Pertinent ingredients for MR-EDF calculations (ESNT Workshop)

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Are two-quasiparticle states pertinent to MR-EDF description of collective states ?

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Aim of the talk

One aim of this work is to find out how relevant are the single particle degrees of freedom in the description of the collective states.

Another interesting point is to know to what degree one can describe collective states like beta and gamma vibrations as genuine superposition of shape fluctuations.

We will also compare calculations in different approaches to pin down the key issues.

We will apply the calculations to the Erbium isotopes ranging from the very soft $^{156}\mathrm{Er}$ to the hard $^{172}\mathrm{Er}$ in the GCM with triaxial shape fluctuation with particle number and angular momentum projection plus two-quasiparticle states.

In this way we will be able to study the evolution of the collectivity and the relevance of the different degrees of freedom.

Theoretical considerations: I.- The constrained HFB equations

Our starting point are the constrained HFB equations

$$\delta\langle\Phi_0(\beta,\gamma)|\hat{H}-\lambda_n\hat{N}-\lambda_p\hat{Z}-\lambda_{q_0}\hat{Q}_0-\lambda_{q_2}\hat{Q}_2|\Phi_0(\beta,\gamma)\rangle=0,$$

with the constraints

$$\langle\Phi_0(\beta,\gamma)|\hat{N}|\Phi_0(\beta,\gamma)\rangle=N,\quad \langle\Phi_0(\beta,\gamma)|\hat{Z}|\Phi_0(\beta,\gamma)\rangle=Z,$$
$$\langle\Phi_0(\beta,\gamma)|\hat{Q}_0|\Phi_0(\beta,\gamma)\rangle=q_0,\quad \langle\Phi_0(\beta,\gamma)|\hat{Q}_2|\Phi_0(\beta,\gamma)\rangle=q_2.$$

This equations are solved in a (β,γ) grid . These states provide basis for the shape fluctuations to be considered in the GCM Ansatz.

For each HFB vacuum $|\Phi_0(\beta,\gamma)\rangle$there is a set of corresponding quasiparticle operators $\alpha_i(\beta,\gamma)$ satisfying

$$\alpha_i(\beta,\gamma)|\Phi_0(\beta,\gamma)\rangle=0,\quad\forall i.$$

Theoretical considerations: II.- The two-quasiparticle states

The second components of our GCM ansatz are the two-quasiparticle states, defined by

$$|\Phi_{ij}(\beta,\gamma)\rangle = \alpha_i^\dagger(\beta,\gamma)\alpha_j^\dagger(\beta,\gamma)|\Phi_0(\beta,\gamma)\rangle.$$

Finally, the HFB vacua and the two-quasiparticle states are projected onto angular momentum and particle number. Thus the complete wave function has the form

$$\begin{aligned}
|\sigma, IM\rangle &= \int d\beta d\gamma \sum_K f_0^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_0(\beta,\gamma)\rangle \\
&\quad + \sum_{ij}\int d\beta d\gamma \sum_K f_{ij}^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_{ij}(\beta,\gamma)\rangle \\
&= \sum_\rho \int d\beta d\gamma \sum_K f_\rho^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_\rho(\beta,\gamma)\rangle \\
&= \sum_\rho \int d\beta d\gamma \sum_K f_\rho^{\sigma,IK}(\beta,\gamma)|IMK,N,\beta,\gamma\rangle_\rho.
\end{aligned}$$

where the index ρ runs over the set $\{0,(ij)\}$ and σ labels the different states. The coefficients $f_\rho^{\sigma,IK}$ are determined by the variational principle which leads to the HWG Equation.

Theoretical considerations: III- Solution of the HWG equation.

The HWG equation looks like the usual ones

$$\sum_{\rho' \beta' \gamma' K'} \left(\mathcal{H}^{IKK'}_{\rho\rho'}(\beta\gamma, \beta'\gamma') - E^{\sigma I} \mathcal{N}^{IKK'}_{\rho\rho'}(\beta\gamma, \beta'\gamma') \right) f^{\sigma I K'}_{\rho'}(\beta'\gamma') = 0$$

with the norms and Hamiltonian overlaps

$$\begin{aligned} \mathcal{N}^{IKK'}_{\rho\rho'}(\beta\gamma, \beta'\gamma') &\equiv {}_{\rho}\langle IMK, N, \beta, \gamma | IMK', N, \beta', \gamma' \rangle_{\rho'} \\ \mathcal{H}^{IKK'}_{\rho\rho'}(\beta\gamma, \beta'\gamma') &\equiv {}_{\rho}\langle IMK, N, \beta, \gamma | H | IMK', N, \beta', \gamma' \rangle_{\rho'}. \end{aligned}$$

Its solution follows the general scheme: First, the norm matrix is diagonalised

$$\sum_{\beta' \gamma' \rho' K'} \mathcal{N}^{IKK'}_{\rho\rho'}(\beta\gamma, \beta'\gamma') u^{\kappa I K'}_{\rho'}(\beta'\gamma') = n^{\kappa I} u^{\kappa I K}_{\rho}(\beta, \gamma).$$

It provides the provides the natural basis

$$|\kappa^{IM}\rangle = \sum_{\beta\gamma\rho K} \frac{u^{\kappa I K}_{\rho}(\beta, \gamma)}{\sqrt{n^{\kappa I}}} |IMK, N, \beta, \gamma\rangle_{\rho}.$$

In this basis the HWG equation becomes a normal Schödinger equation

$$\sum_{\kappa'} \langle \kappa^I | \hat{H} | \kappa'^I \rangle g^{\sigma I}_{\kappa'} = E^{\sigma I} g^{\sigma I}_{\kappa}.$$

Collective wave functions

The collective wave function is given by

$$p^{\sigma I}_{\rho K}(\beta,\gamma) = \sum_{\kappa} g^{\sigma I}_{\kappa} u^{\kappa I K}_{\rho}(\beta,\gamma)$$

remember ρ runs over the ground and 2qp states, i.e, $\{0,(ij)\}$.

They are normalised to the unity

$$\sum_{\beta\gamma\rho K} |p^{\sigma I}_{\rho K}(\beta,\gamma)|^2 = 1, \quad \forall\sigma,$$

and can be interpreted as probability amplitudes.

We furthermore define the partial probability amplitudes:

$$\mathcal{P}^{\sigma I}(\beta,\gamma) = \sum_{K\rho} |p^{\sigma I}_{\rho K}(\beta,\gamma)|^2$$

$$\mathcal{P}^{\sigma I}_{\rm vac}(\beta,\gamma) = \sum_{K} |p^{\sigma I}_{0K}(\beta,\gamma)|^2$$

$$\mathcal{P}^{\sigma I}_{\rm 2qp}(\beta,\gamma) = \sum_{K(i,j)} |p^{\sigma I}_{(ij)K}(\beta,\gamma)|^2$$

Hamiltonian and configuration space

We use the Pairing plus Quadrupole interaction

$$\hat{H} = \hat{H}_0 - \frac{1}{2}\sum_{\tau\tau'}\chi_{\tau\tau'}\sum_{\mu}\hat{Q}^{\dagger}_{\tau\mu}\hat{Q}_{\tau'\mu} - G_M\sum_{\tau}\hat{P}^{\dagger}_{\tau}\hat{P}_{\tau} - G_Q\sum_{\tau\mu}\hat{P}^{\dagger}_{\tau\mu}\hat{P}_{\tau\mu}$$

$$\hat{H}_0 = \sum_k \epsilon_k c^{\dagger}_k c_k, \quad \hat{Q}_\mu = \sum_{k,l}(Q_\mu)_{kl}c^{\dagger}_k c_l,$$

$$\hat{P} = \frac{1}{2}\sum_k c_k c_{\bar{k}}, \quad \hat{P}_\mu = \frac{1}{2}\sum_{k,l}(Q_\mu)_{kl}c_k c_{\bar{l}}.$$

$$G_M = (18.75 \mp 13.00(N-Z)/A)/A$$

$$G_Q = 0.16 G_M$$

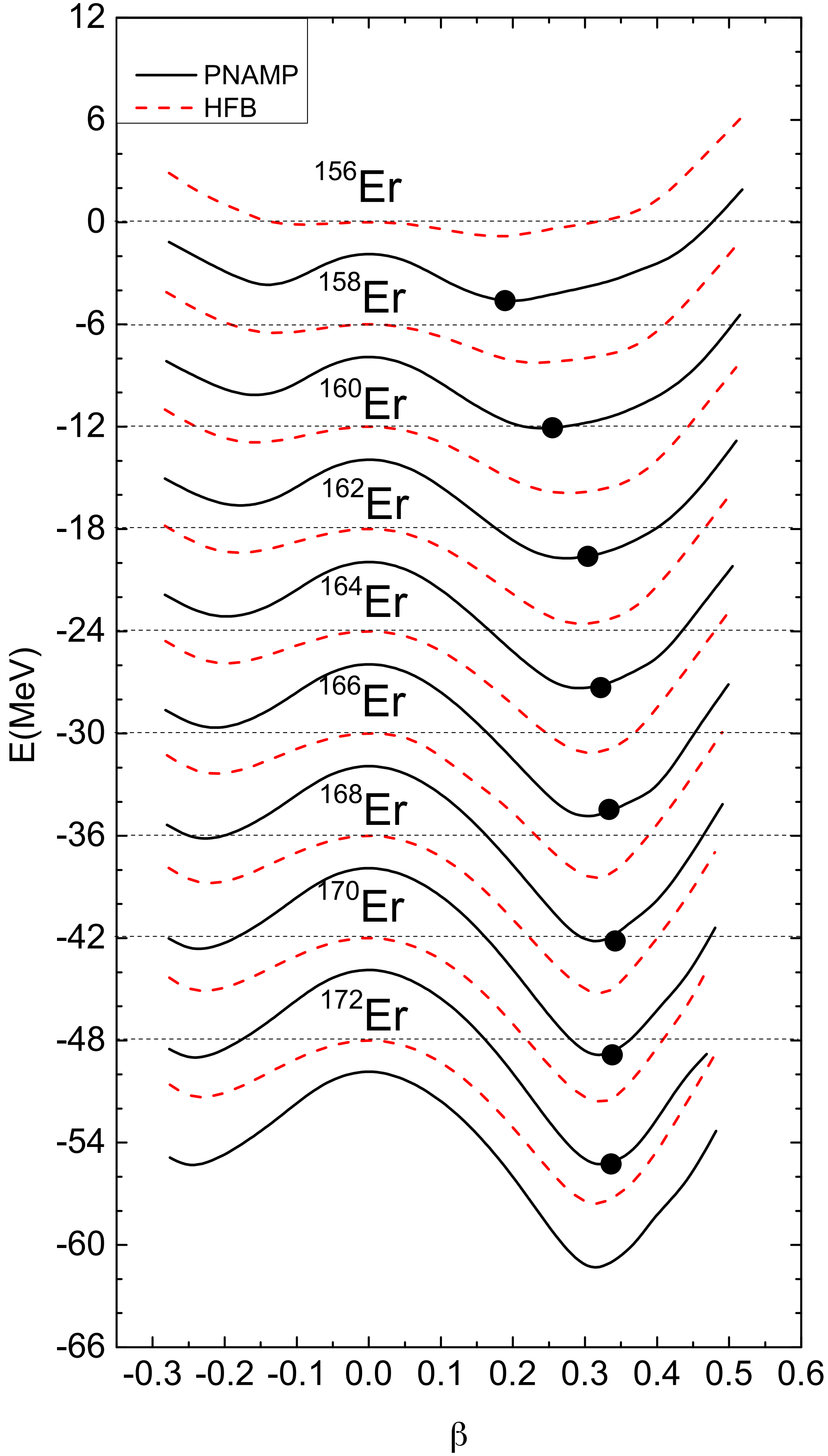
$$\chi_{\tau\tau'} = \chi\alpha_\tau\alpha_{\tau'}, \quad \chi = 70A^{-1.4}b^{-4}MeV, \qquad \alpha_\pi = (2Z/A)^{1/3}, \quad \alpha_\nu = (2N/A)^{1/3}.$$

The s.p.e. are calculated using the the Nilsson parameters of Bengtsson and Ragnarsson. For the present calculations we use a configuration space of $N=3,4,5$ for protons and $N=4,5,6$ for neutrons.

We furthermore use the effective charges of Baranger and Kumar $e^{\pi}_{eff} = 1 + 1.5\frac{Z}{A}$, and $e^{\nu}_{eff} = 1.5\frac{Z}{A}$.

K. Kumar and M. Baranger, Nucl. Phys. A **110**, 529(1968) T. Bengtsson and I. Ragnarsson, Nucl. Phys. A **436**, 14 (1985).

Axially Symmetric Potential Energy Surfaces



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Details of the GCM calculations

The constrained HFB equations are solved in a triangular mesh of 49 points in the intervals

$$0 \leq \beta \leq 0.6, 0 \leq \gamma \leq 60^\circ$$

With respect to the two-quasiparticle states, we set the energy cutoff

$$E_i(\beta,\gamma) + E_j(\beta,\gamma) + E_0(\beta,\gamma) \leq E(\beta_{min},\gamma_{min}) + 3.0 \text{ MeV}$$

With $E_i(\beta,\gamma), E_j(\beta,\gamma)$ the HFB quasiparticle energies in the (β,γ) point and $E_0(\beta,\gamma)$ the HFB energy evaluated in that point:

$$E_0(\beta,\gamma) = \langle \Phi_0(\beta,\gamma)|\hat{H}|\Phi_0(\beta,\gamma)\rangle.$$

Typically we consider about **150-200 two-quasiparticle states**.

We apply the theory to the $^{156-172}\mathrm{Er}$ isotopes.

Calculation of the Potential Energy Surfaces

The symmetries are recovered by means of projection

$$|IMK, N, \beta, \gamma\rangle_0 = \hat{P}^I_{MK} \hat{P}^N \hat{P}^Z |\Phi_0(\beta, \gamma)\rangle,$$

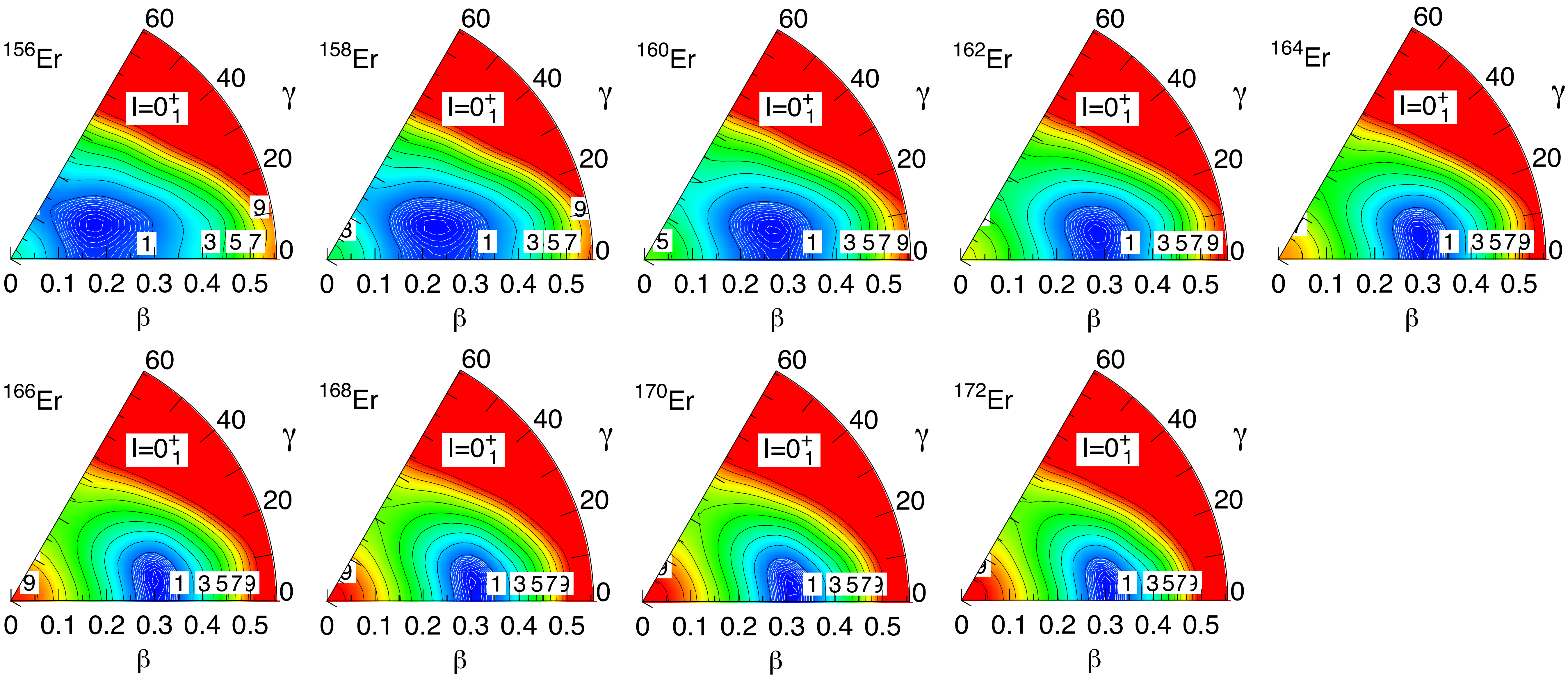
then a linear combination is provided

$$|\sigma, IM, \beta, \gamma\rangle_0 = \sum_K h^{\sigma IK}(\beta, \gamma) |IMK, N, \beta, \gamma\rangle_0$$

finally the coefficients are determined by the variational principle

$$\sum_{K'} \left(\mathcal{H}^{IKK'}_{00}(\beta\gamma, \beta\gamma) - E^{\sigma I}(\beta, \gamma) \mathcal{N}^{IKK'}_{00}(\beta\gamma, \beta\gamma) \right) h^{\sigma IK'}(\beta\gamma) = 0.$$

Ground State (I=0) Potential Energy Surfaces



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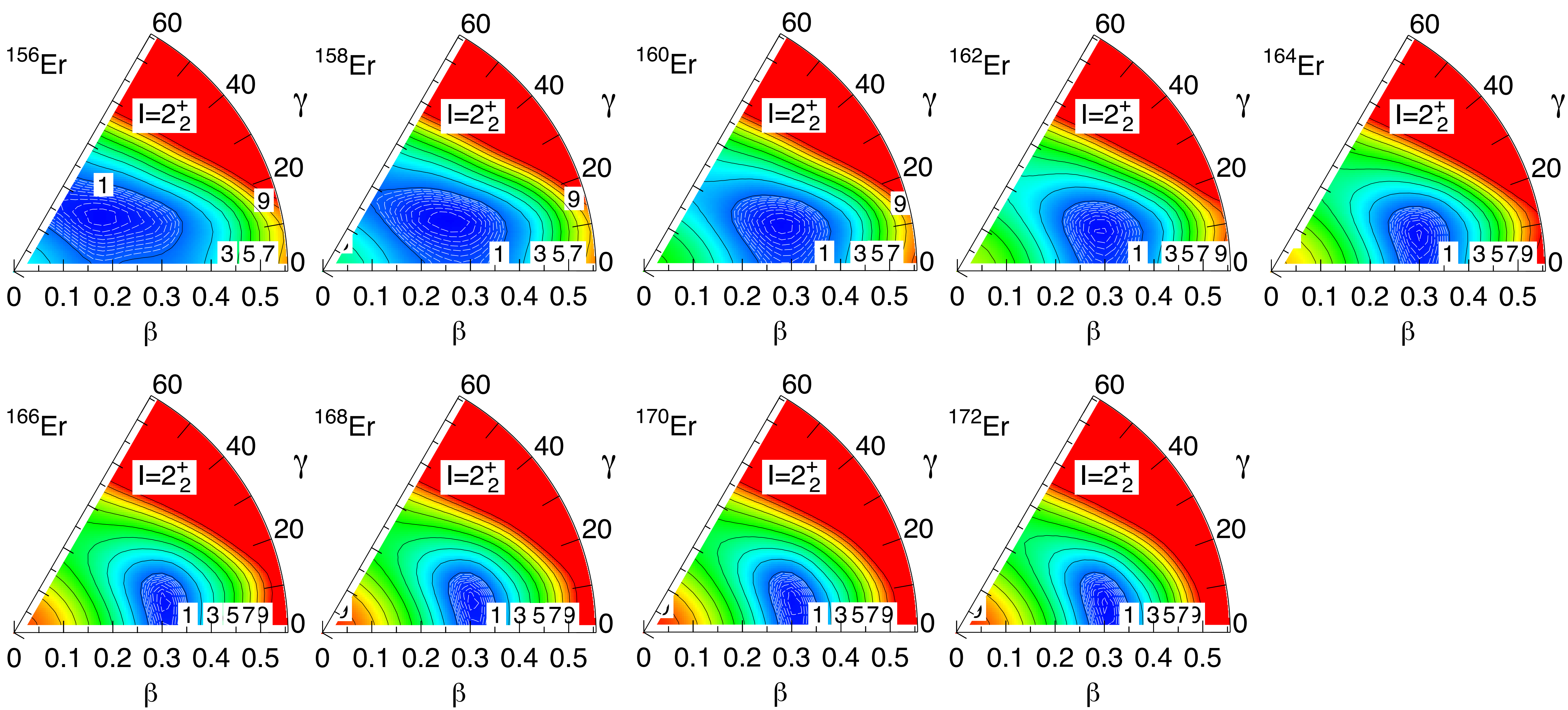
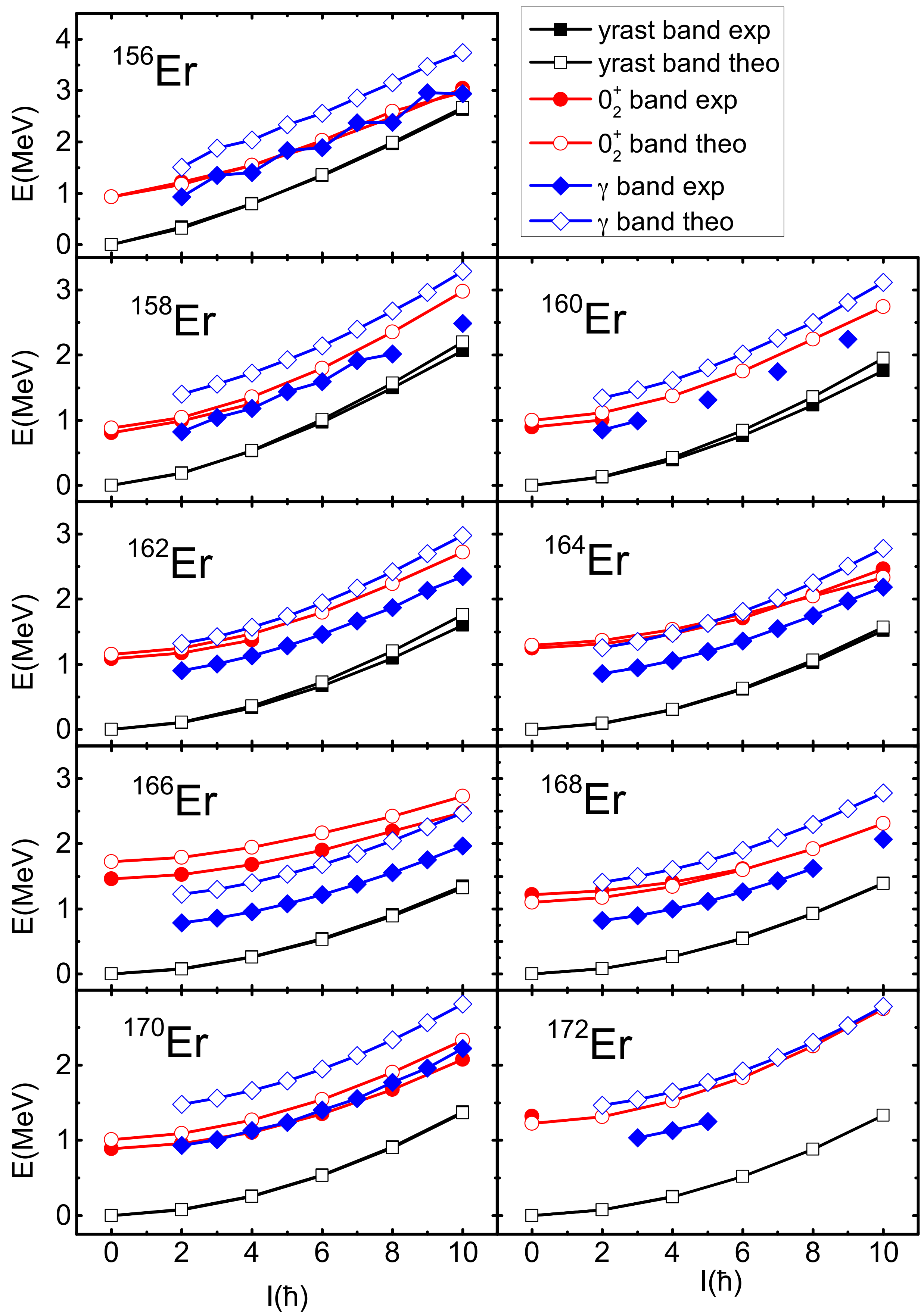
I=2 Potential Energy Surfaces



Excitation energies of the collective bands as a function of spin



Several Approximations for the Collective Bands

Theo0

$$E(2_\gamma^+) = E^{\sigma=2,I=2}(\beta_{\rm min}^{1,0}, \gamma_{\rm min}^{1,0}) - E^{\sigma=1,I=0}(\beta_{\rm min}^{1,0}, \gamma_{\rm min}^{1,0})$$

Theo1

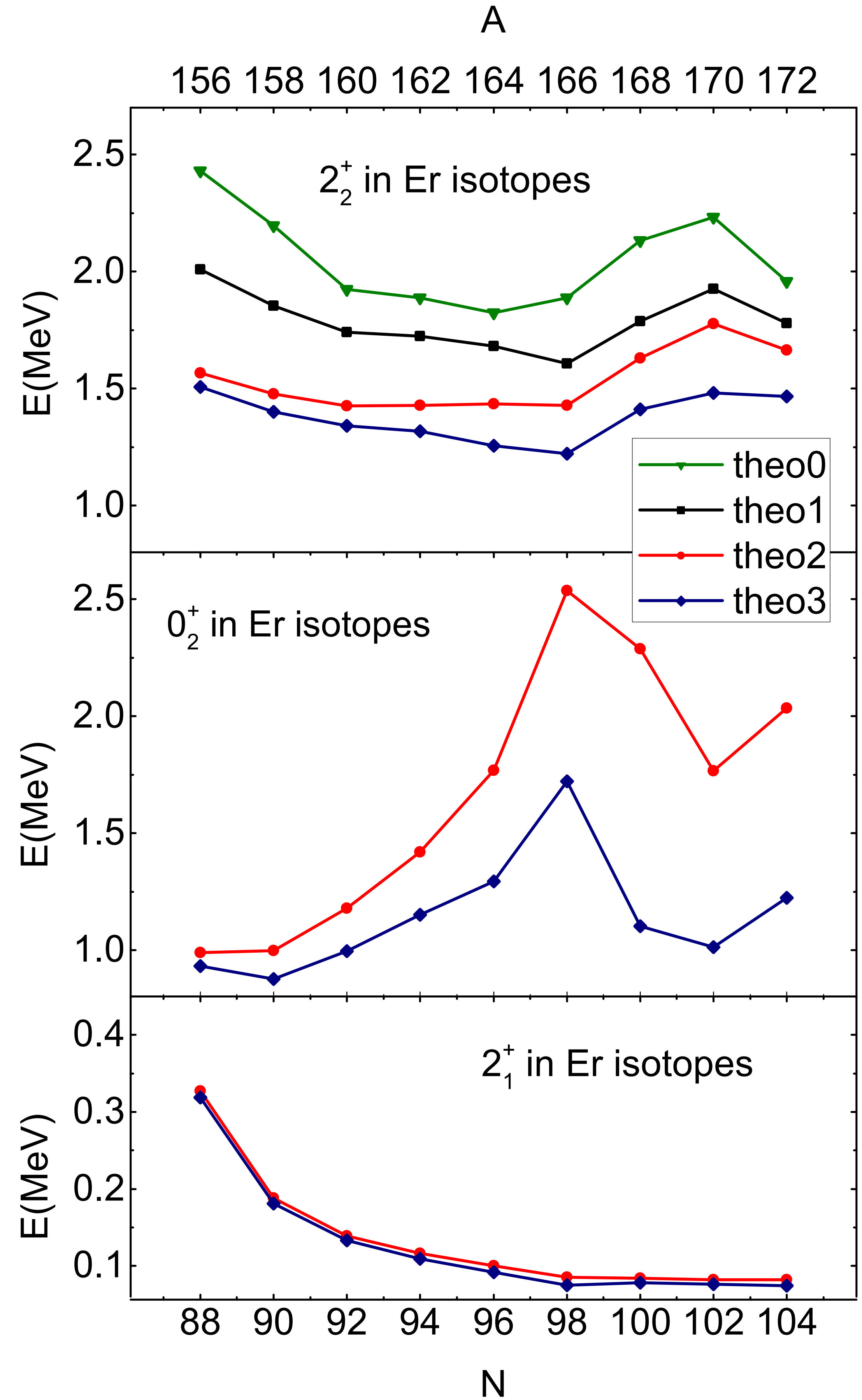
$$E(2_\gamma^+) = E^{\sigma=2,I=2}(\beta_{\rm min}^{2,2}, \gamma_{\rm min}^{2,2}) - E^{\sigma=1,I=0}(\beta_{\rm min}^{1,0}, \gamma_{\rm min}^{1,0})$$

Theo2

$$|\sigma, IM\rangle = \int d\beta d\gamma \sum_K f_0^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_0(\beta,\gamma)\rangle.$$

Theo3

$$|\sigma, IM\rangle = \int d\beta d\gamma \sum_K f_0^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_0(\beta,\gamma)\rangle$$
$$+\sum_{ij}\int d\beta d\gamma \sum_K f_{ij}^{\sigma,IK}(\beta,\gamma)\hat{P}^I_{MK}\hat{P}^N\hat{P}^Z|\Phi_{ij}(\beta,\gamma)\rangle$$



Collective wave functions

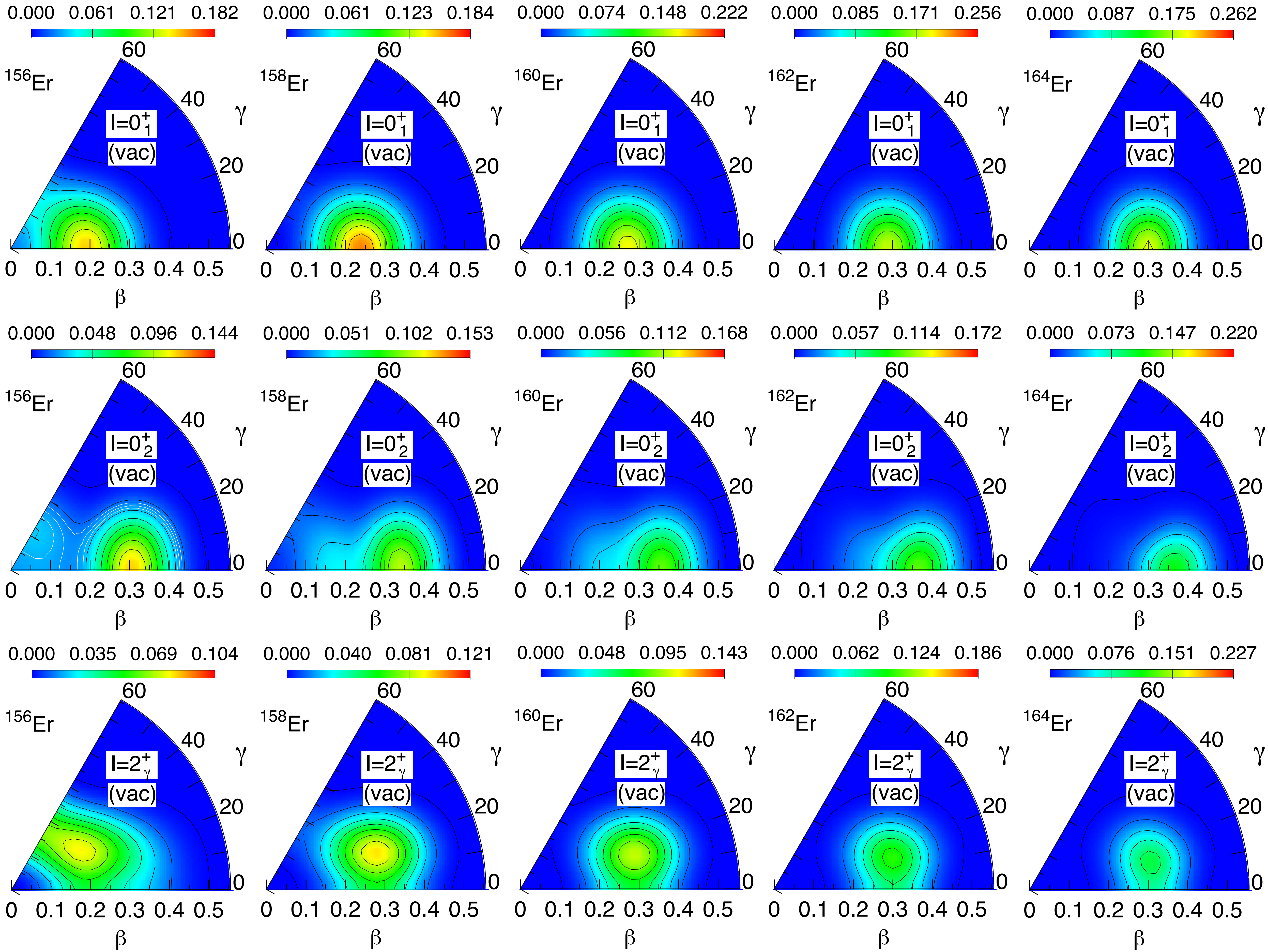
$$p^{\sigma I}_{\rho K}(\beta,\gamma) = \sum_{\kappa} g^{\sigma I}_{\kappa} u^{\kappa I K}_{\rho}(\beta,\gamma) \qquad \sum_{\beta\gamma\rho K} |p^{\sigma I}_{\rho K}(\beta,\gamma)|^2 = 1, \quad \forall \sigma,$$

$$\mathcal{P}^{\sigma I}_{\mathrm{vac}}(\beta,\gamma) = \sum_{K} |p^{\sigma I}_{0K}(\beta,\gamma)|^2$$

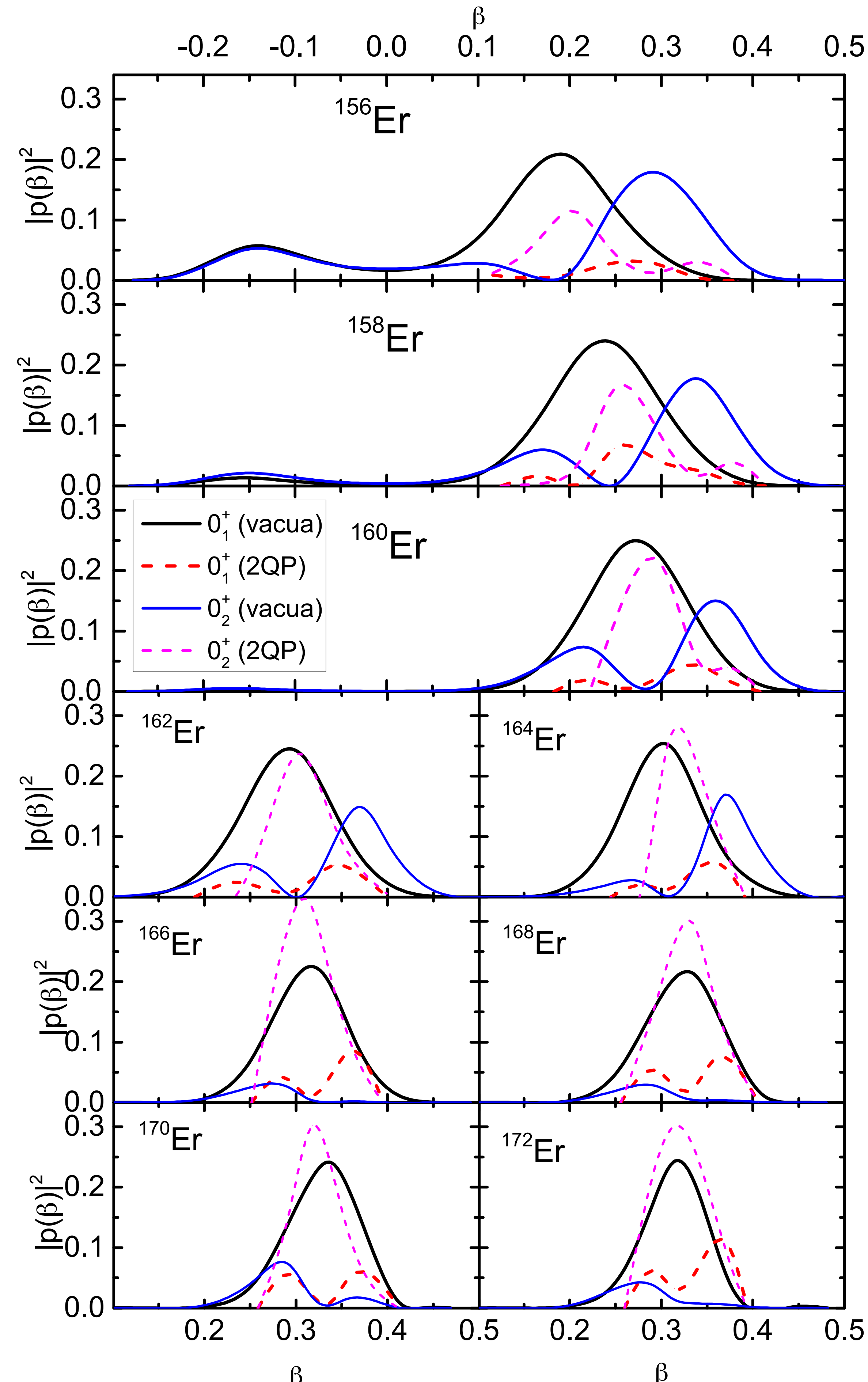
$$\mathcal{P}^{\sigma I}(\beta,\gamma) = \sum_{K\rho} |p^{\sigma I}_{\rho K}(\beta,\gamma)|^2$$

$$\mathcal{P}^{\sigma I}_{\mathrm{2qp}}(\beta,\gamma) = \sum_{K(i,j)} |p^{\sigma I}_{(ij)K}(\beta,\gamma)|^2$$

Collective (only vacua part) wave functions



Axially Symmetric wave functions of the collective states



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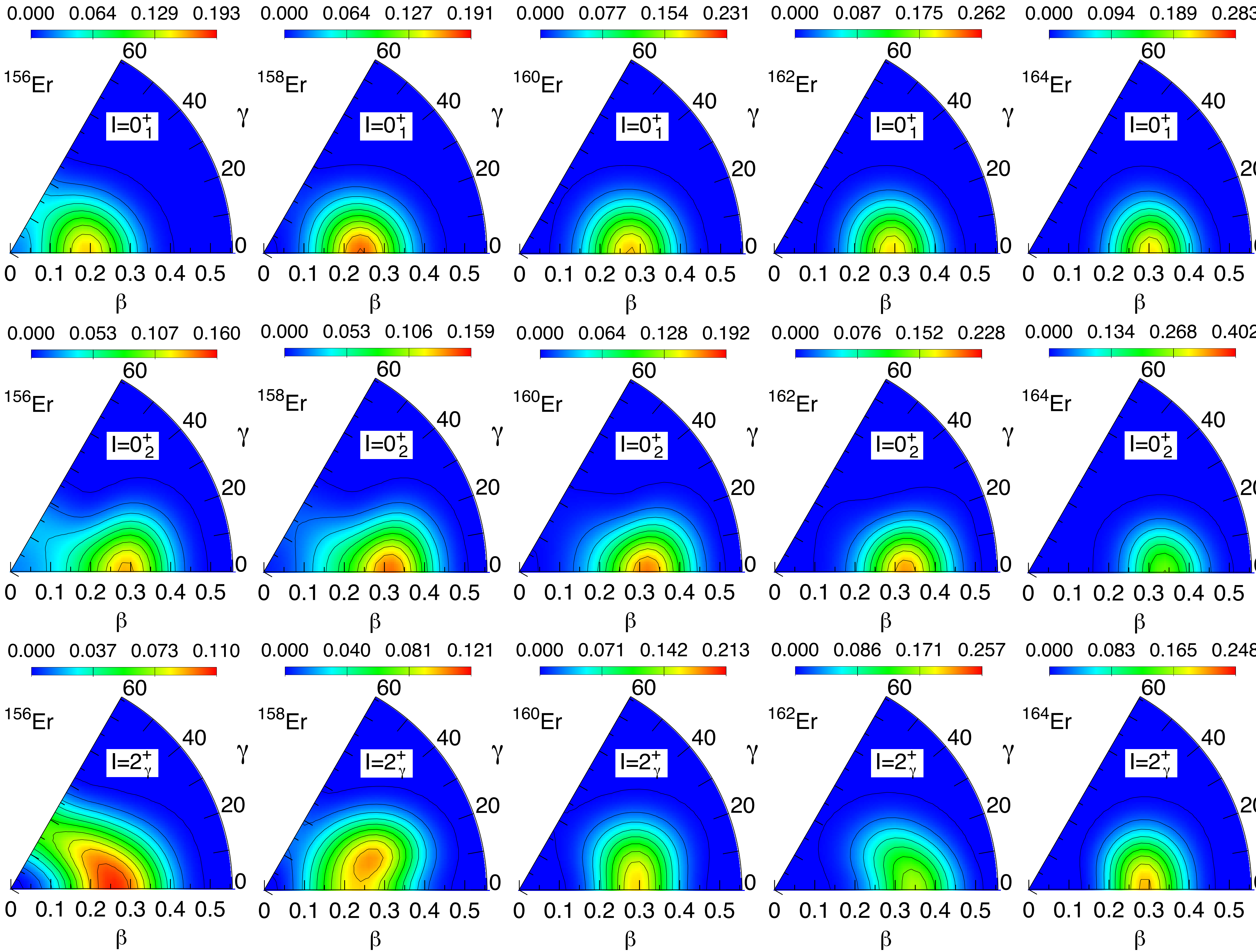
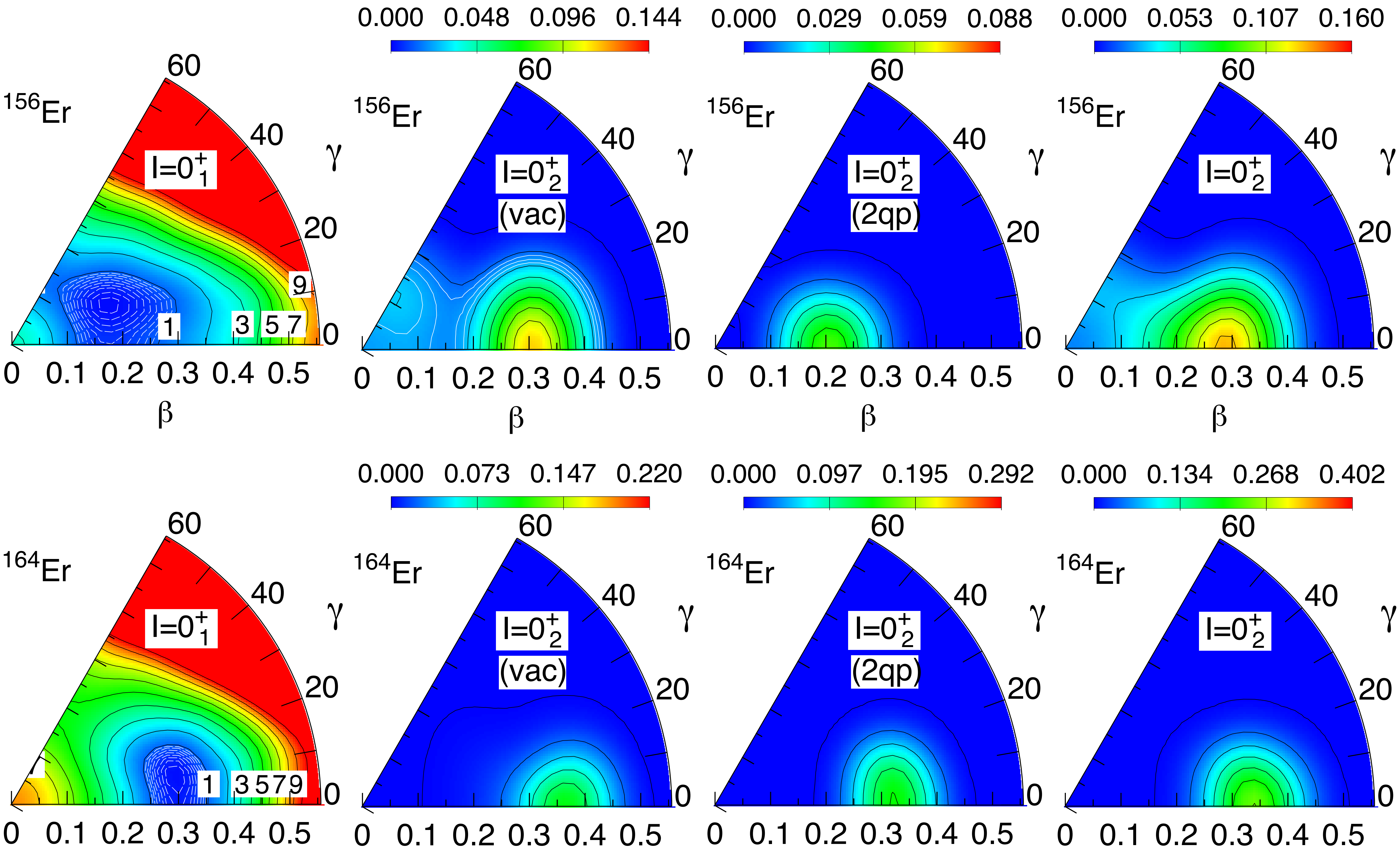
Collective (full, vacua+2qp) wave functions

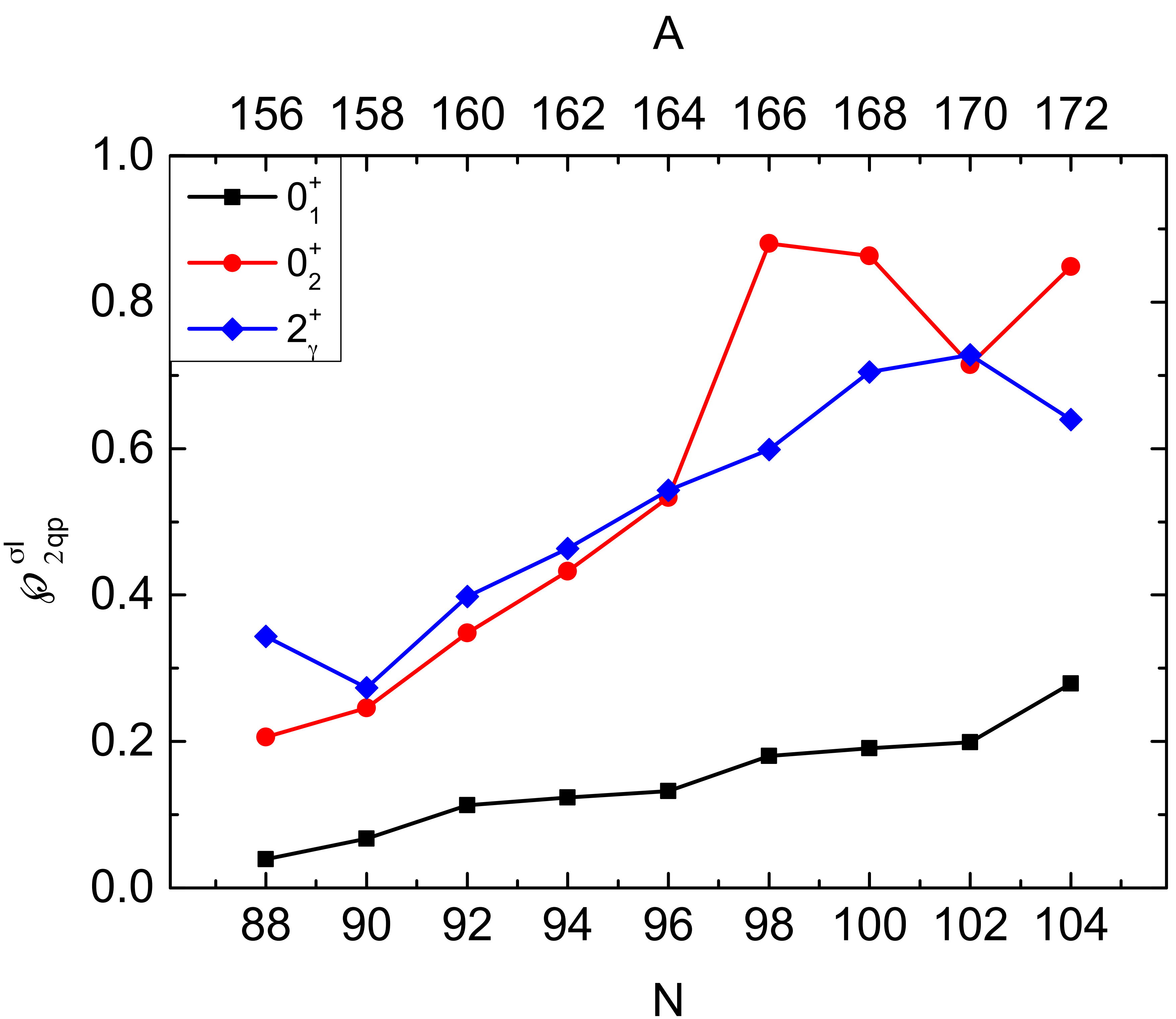


A detailed view of the wave functions

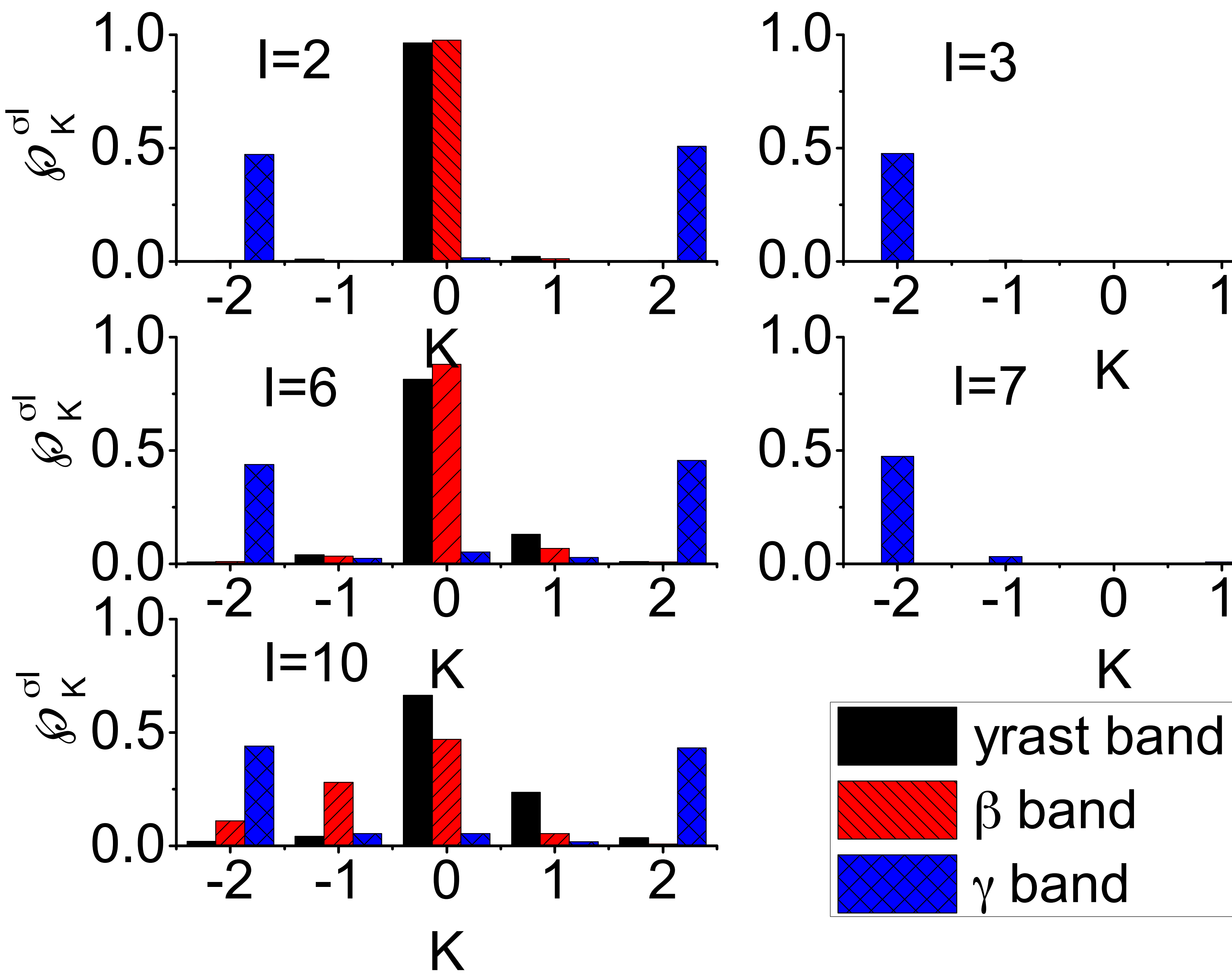


2 qp content of the collective wave functions

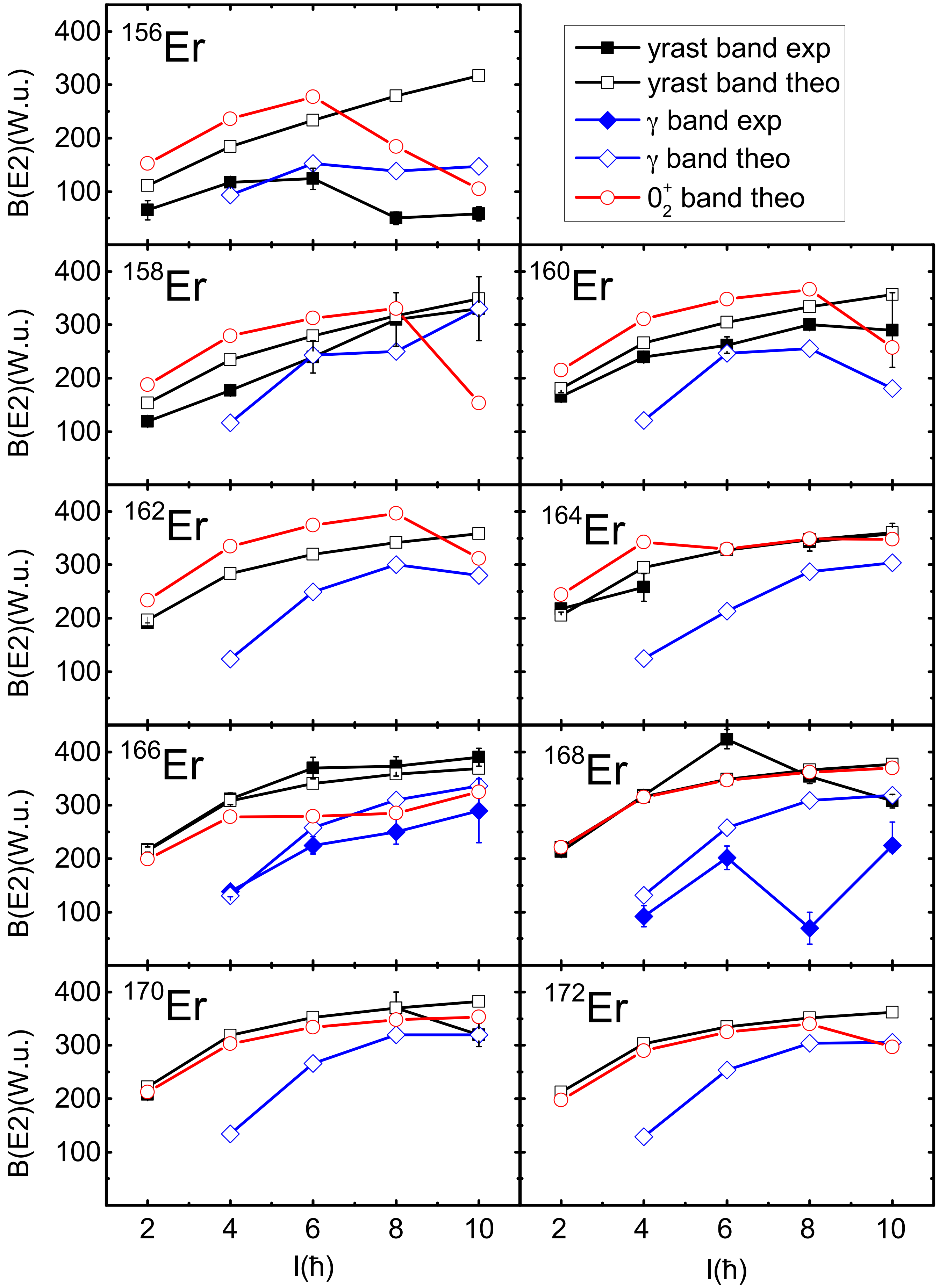
$$\mathcal{P}_{2\mathrm{qp}}^{\sigma I}(\beta,\gamma) = \sum_{K(i,j)} |p_{(ij)K}^{\sigma I}(\beta,\gamma)|^2 \qquad \mathcal{P}_{2\mathrm{qp}}^{\sigma I} = \sum_{\beta\gamma} \mathcal{P}_{2\mathrm{qp}}^{\sigma I}(\beta,\gamma)$$



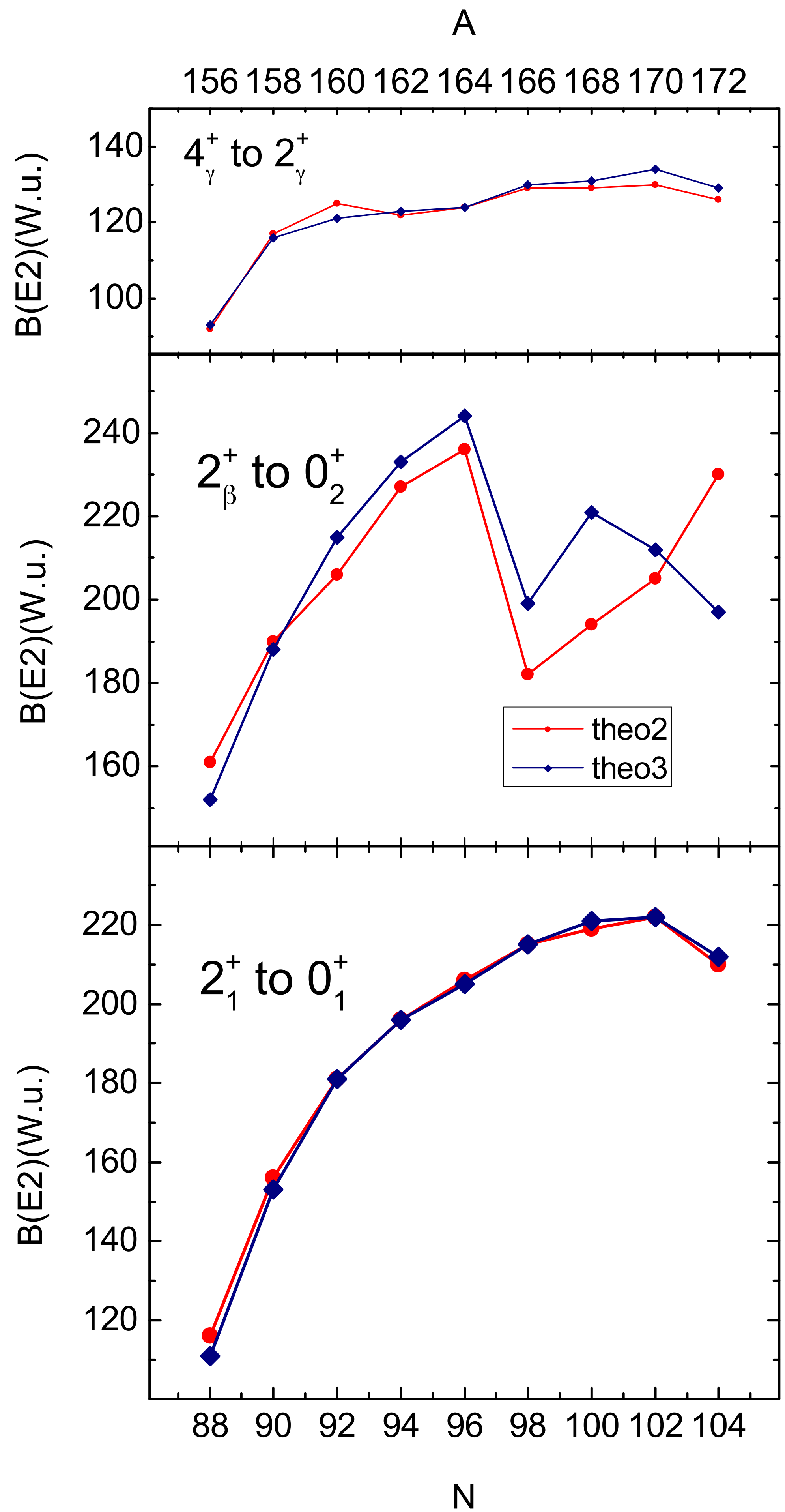
K-distribution of the collective states for several spin values



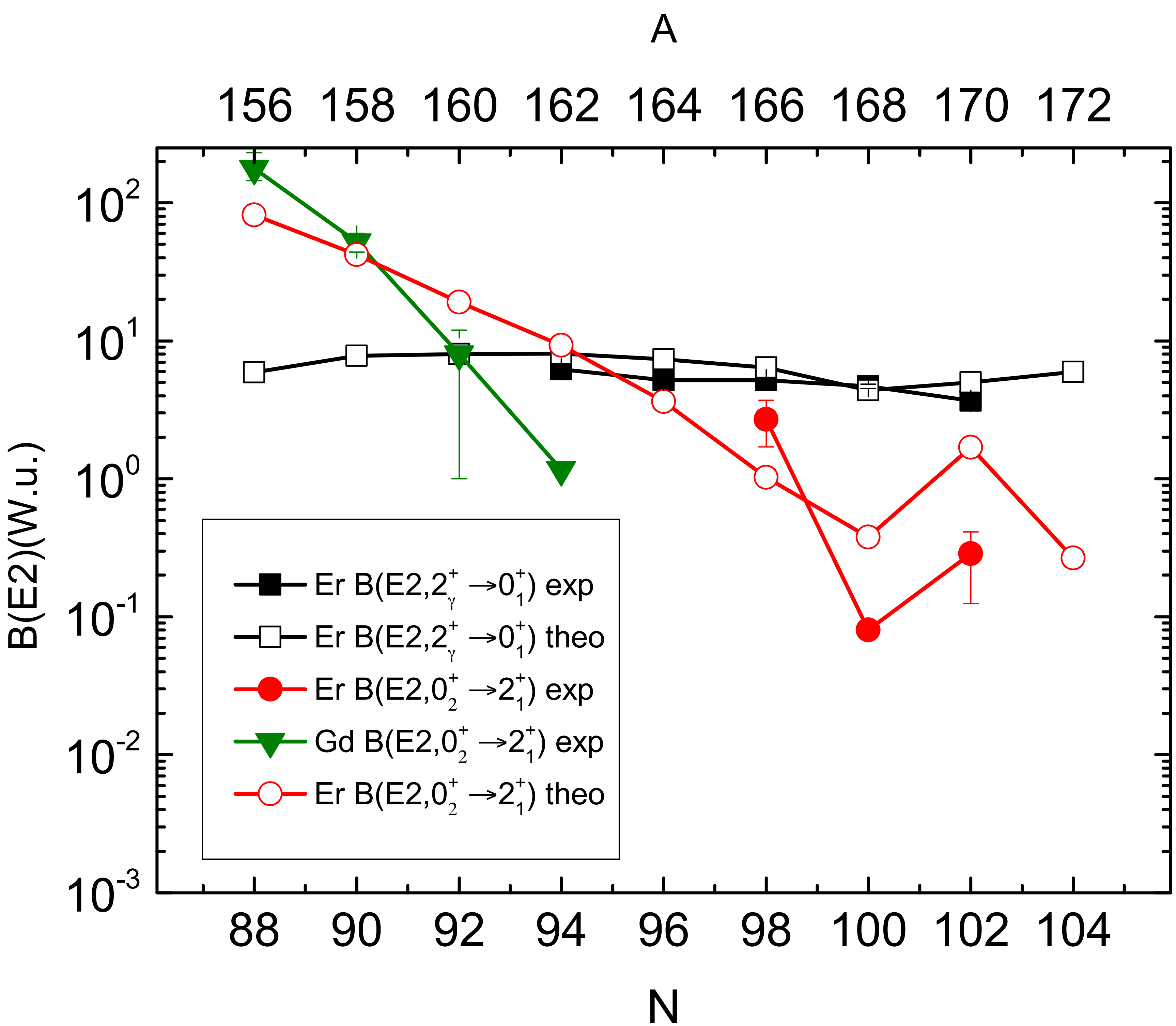
Intraband B(E2) transition probabilities



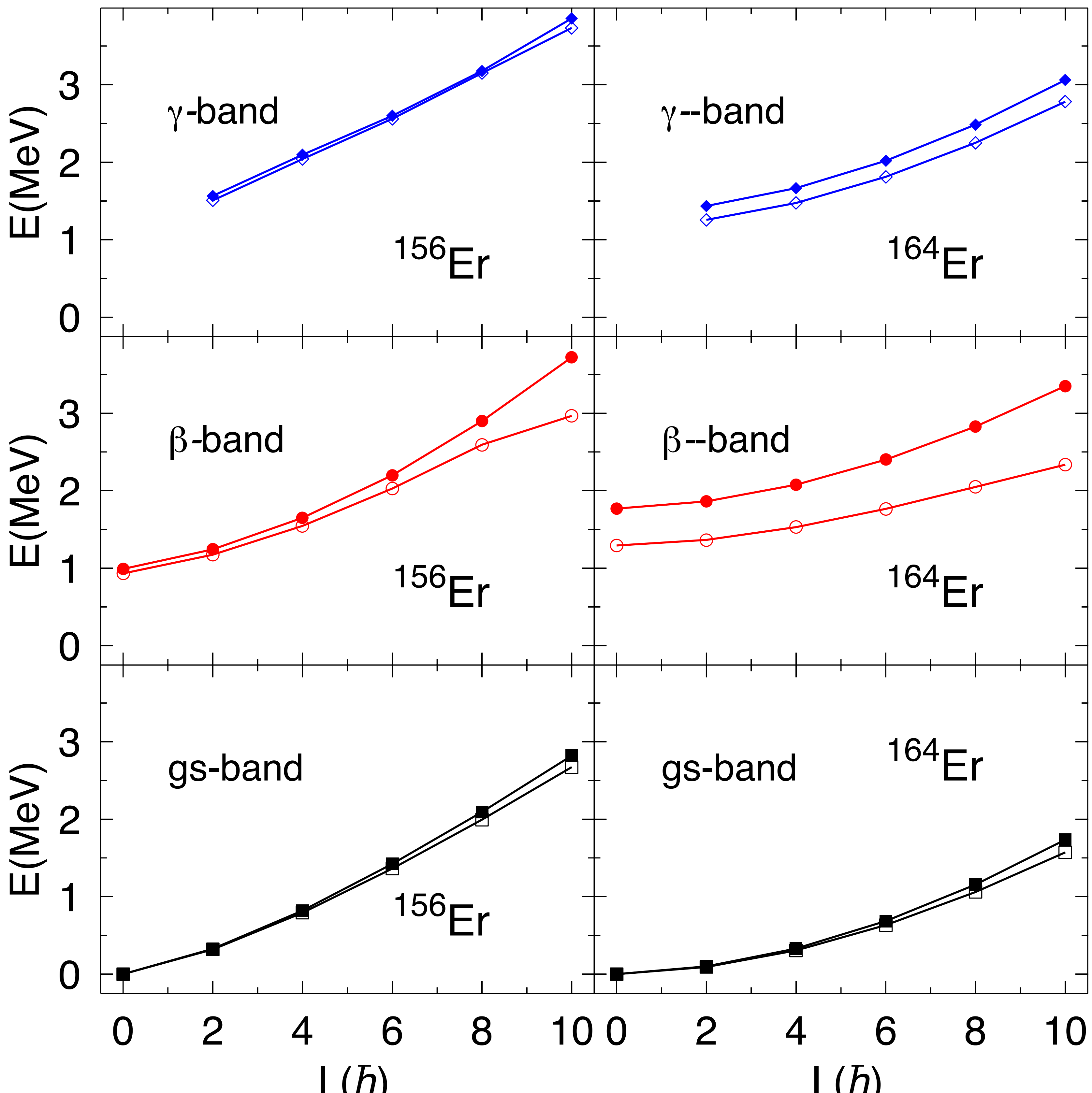
Intraband B(E2) transition probabilities



Interband B(E2) transition probabilities



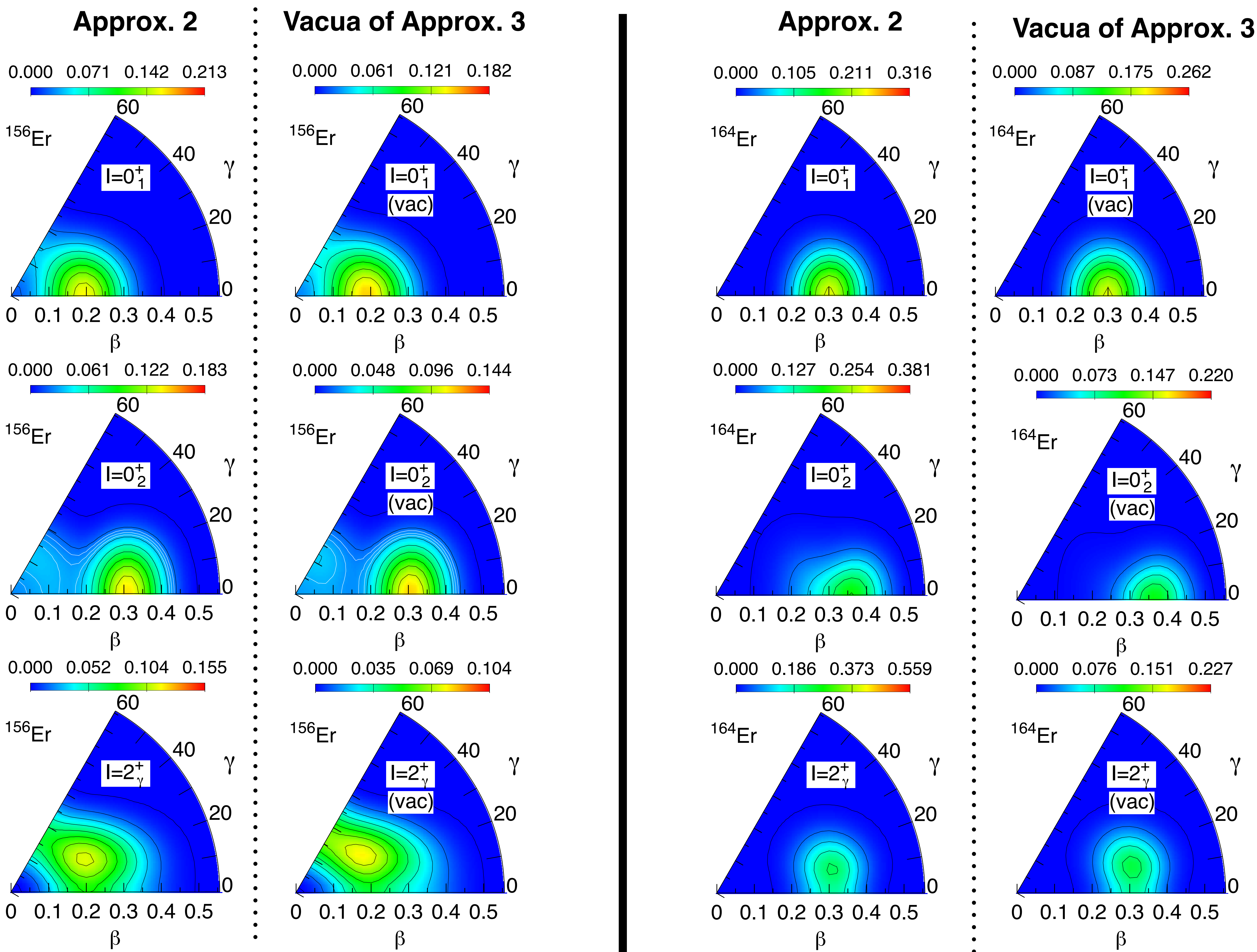
Collective bands with- and without 2qp states



With 2qp states: Open symbols.

Without 2qp states: Filled symbols

Collective wave functions with- and without 2qp states



Conclussion

1.- Our model provides a good overall description of the energies of the collective bands and transition probabilities, over several orders of magnitude, for soft medium and rigid nuclei.

2.-Two-quasiparticle states are relevant for the β and γ bands, specially for the former one.

3.- Two-quasiparticle states are less important for soft nuclei than for rigid ones.

4.- The node of the genuine β-band couples to the triaxiallity and becomes a valley.

5.- Different character of the β and the γ bands.

6.- Mainly five two-quasiparticle states provide the main contribution. Can we find these states in an easy way ?