Recent developments within CI and beyond for nuclear spectroscopy and neutron capture

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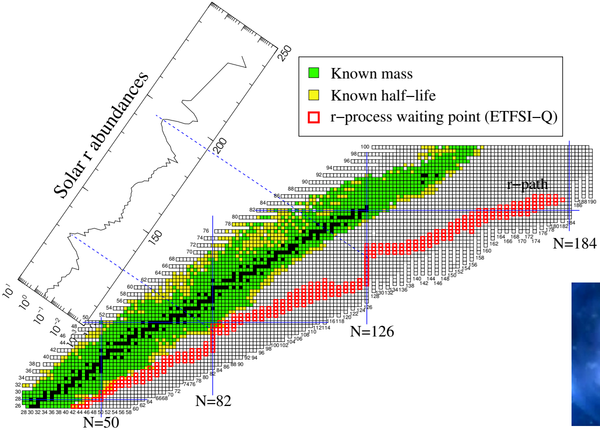
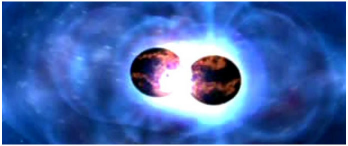
R-process nucleosynthesis

☞Nuclear models are needed to provide input for r-process simulations: *masses*, *neutron-capture rates*, *β-decay rates*, *fission barriers...*





B. Metzger, G. Martinez-Pinedo et al., Monthly Notices of the Royal Astronomical Society. 406, 2650 (2010)

Configuration Interaction approaches

- The wave-function of the ground state is expressed as a sum of the vacuum Φ_0 and particle-hole excitations build on this vacuum state

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{i\alpha} C_{i\alpha}|\Phi_{i\alpha}\rangle + C_{ij\alpha\beta}|\Phi_{ij\alpha\beta}\rangle + \cdots \quad (1)$$

where greek and latin symbols refer to particle and hole states, respectively. In short notation:

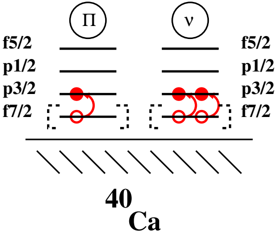
$$|\Psi_0\rangle = \sum_{ph} C_{ph}|\Phi_{ph}\rangle \quad (2)$$

- The equation for the energy reads

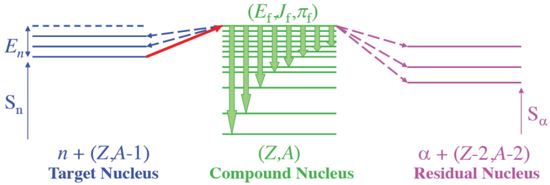
$$E = \langle\Psi_0|\hat{H}|\Psi_0\rangle = \sum_{pp'hh'} C^*_{p'h'}\langle\Phi_{p'h'}|\hat{H}|\Phi_{ph}\rangle C_{ph} \quad (3)$$

and it is solved by diagonalization.

- The vaccum for particle-hole excitations 1p-1h, 2p-2h,..., np-nh can be, e.g. the lowest-filling configuration (Slater determinant) outside a doubly-magic core.



Radiative neutron capture: resonant capture



$$\sigma^{\mu\nu}_{(n,\gamma)}(E_i, n) = \frac{\pi\hbar^2}{2M_{i,n}E_{i,n}} \frac{1}{(2J_i^\mu + 1)(2J_n + 1)} \sum_{J,\pi} (2J+1) \frac{T_n^\mu T_\gamma^\nu}{T_n^\mu + T_\gamma^\nu}$$

for E_n ∼keV $\quad T_n^\mu \gg T_\gamma^\nu \longrightarrow \boldsymbol{\sigma^{\mu\nu} \sim T_\gamma^\nu}$

$E_{i,n}, M_{i,n}$- center-of-mass energy, reduced mass of the system

$J_n = 1/2$-neutron spin

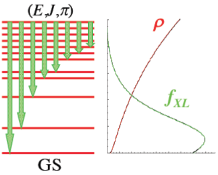
$T_n^\mu = T_n(E, J, \pi; E_i^\mu, J_i^\mu, \pi_i^\mu)$ $T_\gamma^\nu = T_\gamma(E, J, \pi; E_m^\nu, J_m^\nu, \pi_m^\nu)$- transmission coefficients

For a given multipolarity

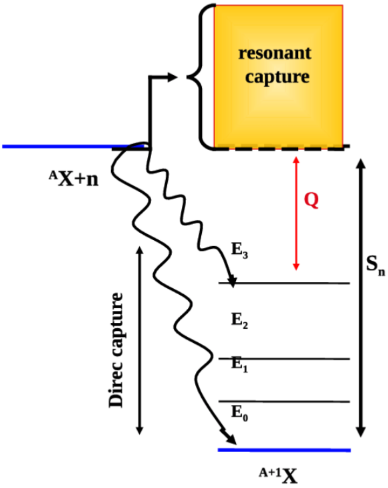
$T_{XL}(E, J, \pi, E^\nu, J^\nu, \pi^\nu) = 2\pi E_\gamma^{2L+1} f_{XL}(E, E_\gamma)$

☞Test, using CI, the key ingredients of Hauser-Feshbach calculations:

- description of γ emission spectra
- Brink-Axel hypothesis



Radiative neutron capture: direct capture



Xi. Yu and S. Goriely, Phys. Rev. C86 (2012) 045801

$$\sigma^{DC}(E) = \sum_{f=0}^{x} S_f \sigma_{dis}(E)$$

$$+ \quad \langle S \rangle \int_{E_x}^{S_n} \sum_{J_f,\pi_f} \rho(E_f, J_f, \pi_f) \times \sigma_f^{cont} dE_f$$

If no experimental data available:

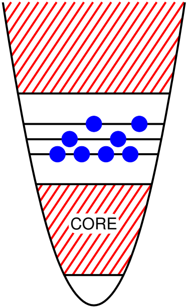
- use combinatorial model for the level density with $\langle S \rangle$=const

☞The key ingredients: low-energy levels and spectroscopic factors

☞Validate theoretical approximations (HFB) in exotic nuclei using CI predictions

Configuration Interaction: generalities

CI relies on the possibility of diagonalizing the Hamiltonian matrix and deriving (constraining empirically) a suitable effective interaction.



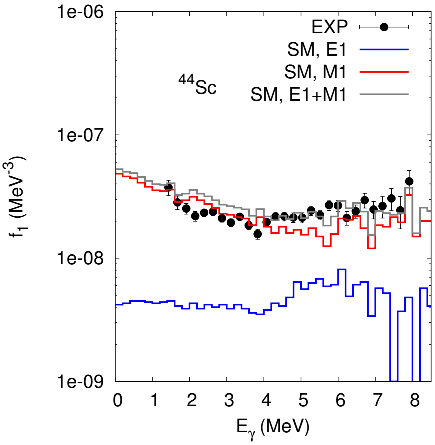
$$H_{eff}|\Psi_{eff}\rangle = E|\Psi_{eff}\rangle$$

- **Direct capture:** knowledge of the lowest-lying levels (energies and spectroscopic factors)$\rightarrow$ quality of the effective Hamiltonian
- **Resonant capture:** knowledge of statistical properties (energies and transitions in nuclear continuum)$\rightarrow$ possibility of computing of hundreds of nuclear levels

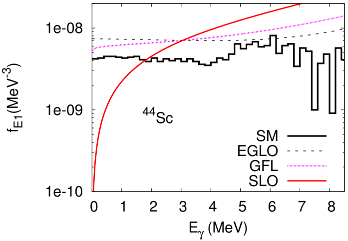
CI computations of γ-decay strength functions

Dipole strength in ^{44}Sc: theory vs exp

K. Sieja, Phys. Rev. Lett. 119 (2017) 052502



$$f_{M1/E1}(E_\gamma) = 16\pi/9(\hbar c)^3 S_{M1/E1}(E_\gamma)$$
$$S_{M1/E1} = \langle B(M1/E1)\rangle \rho_i(E_i)$$

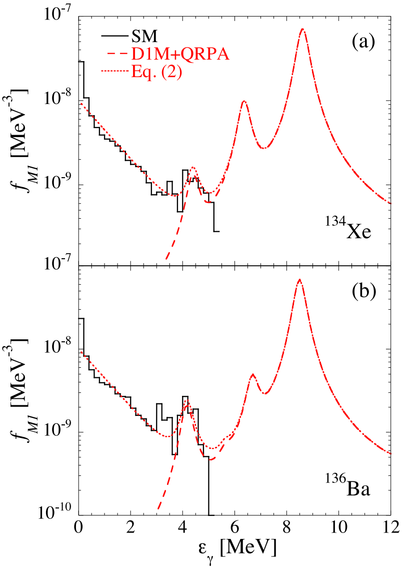


-all states below S_n ∼10MeV
-86642 $M1$matrix elements
-65670 $E1$ matrix elements

☞Qualitative agreement with data:

-the upbend is due to $M1$ transitions
-the $E1$ pattern is flat with the non-zero $E_\gamma \to 0$ limit
-consistent with EGLO model

Application of the low-energy limit to the QRPA results



S. Goriely, S. Hilaire, S. Péru and K. Sieja, PRC98 (2018) 014327

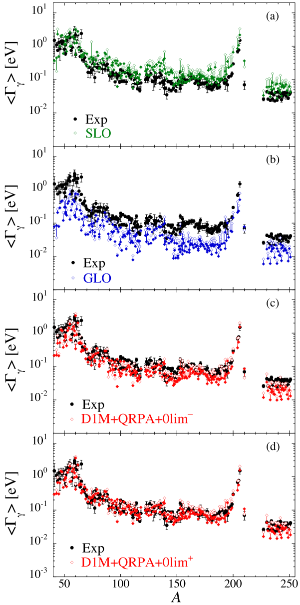
To describe radiative decay, phenomenological low-energy corrections fitted to reproduce CI trends and data are added to microscopic QRPA-Gogny $M1$ and $E1$ PSF:

$$f_{E1}(\epsilon_\gamma) = f_{E1}^{QRPA}(\epsilon_\gamma) + f_0 U/[1+e^{(\epsilon_\gamma-\epsilon_0)}] \quad (4)$$

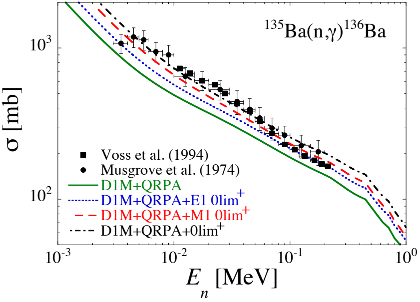
$$f_{M1}(\epsilon_\gamma) = f_{M1}^{QRPA}(\epsilon_\gamma) + Ce^{-\eta\epsilon_\gamma} \quad (5)$$

- upper limit (0lim$^+$)
  $f_0 = 5 \cdot 10^{-10}$MeV^{-4}, ϵ_0=5MeV, C=3·10^{-8}MeV^{-3}, $\eta = 0.8$MeV^{-1}
- lower limit (0lim$^-$)
  $f_0 = 10^{-10}$MeV^{-4}, ϵ_0=3MeV, C=10^{-8}MeV^{-3}, $\eta = 0.8$MeV^{-1}

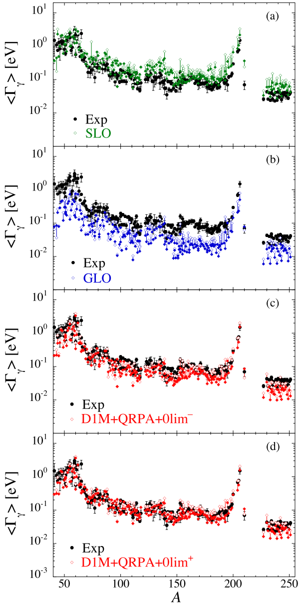
Impact on radiative neutron capture

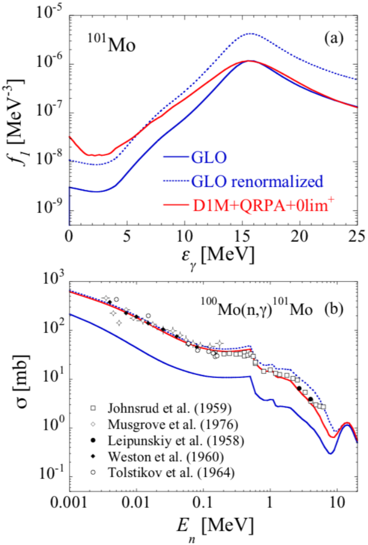


rms/datum		
	$\langle \Gamma_\gamma \rangle$	$\langle \sigma \rangle$
0lim^-(Comb)	0.88	1.07
0lim^-(CT)	0.74	0.95
0lim^+(Comb)	1.02	1.30
0lim^+(CT)	0.90	1.15
GLO(Comb)	0.48	0.61
GLO(CT)	0.38	0.53



Impact on the radiative capture

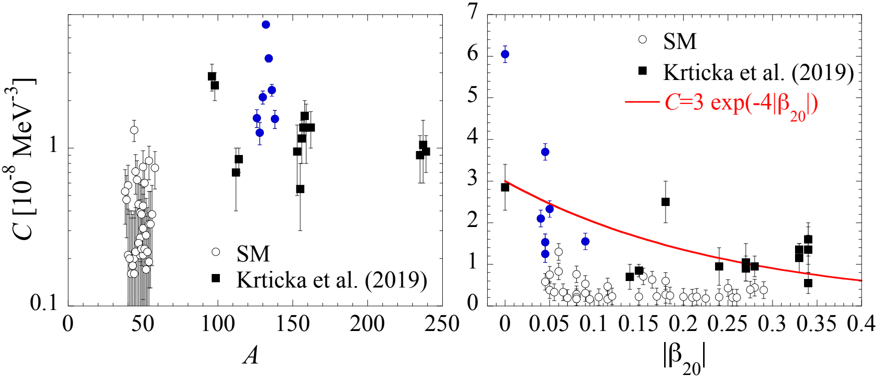




S. Goriely, S. Hilaire, S. Péru and K. Sieja, PRC98 (2018) 014327

Deformation dependence of the low-energy limit

K. Sieja and S. Goriely, Acta. Phys. Pol. B (2020) 535



- no simple deformation dependence with all nuclei included
- further systematic CI studies to characterize the upbend
- benchmark study QRPA/CI with the same Hamiltonian now in progress

Direct capture studies using CI input

$$\sigma^{DC}(E) = \sum_{f=0}^{x} S_f \sigma_{J_f^\pi}(E)$$

- crucial observables: low energy levels and their spectroscopic factors
- E1,M1,E2 transitions
- optical potential

Systematic CI calculations (50 neutron-rich targets from mass 38 to 88) using well-established and newly developed interactions:

- SDPF-U for *sdpf* nuclei

  F. Nowacki and A. Poves,Phys. Rev. C79 (2009) 014310
- LNPS for *fpgd* nuclei

  S.M. Lenzi et al.,Phys. Rev. C82 (2010) 054301
- LNPS+gds for nuclei towards ^{78}Ni

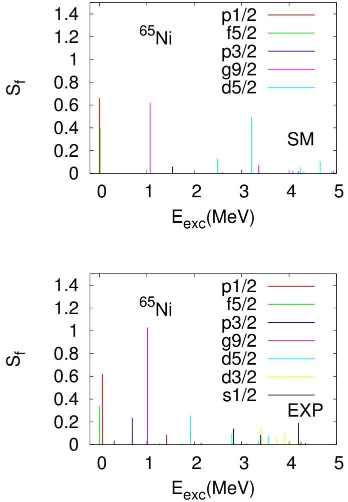
  K. Sieja, unpublished
- Ni78-II for nuclei above ^{78}Ni

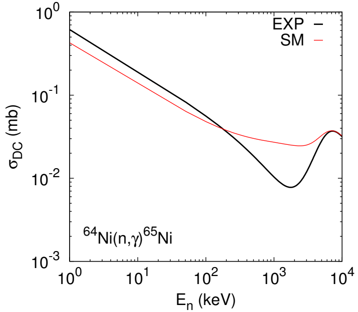
  K. Sieja et al.,Phys. Rev. C88 (2013) 034327

☞Compare global theoretical approximations for spectra and S_f to CI results in unknown nuclei

Direct capture rates using CI results

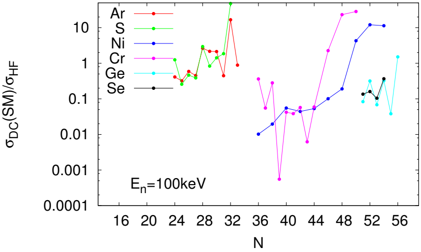
$^{64}Ni(n,\gamma)^{65}Ni$



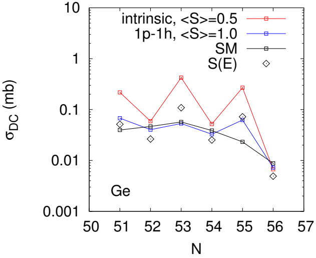


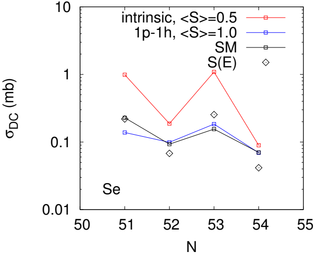
K. Sieja and S. Goriely, Eur. Phys. J A57 (2021) 110

Direct capture vs resonant capture



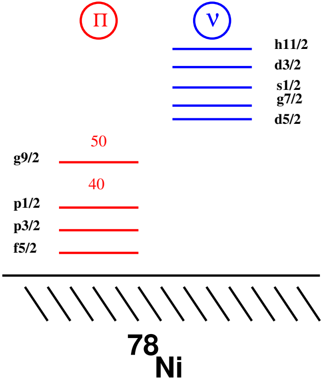
- factor 10 difference after passing $N = 50$ shell closure
- largest discrepancies between models in triaxial nuclei: new model of level densities under way
- different prescription for $S(E)$ used to reduce inter-model differences





K. Sieja and S. Goriely, Eur. Phys. J A57 (2021) 110

CI studies of spectroscopy of fission fragments



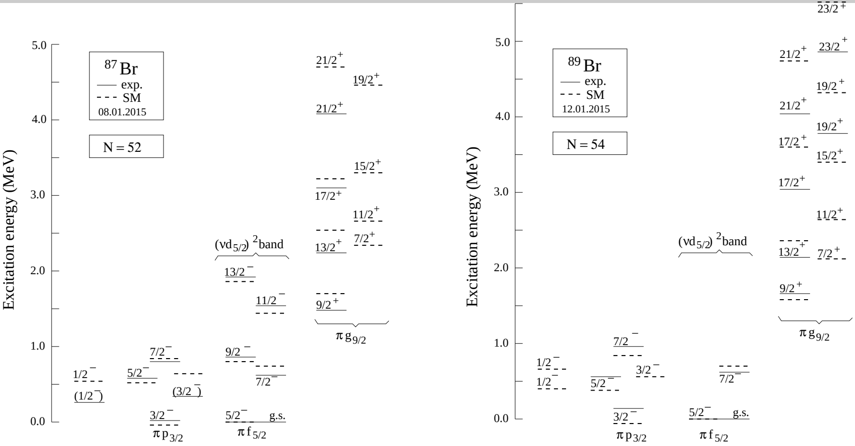
High precision, semi-empirical interactions:
2009-2015: Ni78-I
Since 2015: Ni78-II

- New estimate of proton $f_{5/2}$-$p_{3/2}$ splitting in the core
- New fit of proton-proton interaction for N=50 isotones

Nuclei above ^{78}Ni

- Structure of Sr, Zr nuclei near shape change (N=60)
  K. Sieja et al., Phys. Rev. C79 (2009) 064310; K. Sieja, Universe 8 (2022) 23, PRC104 (2021) 064309
- Isomers and medium-spin structures of ^{95}Y, $^{91-95}$Rb, $^{92-96}$Sr
  PRC 85 (2012) 014329, PRC79 (2009) 024319, PRC82 (2010) 024302, PRC79 (2009) 044304
- Collectivity and j-1 anomaly of ^{87}Se
  PRC88 (2013) 034302
- β-decays of Ga nuclei and structure of $N = 51 - 54$ isotones
  PRC88 (2013) 047301, PRC88 (2013) 044330, PRC88 (2013) 044314, PRC96 (2017) 044320
- Magnetic moments of ^{86}Kr, ^{88}Sr, structure of Kr nuclei
  PRC 80 (2014) 064305, PRC95 (2017)064302, PRC94 (2016) 054323, PRC 94 (2016) 044328
- Collectivity of $N = 52, 54$ nuclei
  PRC88 (2013) 034327, PRC92 (2015) 064322, PRC95 (2017) 051302R, PRC96 (2017) 011301R

CI spectroscopy of fission fragments



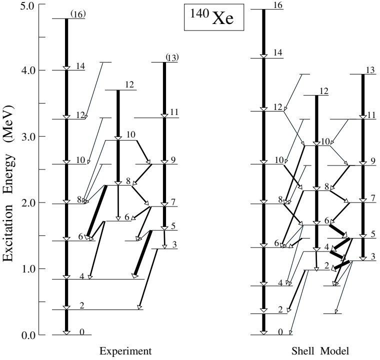
B.M. Nyako et al, PRC104 (2021) 054305, PRC103 (2021) 034304, PRC100 (2019) 054331

- Satisfactory ($rms = 200$keV) description of proton-neutron multiplets in odd-odd nuclei: ^{86,88}Br, ^{90}Rb.

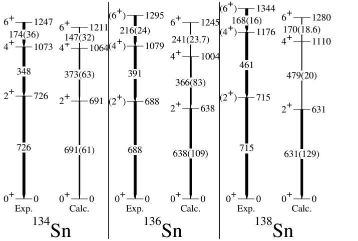
  M. Czerwinski et al., PRC95 (2017) 024321, PRC93 (2016) 034318, PRC94 (2016) 044328

CI spectroscopy of heavier nuclei

Nuclei above ^{132}Sn



Semi-empirical interaction: NL3OP

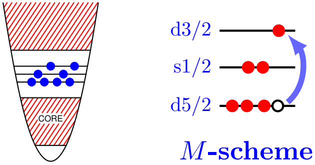


- Seniority isomers in heavy tins
  G.S. Simpson, Phys. Rev. Lett. 113 (2014) 132502
- Prediction of γ-collectivity above ^{132}Sn
  K. Sieja, Acta Phys. Pol.B247 (2016) 883;
  W. Urban, K. Sieja et al, PRC93 (2016) 034326
- Evolution of γ bands at $N = 86$
  H. Naidja et al, PRC95 (2017) 064303

CI versus Beyond Mean-Field Approach

Standard CI approach:

- Valence space
- Spherical SD basis
- Exact diagonalization

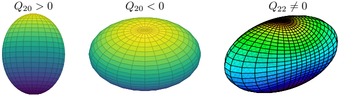


- Advantage: all type of correlations
- Inconvenience: **huge dimensionality**

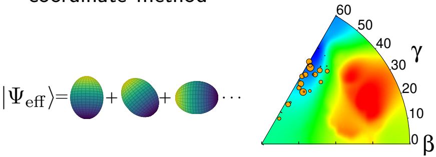
$$dim = \binom{D_\pi}{Z}\binom{D_\nu}{N} \text{ (up to } 10^{12})$$

Beyond mean-field approach:

- Deformed Hartree-Fock (HF) basis (quadrupole, octupole,...)



- Angular momentum projection
- Configuration mixing within the generator coordinate method

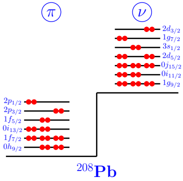


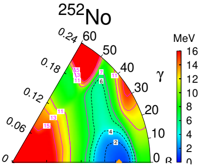
- **Selection of physically important HF states: minimization technique**

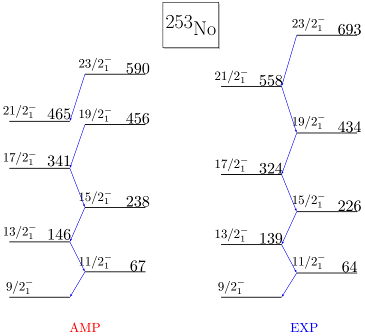
D. D. Dao, F. Nowacki, PRC **105**, *054314 (2022)*

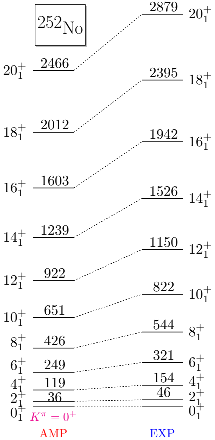
Application: superheavy nuclei ^{252,253,254}No

Angular Momentum Projection (AMP)



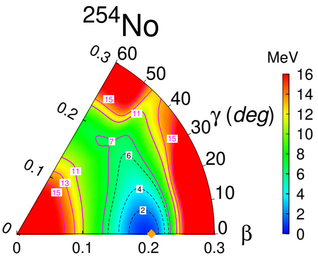


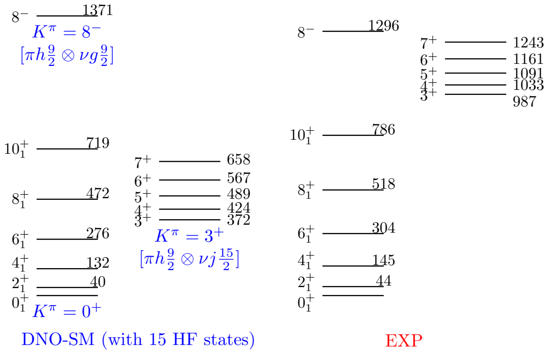




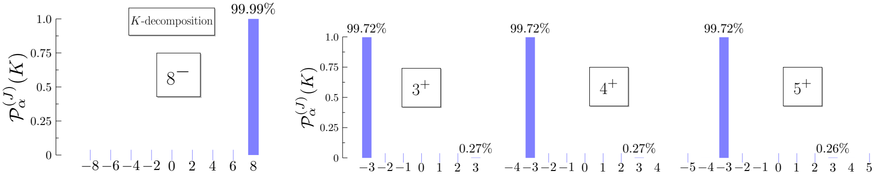
Application: superheavy nuclei ^{252,253,254}No

Comparison with experimental data *D. D. Dao, F. Nowacki, PRC* ***105****, 054314 (2022)*





K-mixing analysis



Future prospects

- Systematics of heavy nuclei with DNO-SM approach: Fm, Rf, U (D. Dao, IPHC)
- Developments of DNO-SM approach to describe dipole transitions (D. Dao, IPHC)
- CI studies of M1 strength functions: low energy behavior and its relation with level densities and deformation (P. Kumar, GSI)
- CI benchmark of other many-body methods: CI vs QRPA for strength functions (W. Ryssens, Brussels)
- Calculations of (n, γ) cross sections with CI input vs Hauser-Feshbach model

Thanks to:
IEA project "Radiative Neutron Capture": collaboration with ULB Brussels