precise enough to unambiguously identify the shape of the ground states.
- This discrepancy of theoretical calculations and data in these region remains a challenge to nuclear theories.
- The computations presented here provide us with a useful step towards the description of deformed nuclei in heavy-ion collisions, and for tests of fundamental symmetries