First complete shell-model description of ^{254}No: a new paradigm for superheavy nuclear structure studies

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Introduction

- In the search of unknown elements that delineates the border of the periodic table, superheavy nuclear elements (**SHE**), loosely defined with $Z \geq 102$, represent one of the most challenging regions both experimentally and theoretically.

- Covariant and nonrelativistic mean field models with density-dependent forces such as ***Skyrme*** and ***Gogny*** forces, generically designated as Energy Density Functionals (**EDFs**), are so far the only microscopic tools to study these exotic nuclei.

- a large amount of spectroscopic data has been accumulated for heavy actinides surrounding the $N = 152$:
  nuclear masses, deformation landscapes, fission related properties, and the pattern of single-particle spectra.

Introduction

Current theoretical approaches for these actinide nuclei

- Average potential (e.g., Woods-Saxon) + pairing treatment.
- HFB approximation derived from the EDFs.
- Beyond-mean-field within the EDFs.
  - Angular-momentum and particle-number projections of one single HFB state.
  - Configuration mixing of projected HFB states.
- Application of shell model to ^{254}No is out of reach.
- A approximate "shell model": GCM combined with the AMP using Kuo-Herling effective interaction showed a surprising agreement with data for the rotational band at the price of one Slater determinant.

Introduction

Previously, the authors developed discrete nonorthogonal shell model (DNO-SM) .

Diagonalize valence shell-model Hamiltonians in a nonorthogonal basis with the use of beyond-mean-field techniques. i.e., a GCM-like method mixing nonorthogonal angular-momentum projected HF states

In this paper, the authors extend the DNO-SM in a variation-after-projection scheme: DNO-SM(VAP). They perform a systematic shell-model comparison of spectra for nuclei around A ~ 254, and assess the ground and various excited structures of ^{254}No.

The Model

Generator-coordinate method (GCM)

The GCM is based on the assumption that the trial wave function $|\Psi_\alpha\rangle$ of a nuclear state labeled with α is written as a continuous superposition of the basis functions $|\phi_q\rangle$, with a continuous parameter set q,

$$|\Psi_\alpha\rangle = \int dq f_q^\alpha |\phi(q)\rangle$$

where the parameters q denote a set of collective variables — the so-called generator coordinates and they do not appear in the nuclear state wave function $|\Psi_\alpha\rangle$. The weight f(q) also called "generator function" is folded into the basis functions to produce the wave function $|\Psi_\alpha\rangle$. The internal degrees of freedom are supposed to be taken into account by the functions $|\phi_q\rangle$

In practical, the generator coordinate q is discretized.

$$|\Psi\rangle = \sum_{i=0}^{\infty} f(q_i)\,|\Phi(q_i)\rangle,$$

The Model

Generator-coordinate method (GCM)

Variation of the energy w.r.t. the weight function corresponds to a diagonalization of ***H*** spanned in the subspace consisting of projected wave function. It leads to the Hill-Wheeler-Griffin equations

$$\sum_{i=0}^{\infty}[\mathcal{H}(q_{i'}, q_i) - E\ \mathcal{N}(q_{i'}, q_i)]f(q_i) = 0,$$

where $\mathcal{O}(q_{i'}, q_i) = \langle\Phi(q_{i'})|\hat{\mathcal{O}}|\Phi(q_i)\rangle \quad (\hat{\mathcal{O}} = \hat{\mathcal{H}}, \mathbf{1})$

are Hamiltonian kernels and norm kernels.

The truncation of the infinite countable set could be done in a variational way such that the finite sum

$$|\Psi\rangle \approx \sum_{i=0}^{n} f(q_i)|\Phi(q_i)\rangle$$

yields an optimal approximation.

The Model

Projected constrained Hartree-Fock basis

The basis are built upon the constrained Hartree-Fock calculations under the conditions

$$\frac{1}{2}\langle\Phi|\hat{Q}_{\lambda\mu} + (-)^{\mu}\hat{Q}_{\lambda-\mu}|\Phi\rangle = Q_{\lambda\mu},$$

$$\langle\Phi|\hat{J}_m|\Phi\rangle = \langle\hat{J}_m\rangle \ \ (m = x, z),$$

where $\hat{Q}_{\lambda\mu} = r^{\lambda}Y_{\lambda\mu}(\theta, \varphi)$ is the multipole operator expressed in terms of the spherical harmonics, and $\hat{J}_m$ the components of the total angular momentum operator $\hat{\mathbf{J}}$.

the resulting HF state is projected onto good angular momentum *J*. This provides us a family of PCHF states characterized by the angular momentum projection onto the intrinsic axis |*K*| ≤ *J* and the coordinate *q* for a given J.

The Model

Truncation of the PCHF basis with the generalized minimization technique

Based on the selection of discrete values of the coordinate(s) q which minimizes the energy, we let the Hamiltonian itself choose what is the best state from a variational viewpoint.

- Fix the state $E_\alpha(J)$ to be minimized with α indexing energy levels
- Define a searching region of the coordinate(s) q.
- Start from the first point which can be chosen as the HF minimum.
- The second point is chosen in such a way that the energy obtained from solving the HWG equations in the 2-dimensional space spanned by these two basis be a minimum.
- Proceed the same way in next iterations until the convergence of $E_\alpha(J)$.

In practice, the convergence criterion is defined by the absolute energy gain $\Delta E_\alpha^{(J)}(k) = E_\alpha^{(J)}(k) - E_\alpha^{(J)}(k-1)$ at the iteration number k.
If $\Delta E_\alpha^{(J)}(k) > \epsilon > 0$ we keep the CHF state; otherwise it is not retained.

The Model

Truncation of the PCHF basis with the generalized minimization technique

The key point is thus that minimizing as many excited states at the same time as possible.

This is done by comparing the energy differences $\{E_\alpha(J)\}$ for every state (α, J) in a given set of nuclear states which we want to describe. The procedure then continues until we find no more states satisfying the condition $\max\{\Delta E_\alpha^{(J)}\} > \epsilon$

The Model

From DNO-SM to DNO-SM (VAP)

Owing to the Thouless theorem, an arbitrary non-orthogonal Slater state can be defined as

$$|\phi_i\rangle = \mathcal{N} e^{\hat{T}} |\phi_0\rangle = \mathcal{N}\left(\mathbb{1} + \hat{T} + \frac{\hat{T}^2}{2!} + \frac{\hat{T}^3}{3!} + \cdots\right)|\phi_0\rangle$$

with the one-body operator

$$\hat{T} = \sum_{nm} Z^{(i)}_{nm} a^\dagger_n a_m$$

The fully projected wavefunction can be denote by

$$|\psi^{\pi JM}_\alpha\rangle = \sum_{i,K} C^{\pi J}_\alpha(i,K) \mathcal{P}^J_{MK}\, P^\pi |\phi_i\rangle$$

The Slate state $|\phi_i\rangle$ is determined by variation of the energy functional $\delta E^J_\alpha / \delta \phi_i$

where $$E^J_\alpha = \frac{\langle \psi^{\pi JM}_\alpha | \hat{H} | \psi^{\pi JM}_\alpha \rangle}{\langle \psi^{\pi JM}_\alpha | \psi^{\pi JM}_\alpha \rangle}.$$

The Model

From DNO-SM to DNO-SM (VAP)

In this way, by breaking and restoring the SO(3) symmetry simultaneously, one explicitly incorporates 1*p*1*h*, 2*p*2*h*, . . . , *NpNh* (*N* being the particle number of the system) into the non-orthogonal states $\{|\phi_i\rangle\}$ and takes full advantage of angular momentum projection.

The model space

Valence protons ($82 < Z < 126$):

$$0h_{9/2}, 0i_{13/2}, 1f_{7/2}, 1f_{5/2}, 2p_{3/2}, 2p_{1/2}$$

Valence neutron: ($126 < N < 184$)

$$0i_{11/2}, 0j_{15/2}, 1g_{9/2}, 1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}$$

Interaction: the effective Kuo-Herling interaction

- G. Herling and T. Kuo, Nucl. Phys. A 181, 113 (1972)
- E. Caurier, M. Rejmund, and H. Grawe, Phys. Rev. C 67, 054310 (2003).

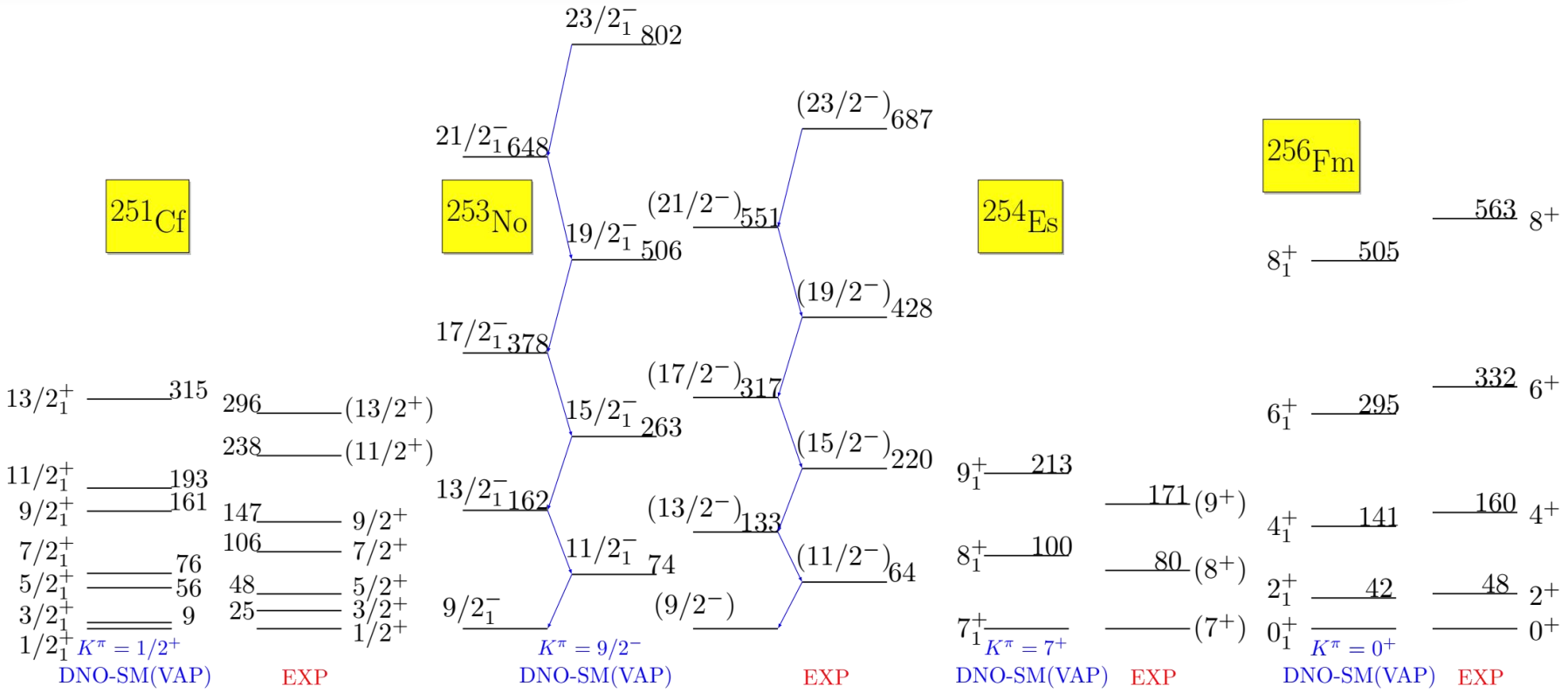
Results and discussions

To test the validity of the Kuo-Herling interaction, the calculated magnetic dipole moment μ and the spectroscopic quadrupole moment Q_s are compared with the experimental data.

J^π_{gs}		E (MeV)		$\mu(\mu_N)$			Q_s (eb)		
		PAV	VAP	PAV	VAP	EXP	PAV	VAP	EXP
^{253}No	$9/2^-$	−241.818	−242.816	+0.591	−0.493	−0.527(33)(75)	−3.5	+7.2	+5.9(1.4)(0.9)
^{253}Cf	$7/2^+$	−253.402	−253.818	−0.677	−0.556	−0.731(35)	+5.77	+5.78	+5.53(51)
^{251}Cf	$1/2^+$	−241.321	−241.724	−0.727	−0.610	−0.571(24)	-	-	-
^{249}Cf	$9/2^-$	−229.021	−229.381	−0.480	−0.461	−0.395(17)	+6.62	+6.63	+6.27(33)
^{255}Es	$7/2^+$	−263.512	−264.695	−1.10	+3.94	+4.14(10)	+6.0	+5.8	+5.1(1.7)
^{254}Es	7^+	−257.492	−258.441	+0.778	+3.36	+3.42(7)	+1.8	+8.4	+9.6(1.2)
^{253}Es	$7/2^+$	−251.837	−252.280	+3.63	+3.93	+4.10(7)	+5.87	+5.9	+6.7(8)
^{256}Fm	0^+	−268.999	−269.717	+0.87	+0.89	-	−3.57	−3.60	-
^{254}No	0^+	−249.568	−250.187	+0.87	+0.91	-	−3.78	−3.75	-

These calculations are performed using 1 Slater state in both PAV and VAP schemes. In the former, we use the cranking method with the constraint on the expectation value of the third angular moment component $\langle J_z \rangle = J_{\rm gs}$

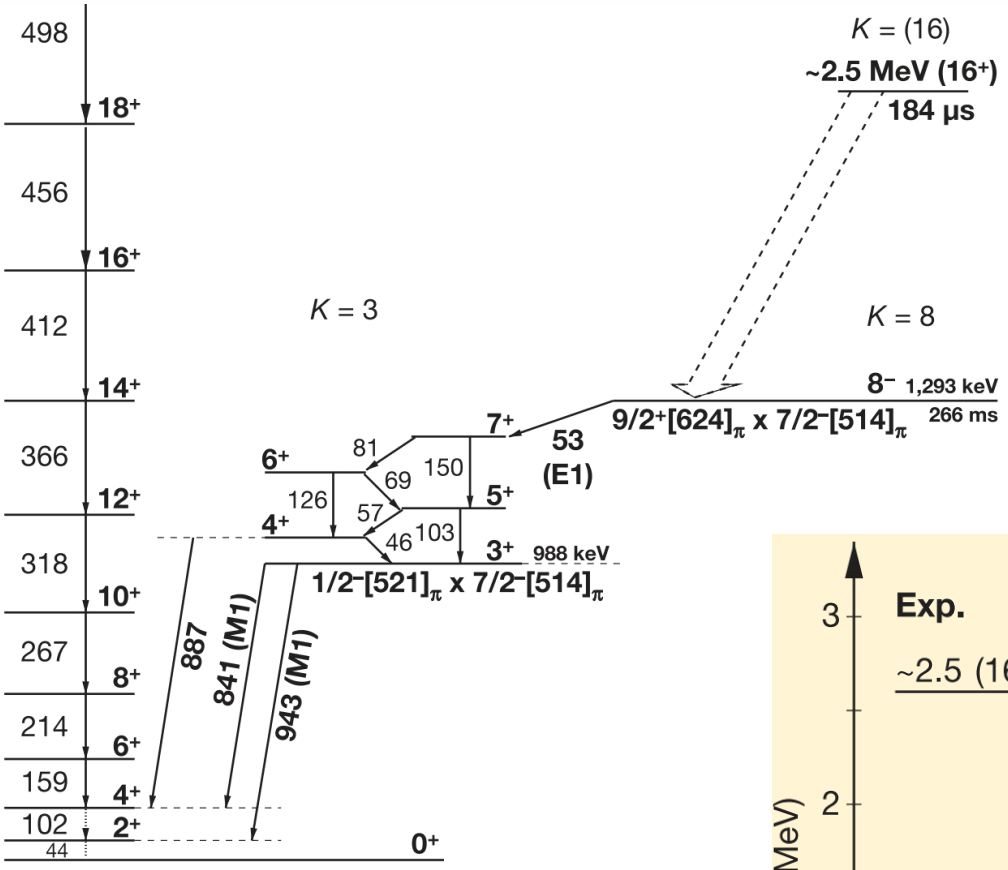
Results and discussions



Yrast bands computed by the DNO-SM(VAP) with 1 Slater state reproduce well the experimental data.

The extented DNO-SM(VAP) treate both odd and even systems on an equal footing, with a better incorporation of correlations providing at the same time the yrast spectra and ground state moments.

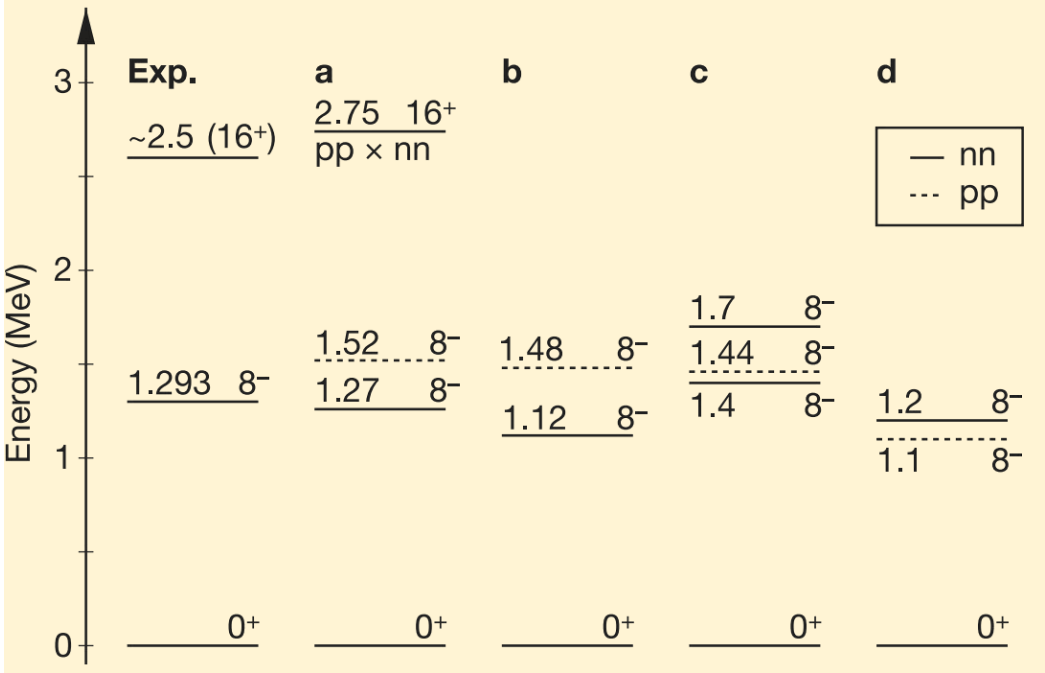
Specified case of ^{254}No



Calculated 2-neutron and 2-proton $K = 8^-$ configurations are close to each other. It is difficult to determine the neutron or proton nature of $K = 8^-$ isomer experimentally.

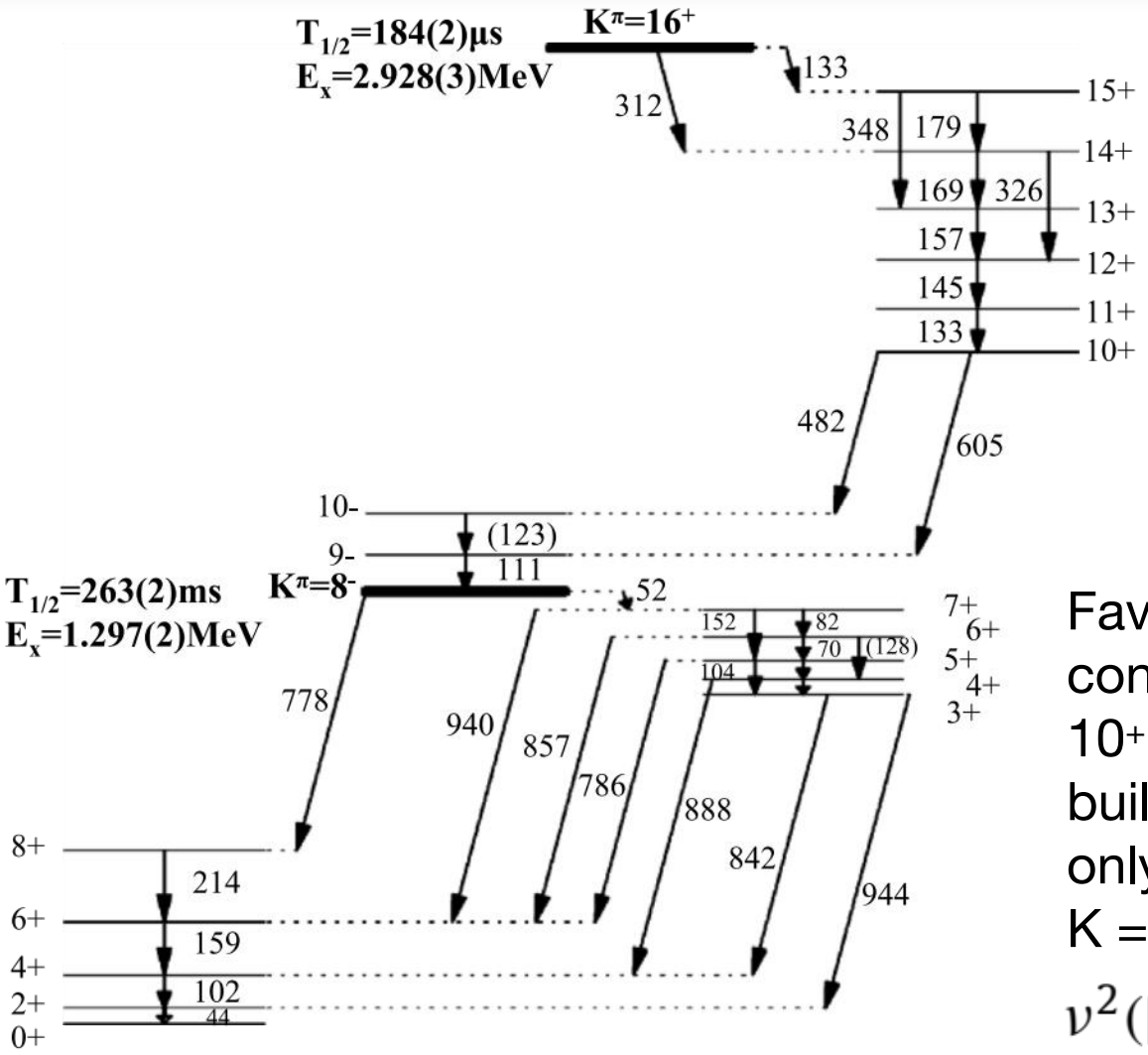
2p: $\{\bar{7}/2^-[\bar{5}14]_\pi \times 9/2^+[6\bar{2}4]_\pi\}^{(8-)}$

2n: $\{7/2^+[613]_\upsilon \times 9/2^-[734]_\upsilon\}^{(8-)}$



R.-D. Herzberg, et. al., Nature 442, 896 (2006)

Specified case of ^{254}No



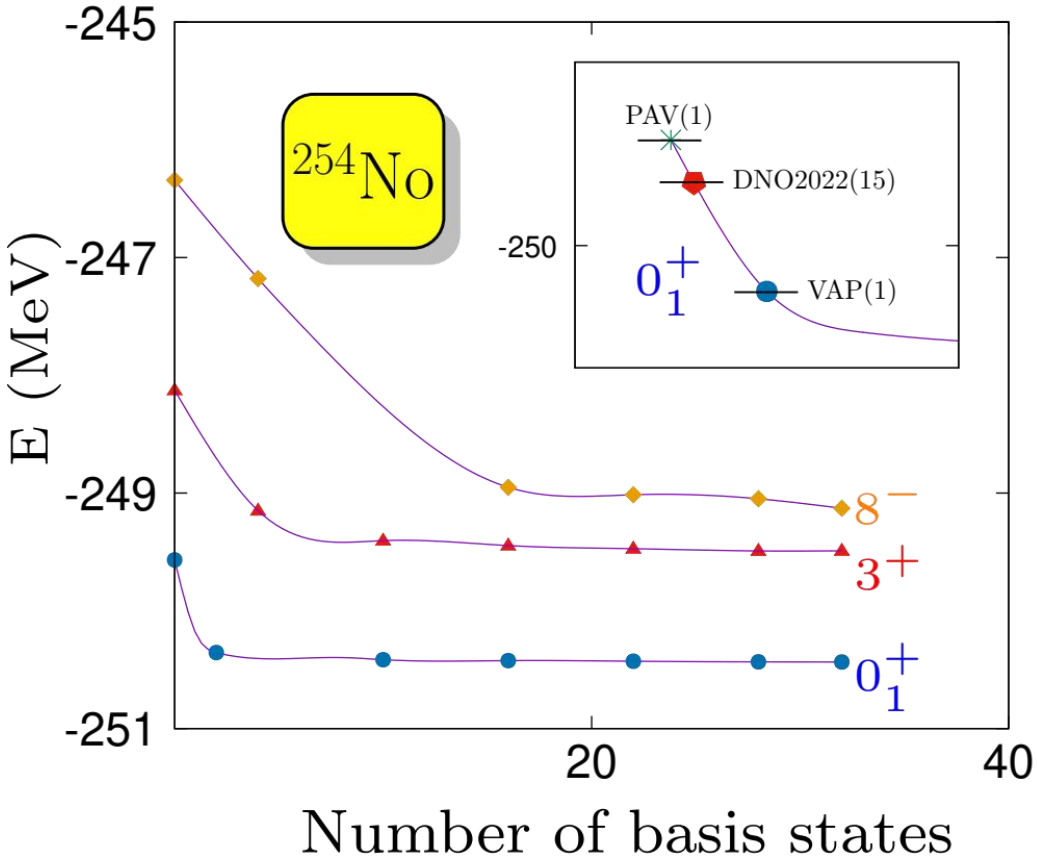
Favors 2-neutron $K = 8^-$ configuration because K = 10^+ state decay into the band built on $K = 8^-$ isomer, and only possible configuration of K = 10^+ state is

$$\nu^2([734]9/2^- \otimes [725]11/2^-).$$

R.M. Clark, et. al., Phys. Lett. B 690, 19 (2010)

Specified case of ^{254}No

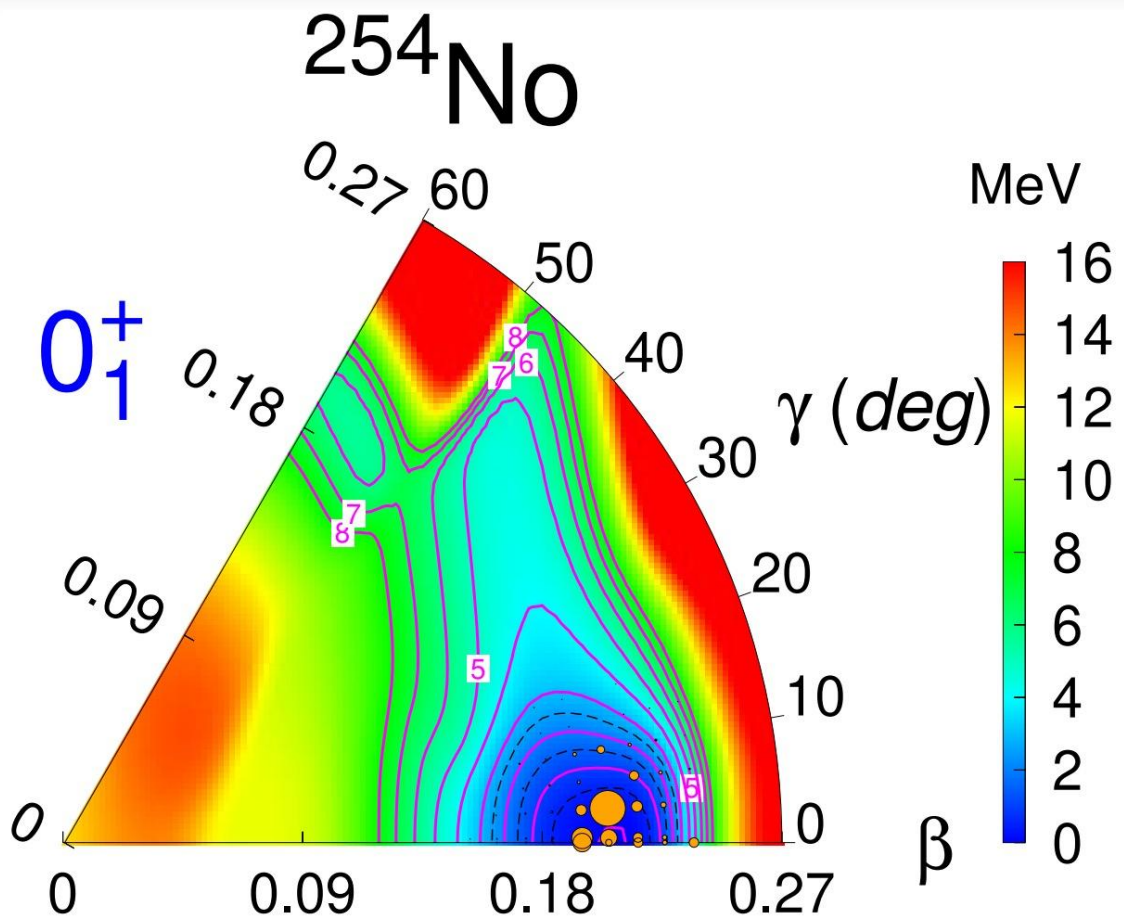
Point of view: "*this situation is a priori understandable, since rigorously one needs to go beyond the intrinsic mean field that breaks the symmetries of the Hamiltonian to include correlations which cannot be described by a single mean-field state. Configuration-mixing calculations are therefore desirable.*"



The convergence of the band heads 0_1^+, 3^+, and 8^-.

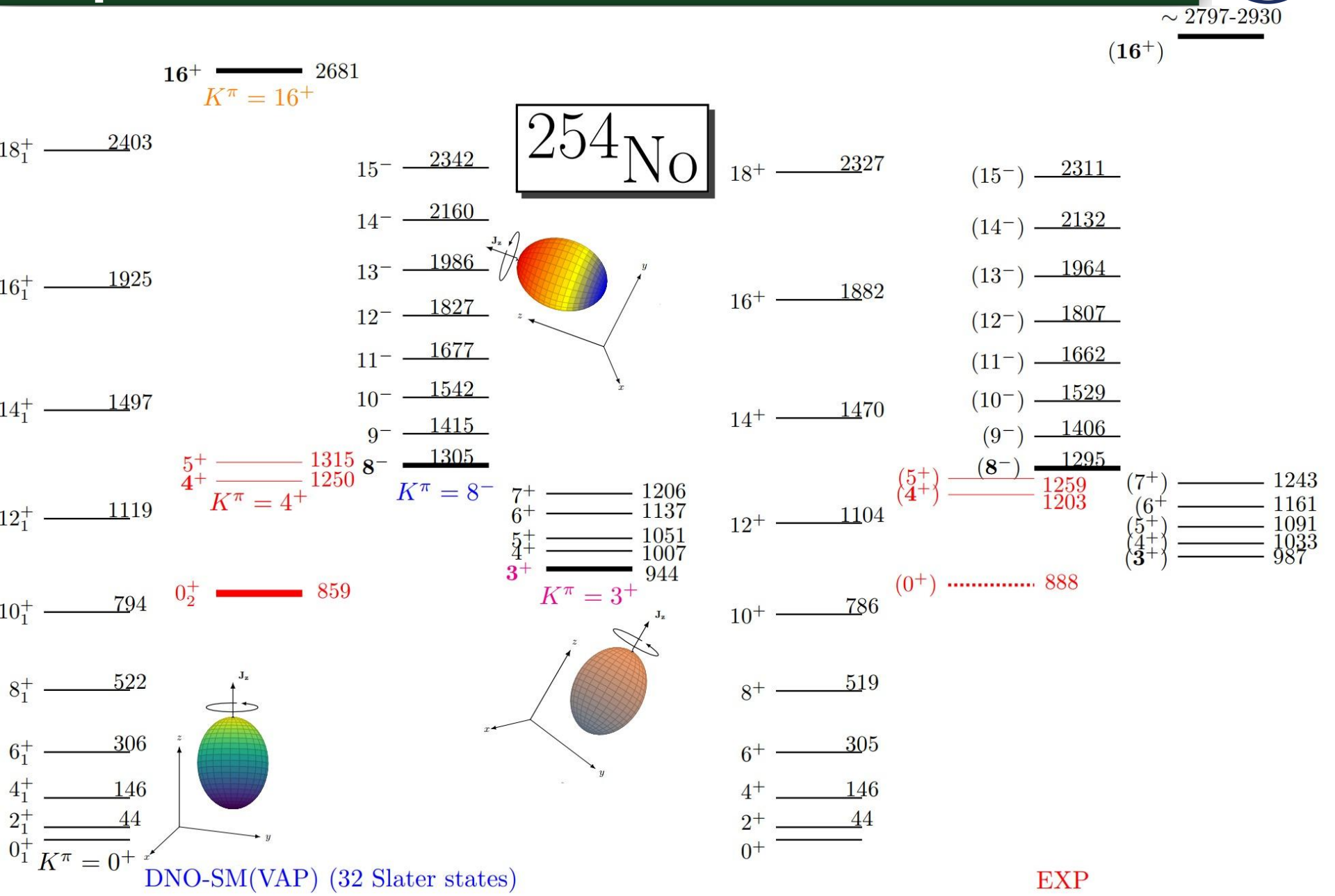
The inset shows the comparison of the ground state binding computed with AMP of the HF minimum, the previous DNO-SM calculation with 15 CHF states, and the present Variation-After Projection calculation with 1 Slater state.

Specified case of ^{254}No



The ground state wave function is found to be strongly dominated by $\gamma \sim 0^\circ$ configurations centered around the HF minimum, which implies a predominant axially deformed structure.

Specified case of ^{254}No



Specified case of ^{254}No

Proton orbits	$0h_{9/2}$	$0i_{13/2}$	$1f_{7/2}$	$1f_{5/2}$	$2p_{3/2}$	$2p_{1/2}$
0_1^+	6.03	7.75	3.43	1.49	0.77	0.52
0_2^+	7.08	7.91	3.23	0.89	0.69	0.21
$3^+(K=3)$	6.47	7.98	3.34	1.15	0.72	0.34
$4^+(K=4)$	6.50	7.83	3.41	1.18	0.72	0.36
$8^-(K=8)$	6.48	7.90	3.36	1.19	0.70	0.37
$16^+(K=16)$	6.39	8.82	3.18	0.78	0.68	0.15

Neutron orbits	$0i_{11/2}$	$0j_{15/2}$	$1g_{9/2}$	$1g_{7/2}$	$2d_{5/2}$	$2d_{3/2}$	$3s_{1/2}$
0_1^+	7.30	9.91	5.43	1.00	1.09	0.84	0.43
0_2^+	7.36	9.95	5.45	0.96	1.05	0.80	0.42
$3^+(K=3)$	7.32	9.94	5.46	0.97	1.07	0.81	0.42
$4^+(K=4)$	7.34	9.79	5.48	1.03	1.11	0.81	0.44
$8^-(K=8)$	7.42	9.00	6.30	0.98	1.06	0.81	0.43
$16^+(K=16)$	7.46	8.99	6.30	0.97	1.05	0.80	0.42

The spherical occupancies of the different band heads

The 8^- isomer essentially originates, w. r. t. the g.s., from a proton-neutron coupling [$\pi h_{9/2} \otimes \nu j_{15/2}$] with some slight residual mixing of the other orbitals.

The 16^+ is predicted to be lying at 2.68 MeV. With respect to the ground state, the spherical occupancy shows its shell structure originates mainly from the large-*j* orbitals $\pi i_{13/2}$ and $\nu j_{15/2}$.

Summary

- Have presented the implementation of the Variation-After-Projection scheme applied to the DNO-SM many-body approach.
- The VAP is able to capture important correlations beyond the mean field with respect to the usual PAV scheme.
- Have applied the DNO-SM(VAP) to the description of exotic nuclei in the mass region around ^{254}No.
- Pave an appealing route for the microscopic description of very heavy and very deformed nuclei within the shell-model framework.
- The present description proposes a benchmark to be confronted to modern shell-model interactions from ab-initio Valence-Space IM-SRG approaches.