9th International Workshop on
Quantum Phase Transition in Nuclei and Many-Body Systems
22-25 May 2018, Padova (Italy)

Symmetry Conserving Configuration Mixing description of odd-mass nuclei
and
some comments on shape coexistence and pairing transitions

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Departamento de Física Teórica

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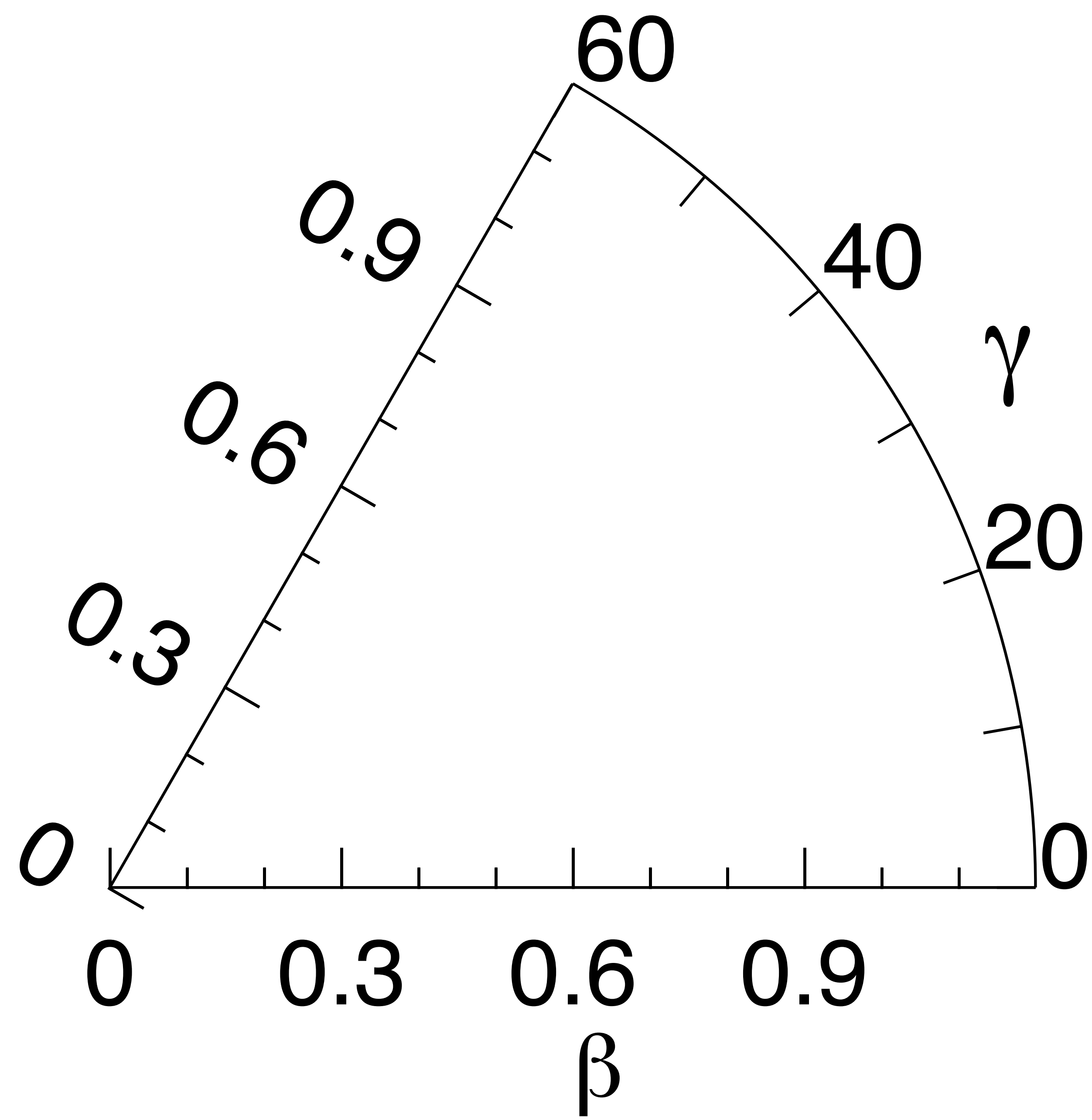
Aim of the talk…



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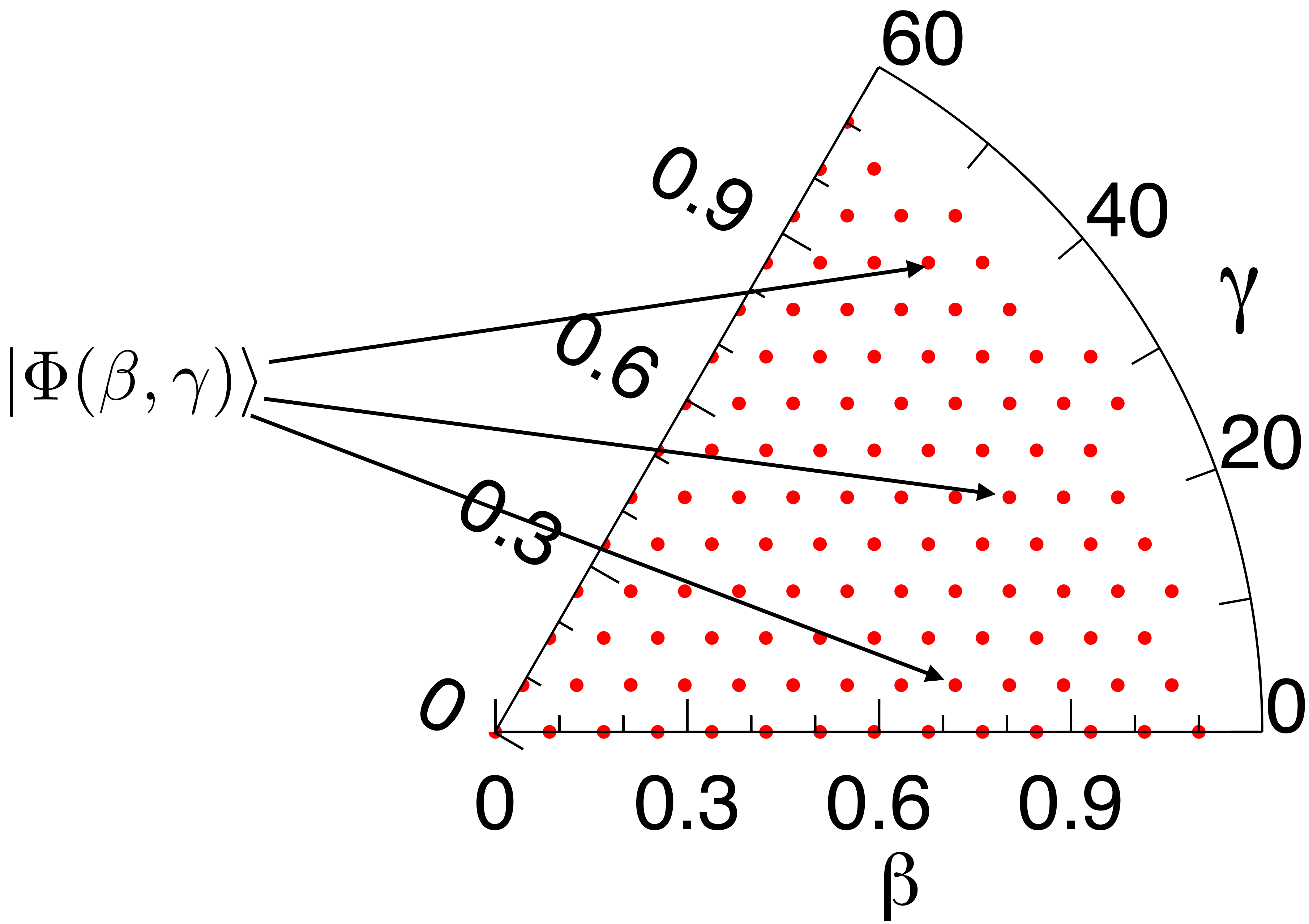

… to perform configuration mixing calculations

… I am going to talk about the theoretical description of odd-A nuclei using the Finite Range density dependent Gogny interaction and sophisticated microscopical approaches namely the symmetry conserving configuration mixing theory

Calculations:

1.- **Systematic study of bulk properties** (binding energies, energy gaps, radii and electromagnetic moments, etc) in the Mg isotopic chain with particle number and angular momentum projection.

2.- As an example of full spectroscopy I will show the spectrum and the transition probabilities of the **odd nucleus ^{25}Mg** a symmetry conserving approach with triaxial shape fluctuations and alignment fluctuations.

3.- Some comments on shape coexistence and pairing phase transitions

Symmetry conserving mean field theory (SCMFT): EXACT

A good approximation to a many-body wave function is provided by HF, BCS or HFB

$$|\Phi\rangle = \prod_\mu \alpha_\mu |-\rangle \qquad \text{(even-even)}, \qquad |\tilde{\Phi}\rangle = \alpha^\dagger_{\rho_1} |\Phi\rangle \qquad \text{(odd-even)}$$

with

$$\alpha^\dagger_\rho = \sum_\mu U_{\mu\rho} c^\dagger_\mu + V_{\mu\rho} c_\mu$$

To recover symmetries we perform exact projections

$$|\Psi^{N,I,\pi}_{M,\sigma}\rangle = P^N P^I_M \, |\tilde{\Phi}^\pi\rangle = \sum_K g^I_{K\sigma} P^N P^I_{MK} \, |\tilde{\Phi}^\pi\rangle,$$

with the parameters U, V and g's determined by the variational principle:

$$\delta E^{N,I,\pi} = \delta \frac{\langle \tilde{\Phi}^\pi | \hat{H} \hat{P}^N P^I_M | \tilde{\Phi}^\pi \rangle}{\langle \tilde{\Phi}^\pi | \hat{P}^N P^I_M | \tilde{\Phi}^\pi \rangle} = 0.$$

This equation provides only the energy minimum in the (β, γ) plane.

Symmetry conserving mean field theory (SCMFT): EXACT

To generate all possible configurations one has to solve

$$\delta E^{N,I,\pi} = \delta \frac{\langle \tilde{\Phi}^{\pi} | \hat{H} \hat{P}^{N} P^{I}_{M} | \tilde{\Phi}^{\pi} \rangle}{\langle \tilde{\Phi}^{\pi} | \hat{P}^{N} P^{I}_{M} | \tilde{\Phi}^{\pi} \rangle} = 0.$$

with the constraints

$$\langle \tilde{\Phi}^{\pi} | \hat{Q}_{20} | \tilde{\Phi}^{\pi} \rangle = q_{20}, \qquad \langle \tilde{\Phi}^{\pi} | \hat{Q}_{22} | \tilde{\Phi}^{\pi} \rangle = q_{22}$$

for a set of (q_{20}, q_{22}) values. This provides a set of wave functions $|\tilde{\Phi}^{\pi}(q_{20}, q_{22})\rangle$, **or equivalently** $|\tilde{\Phi}^{\pi}(\beta, \gamma)\rangle$.

In a second step we mix all (β, γ) configurations

$$|\Psi^{N,I,\pi}_{M,\sigma}\rangle = \sum_{K,\beta,\gamma} f^{I}_{K\sigma}(\beta,\gamma) P^{N} P^{I}_{MK} \, |\tilde{\Phi}(\beta,\gamma)\rangle,$$

and determine the mixing coefficients by diagonalization of the full Hamiltonian and obtain wave functions and energies.

The determination of the wave functions $|\tilde{\Phi}_{\pi}(\beta, \gamma)\rangle$ is very time consuming, therefore

A symmetry conserving mean field approach (SCMFA)

… much simpler is to solve

$$\delta E^{N,\pi} = \delta \frac{\langle \tilde{\Phi}^{\pi} | \hat{H} \hat{P}^{N} | \tilde{\Phi}^{\pi} \rangle}{\langle \tilde{\Phi}^{\pi} | \hat{P}^{N} | \tilde{\Phi}^{\pi} \rangle} = 0,$$

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An important quantity is the potential energy surface (PES) for different angular momentum. It provides insight in the physics of the results

$$E^{N,I,\pi}(\beta,\gamma) = \frac{\langle \tilde{\Phi}^{\pi}(\beta,\gamma) | \hat{H} \hat{P}^{N} P^{I}_{M} | \tilde{\Phi}^{\pi}(\beta,\gamma) \rangle}{\langle \tilde{\Phi}^{\pi}(\beta,\gamma) | \hat{P}^{N} P^{I}_{M} | \tilde{\Phi}^{\pi}(\beta,\gamma) \rangle}$$

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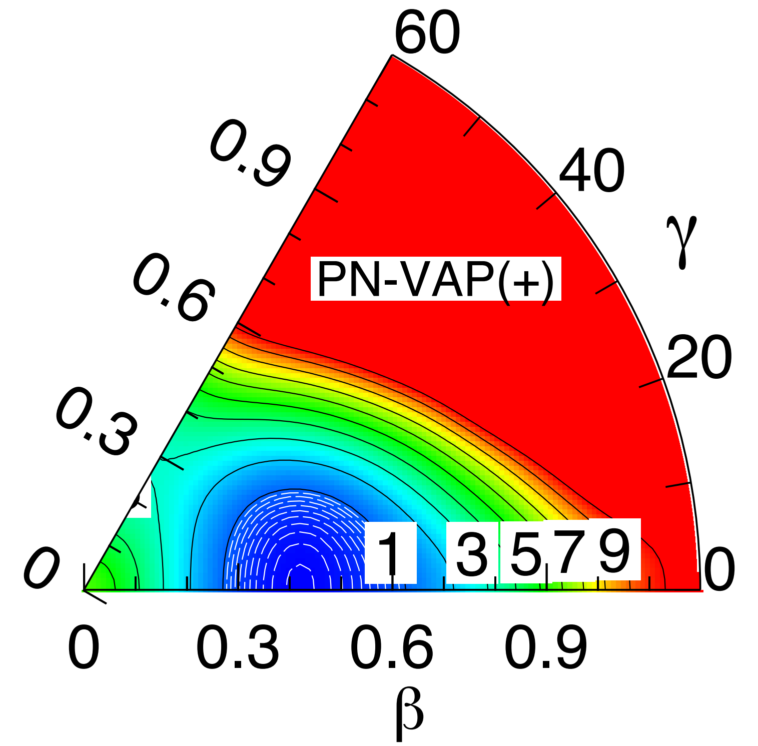

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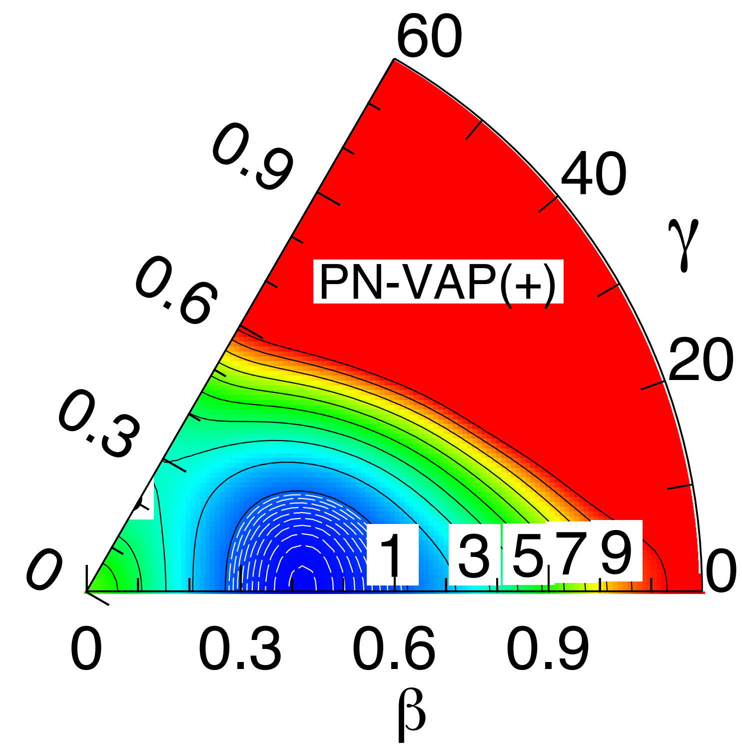

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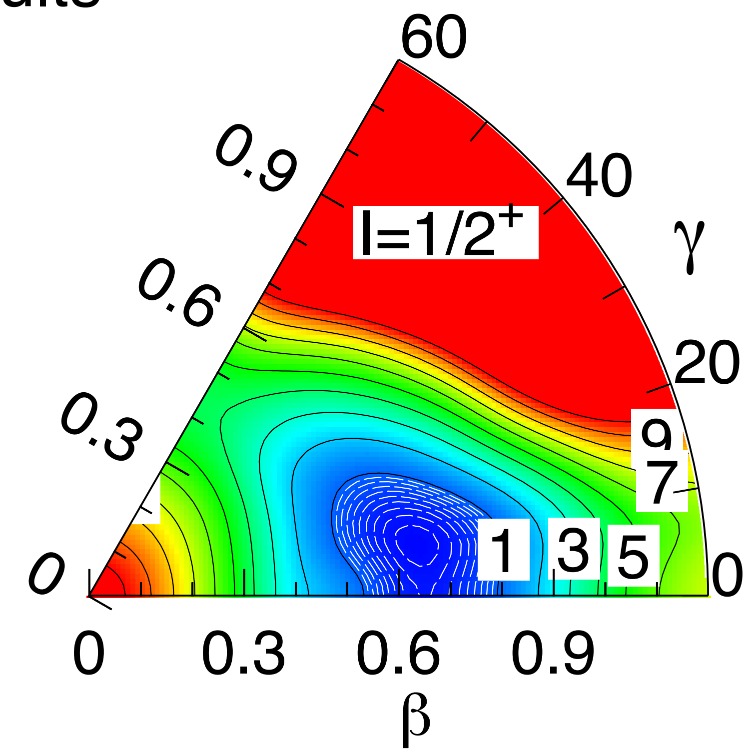

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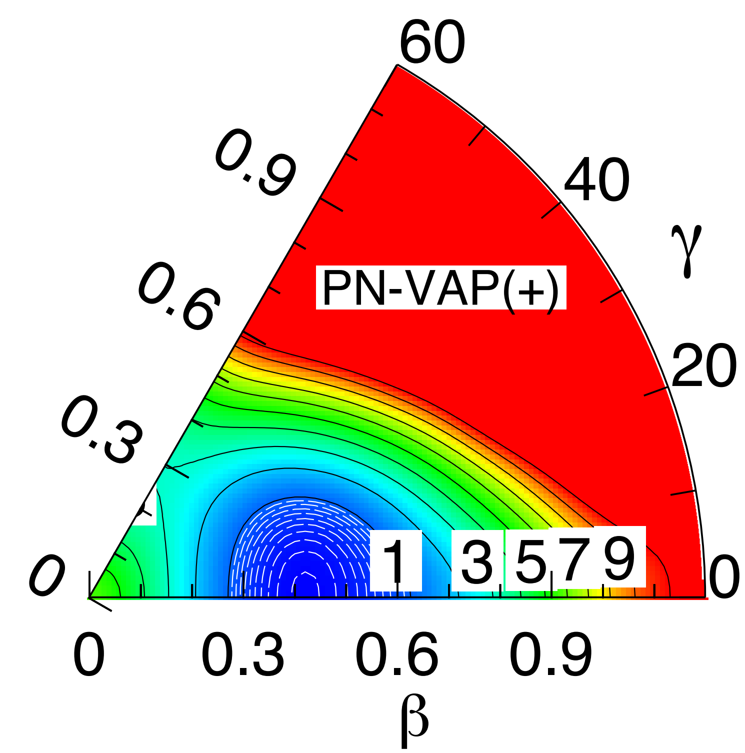

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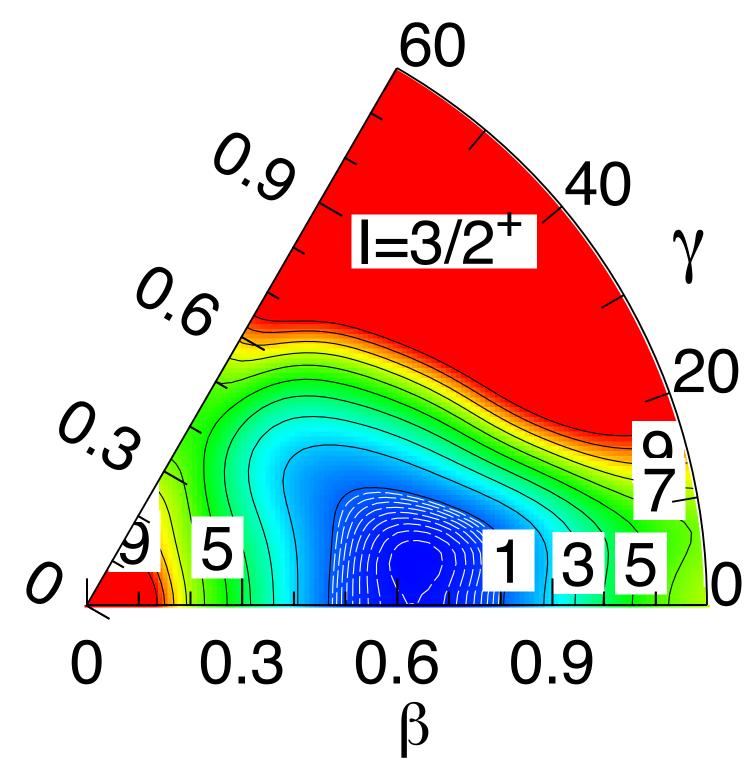

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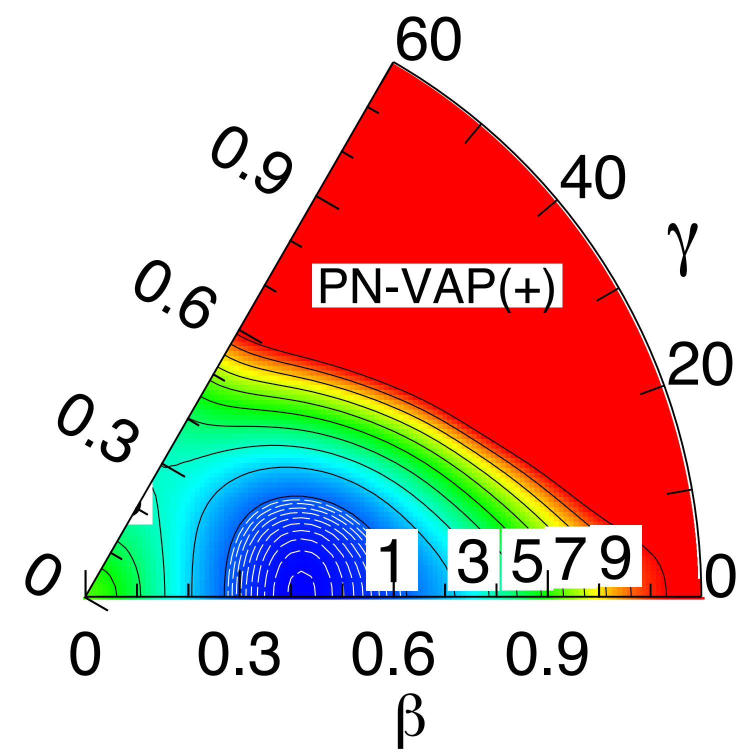

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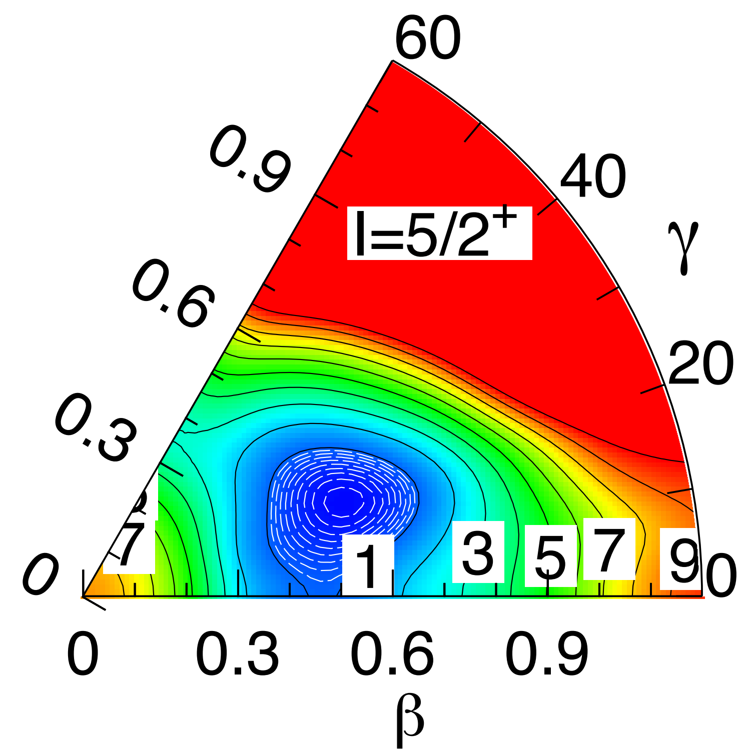


Ground state properties
of the
Magnesium Isotopes
in the
Symmetry Conserving Mean Field Approximation

The Gogny Interaction

J. Dechargé, D. Gogny, Phys. Rev. C 21, 1568 (1980)

In the calculations we use large configuration spaces (8 or 9 Oscillator shells.Therefore no effective charges are needed. We use the D1S parametrisation of the Gogny force:

$$V(1,2) = \sum_{i=1}^{2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2} \left(W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau\right) \quad \text{central term}$$

$$+iW_0(\sigma_1+\sigma_2)\vec{k} \times \delta(\vec{r}_1-\vec{r}_2)\vec{k} \quad \text{Spin-orbit term}$$

$$+t_3(1+x_0P^\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha((\vec{r}_1+\vec{r}_2)/2) \quad \text{density-dependent term}$$

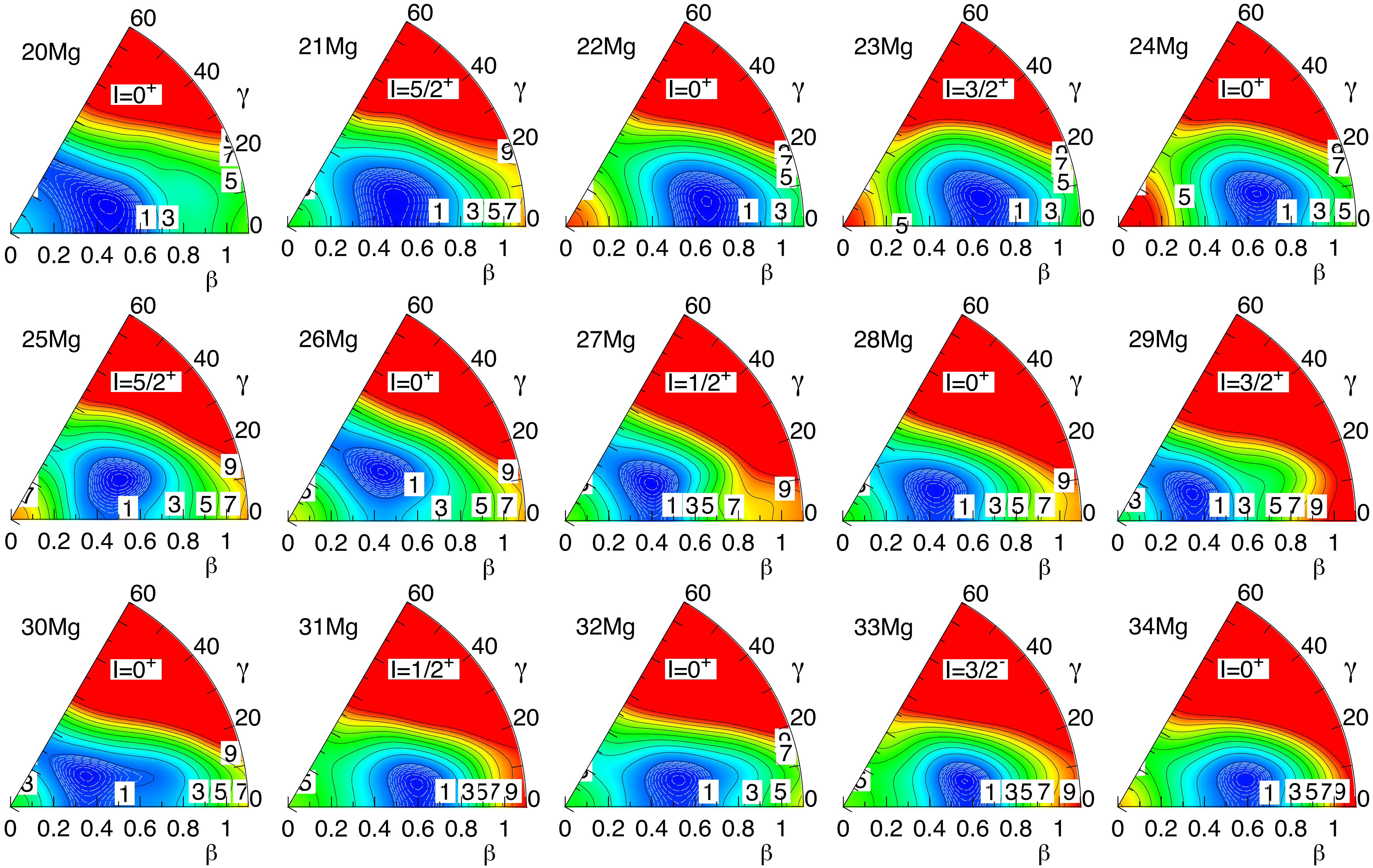
$$+V_{\text{Coulomb}}(\vec{r}_1,\vec{r}_2) \quad \text{Coulomb term}$$

D1S Parametrization (Berger et al. 1984)

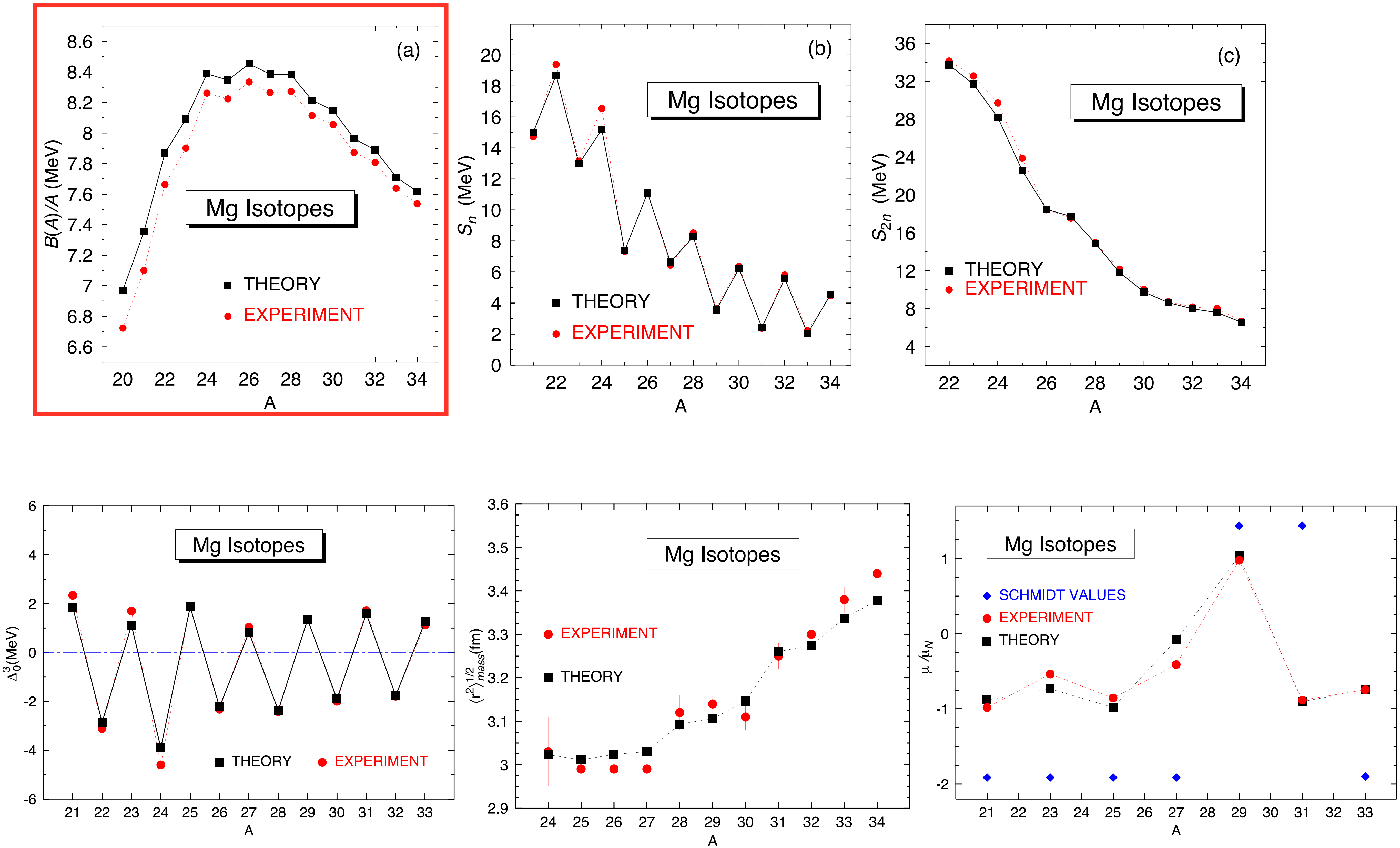
i	$\mu(\text{fm})^2$	W	B	H	M
1	0,7	-1720,3	1300	-1813,53	1397,6
2	1,2	103,638	-163,48	162,81	-223,93

W_0=130 MeV fm^5
x_0=1.0, α =1/3
t_3=1390.6 MeV fm^4

Particle Number and Angular Momentum Projected Potential Energy Surfaces of Mg isotopes



Bulk properties of the Mg isotopes



M. Borrajo, J.L. E., Phys. Lett. B 764 (2017)328-334

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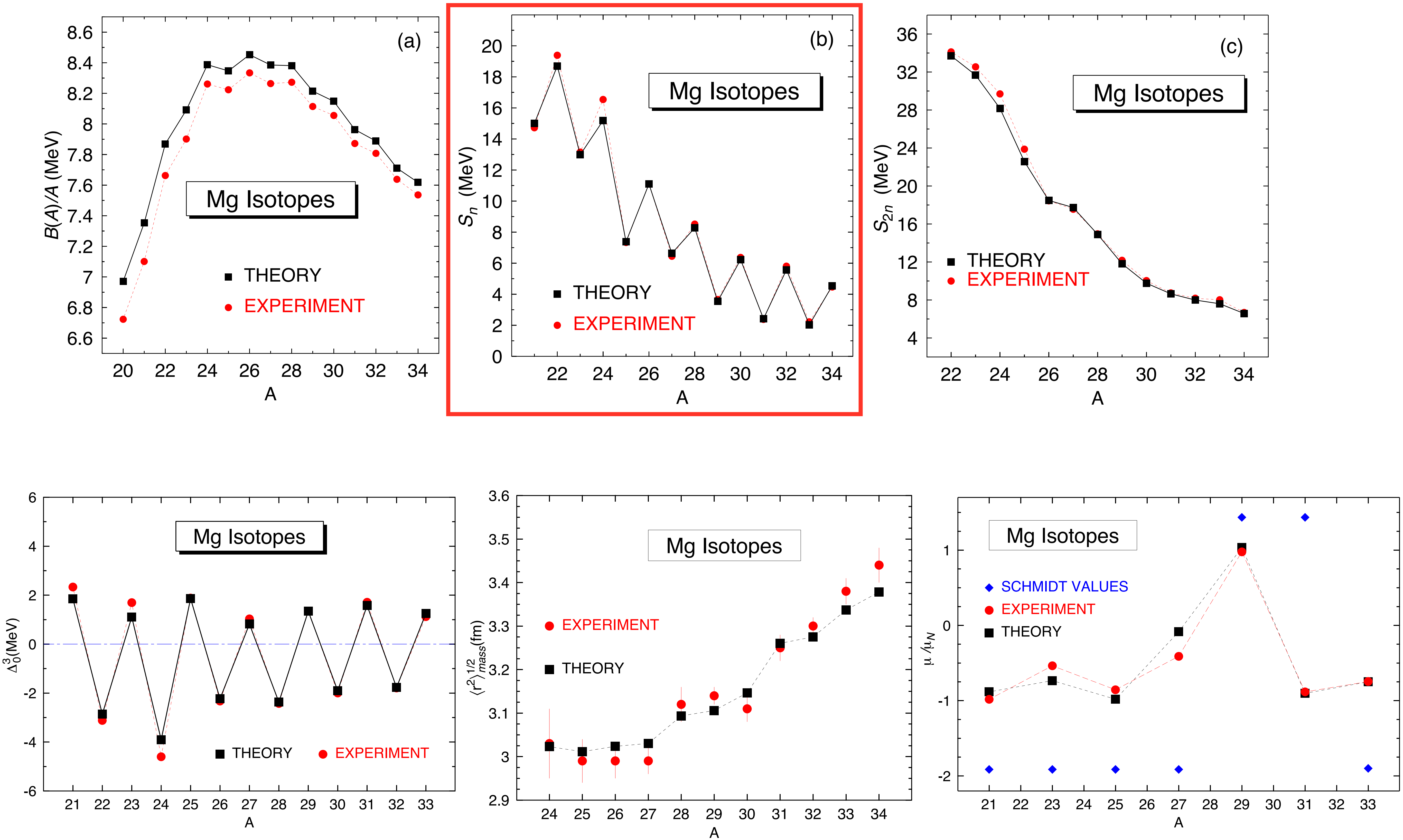

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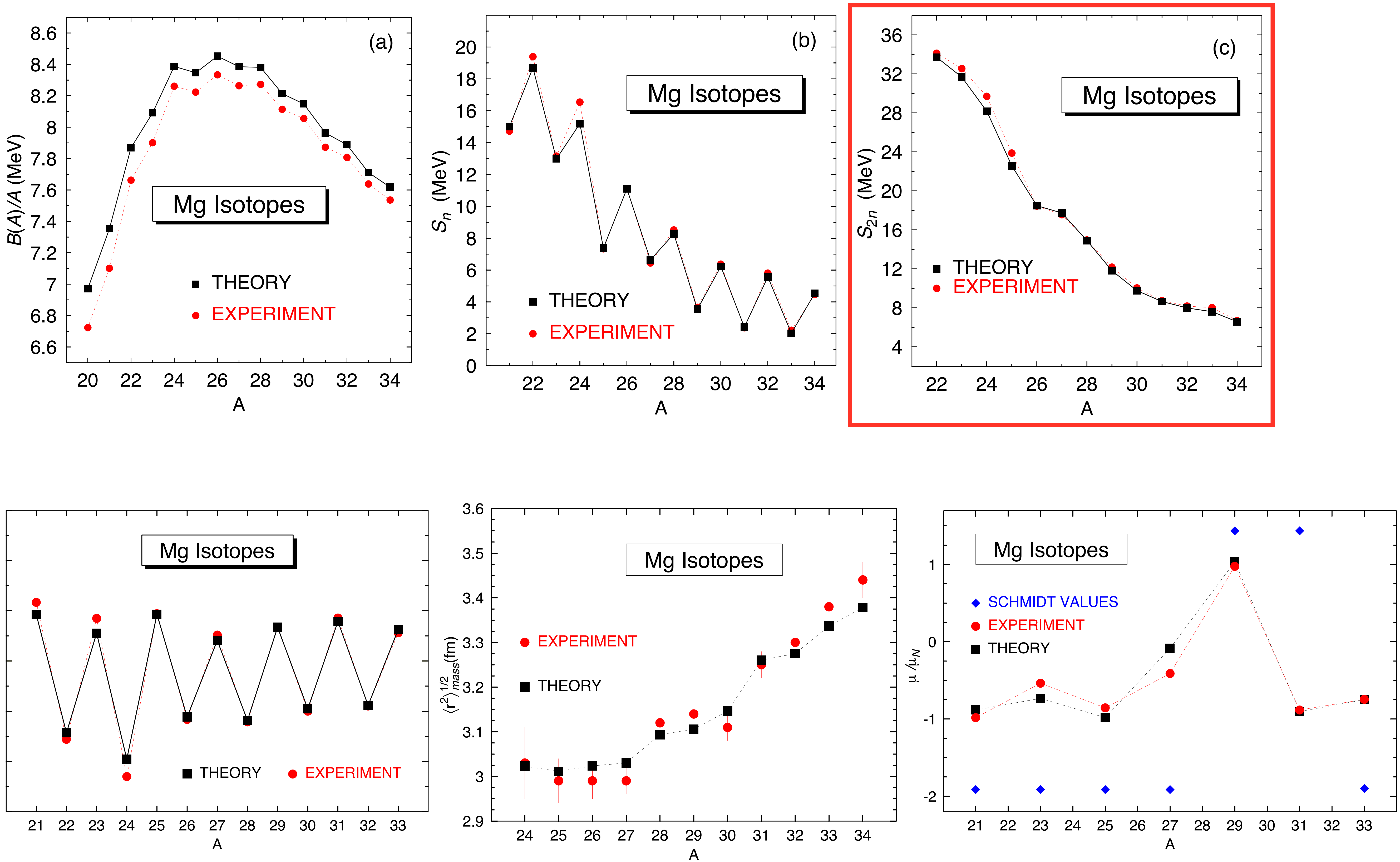

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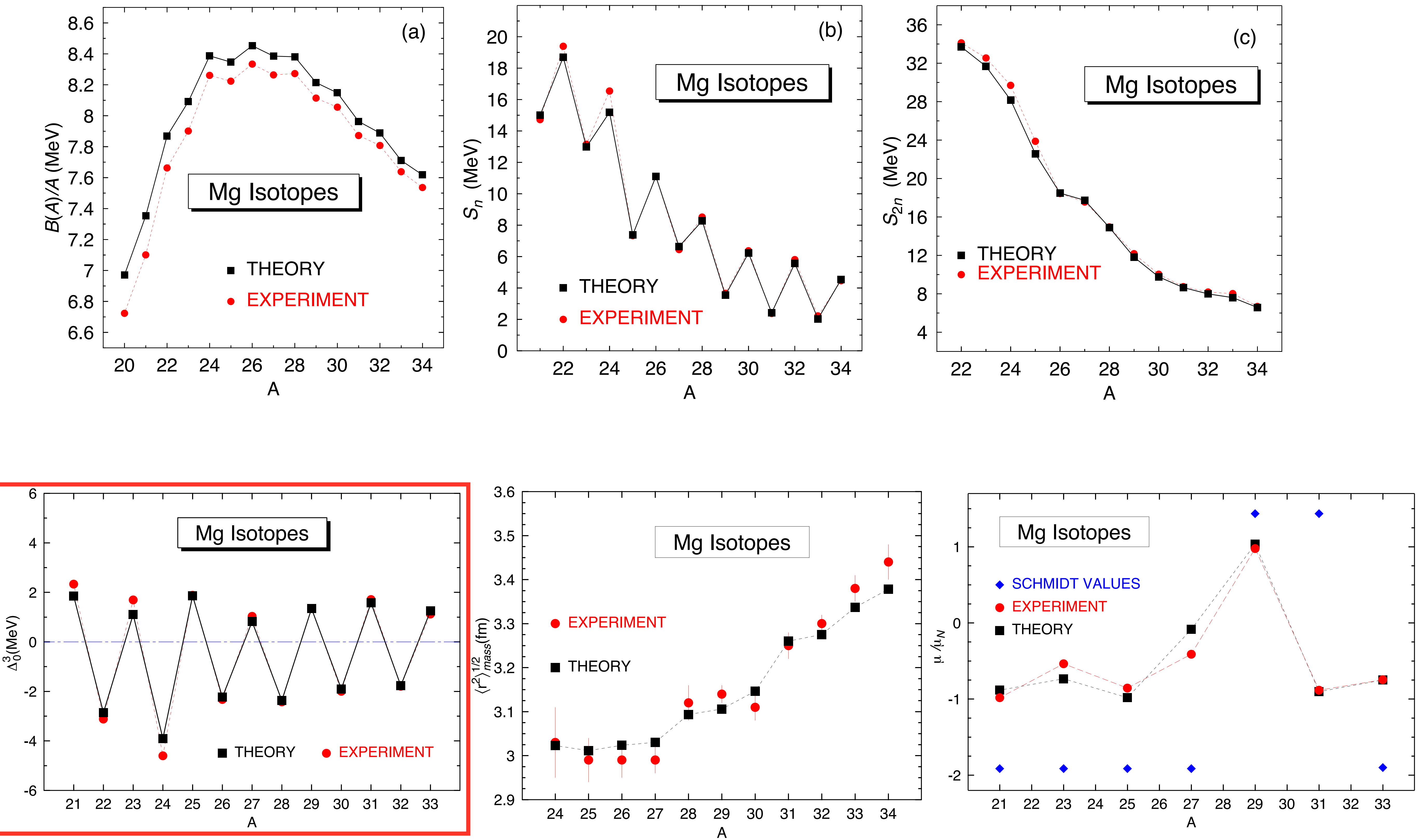

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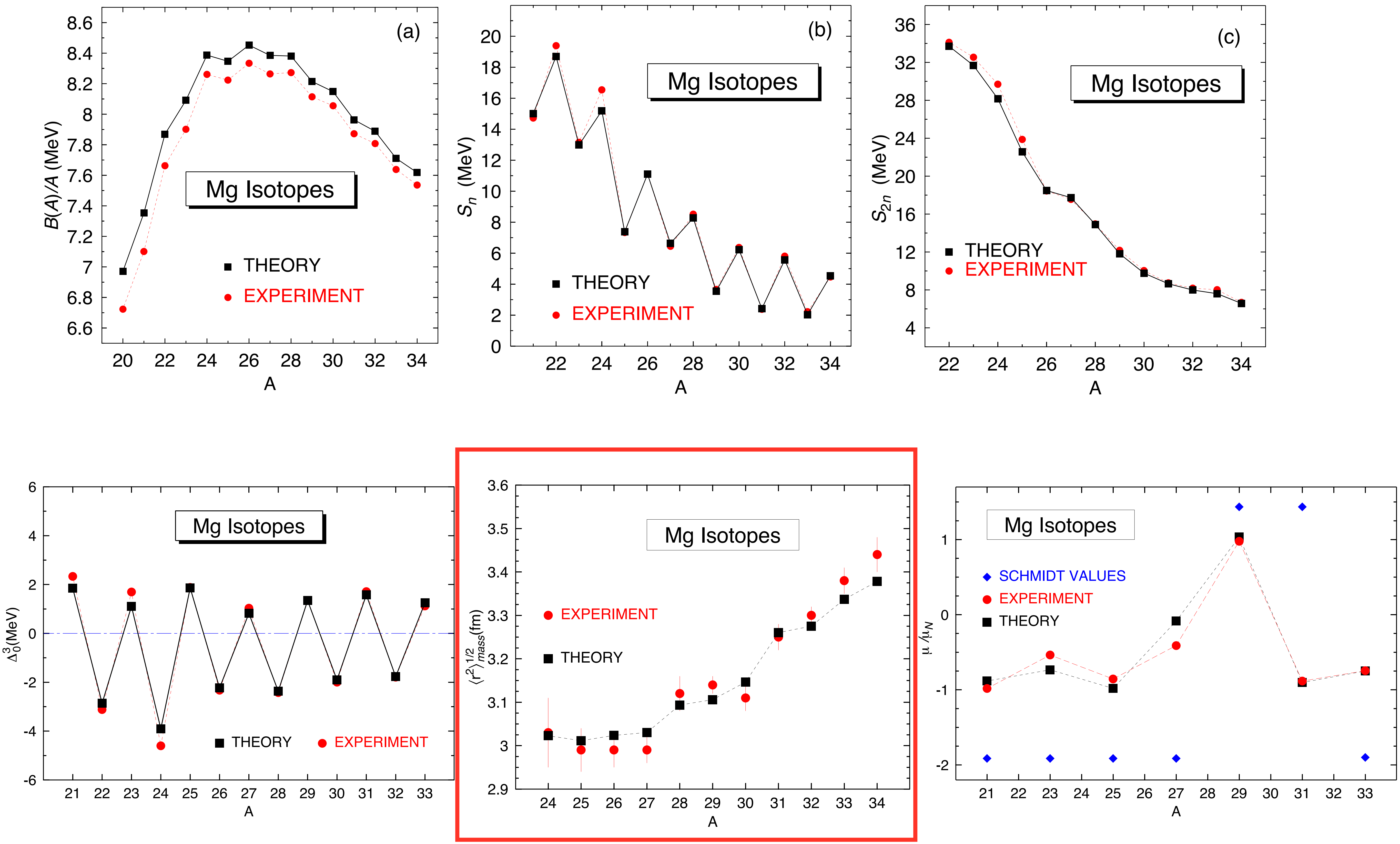

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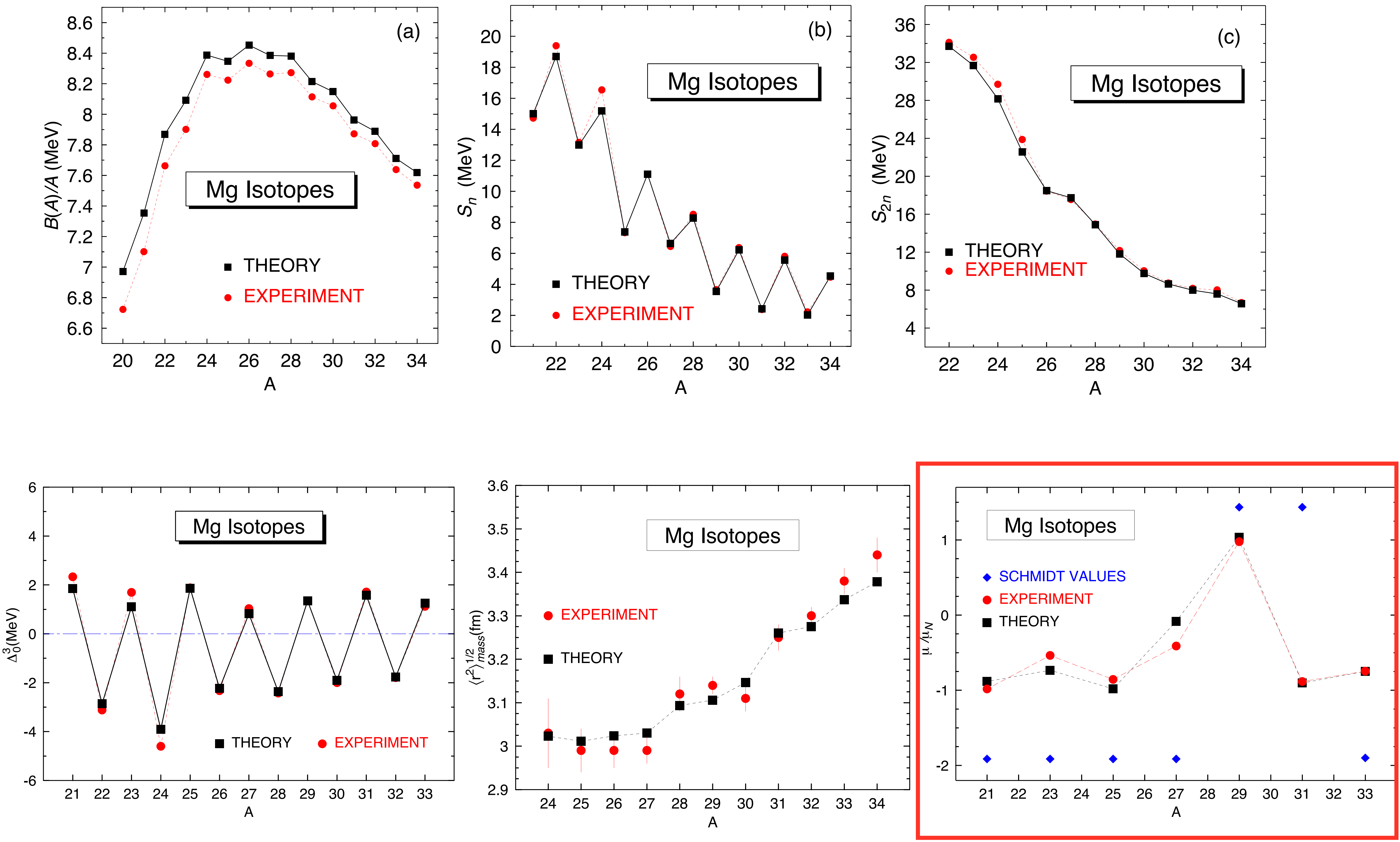

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The spectrum of ^{25}Mg

The Symmetry Conserving Configuration Mixing Approach

We now mix all (β, γ) configurations

$$|\Psi^{N,I,\pi}_{M,\sigma}\rangle = \sum_{K,\beta,\gamma} f^{I}_{K\sigma}(\beta,\gamma) P^N P^I_{MK} |\tilde{\Phi}(\beta,\gamma)\rangle,$$

and diagonalize the Hamiltonian. The mixing coefficients are provided by the Hill-Wheeler-Griffin equation

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

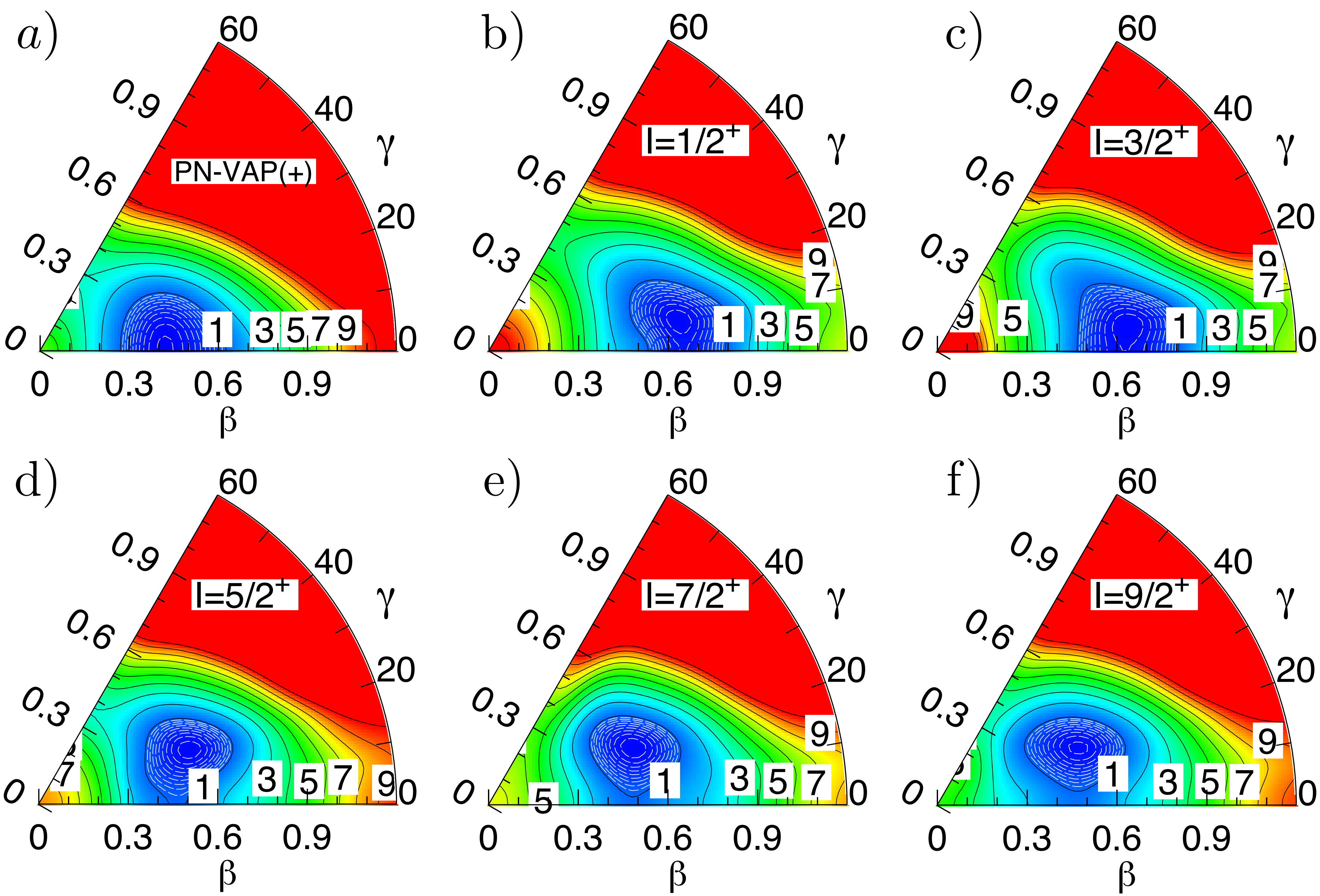
The collective wave functions are given by

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

where

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

Potential Energy Surfaces Positive Parity



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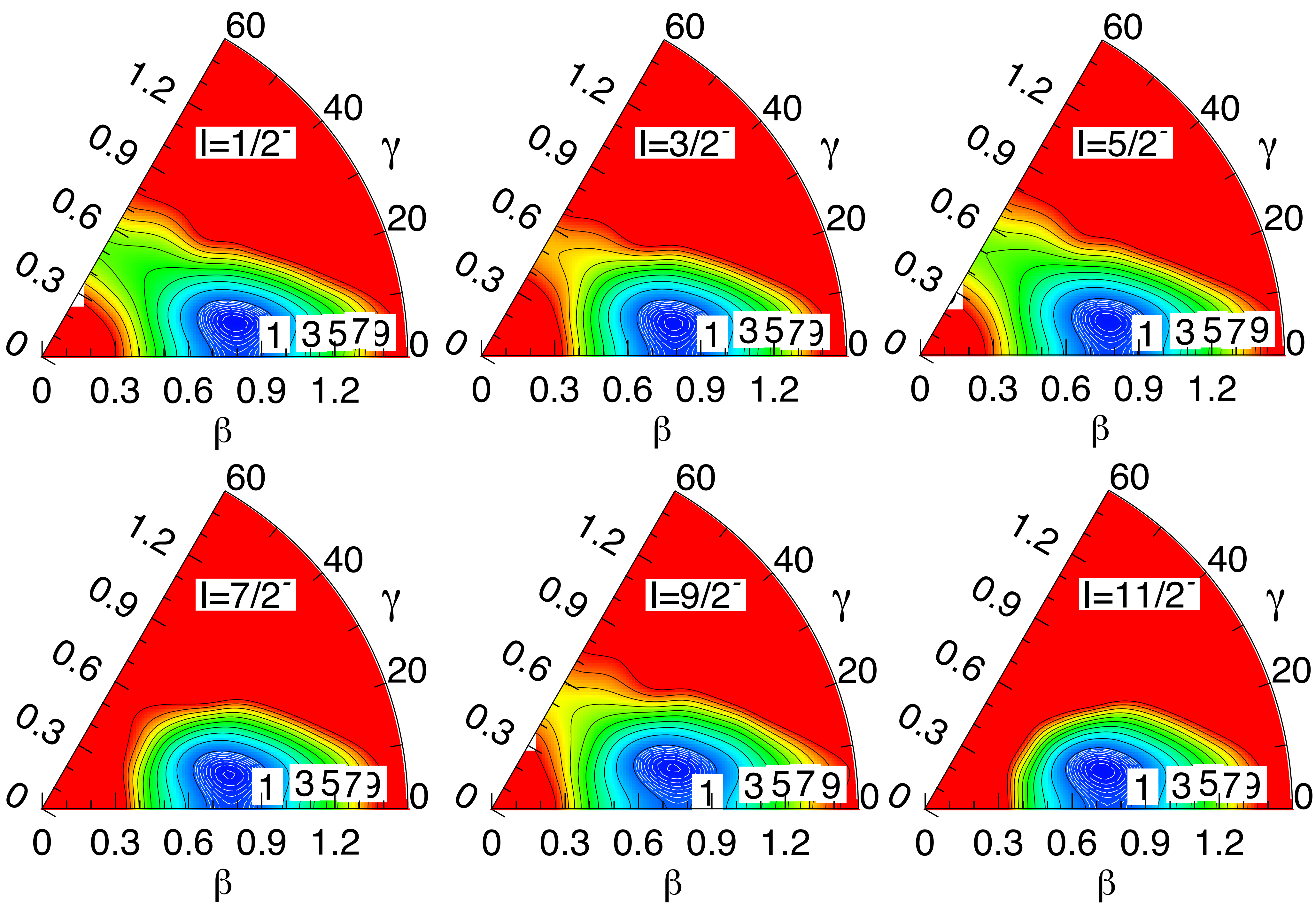
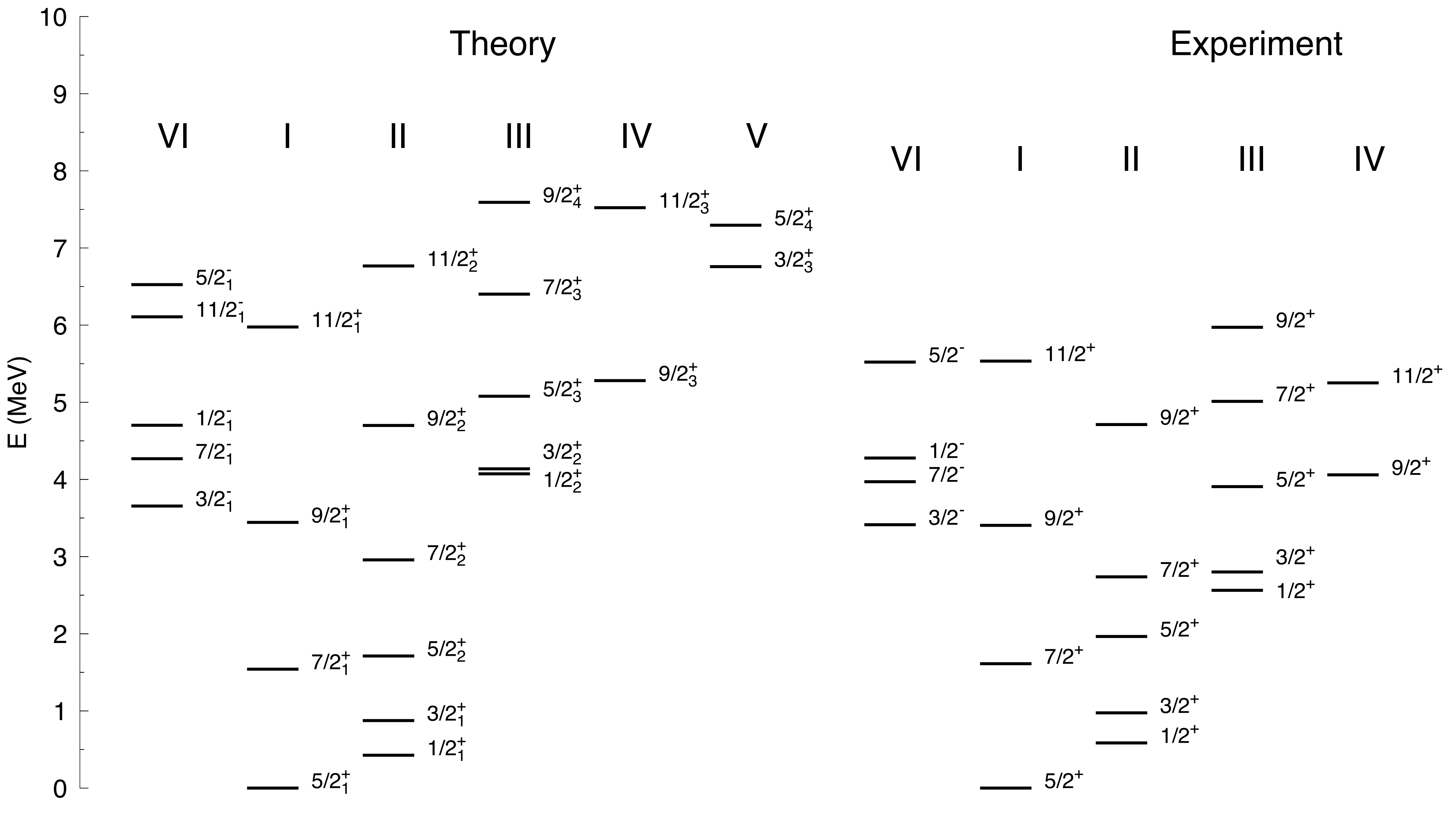
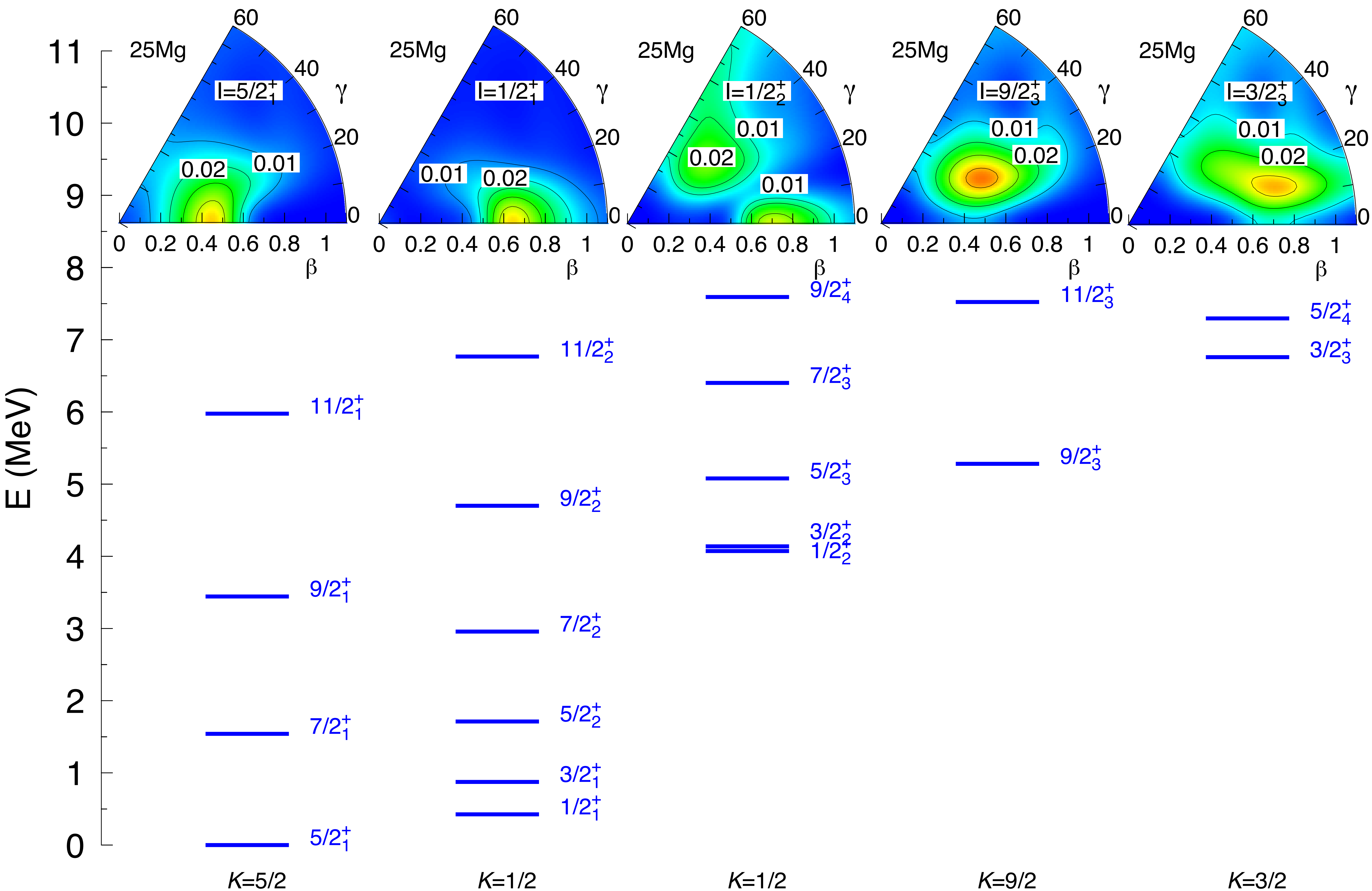


The nucleus ^{25}Mg in the triaxial GCM



M. Borrajo, J.L. E., to be published

Positive Parity bands in ^{25}Mg in the triaxial GCM



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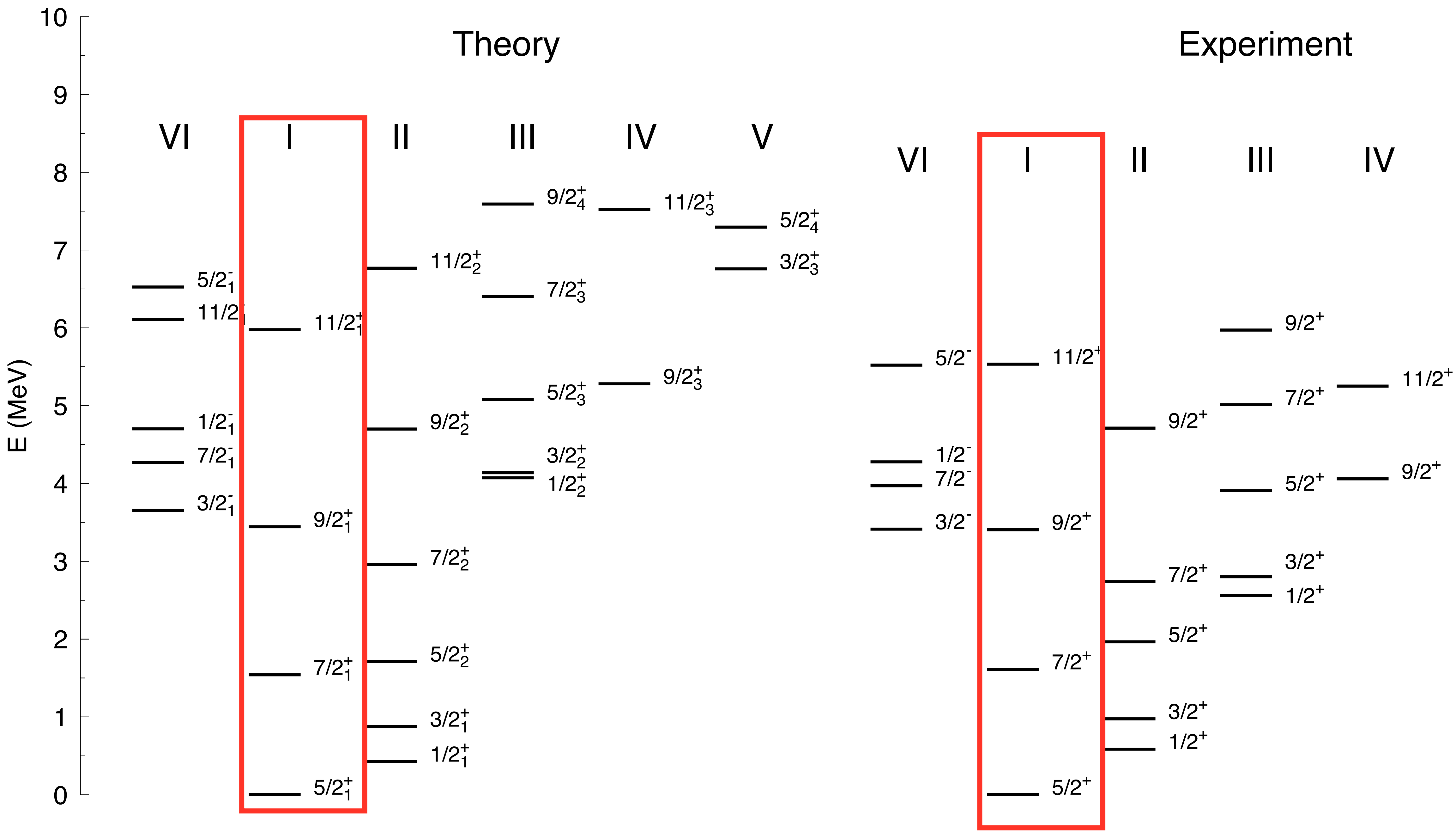
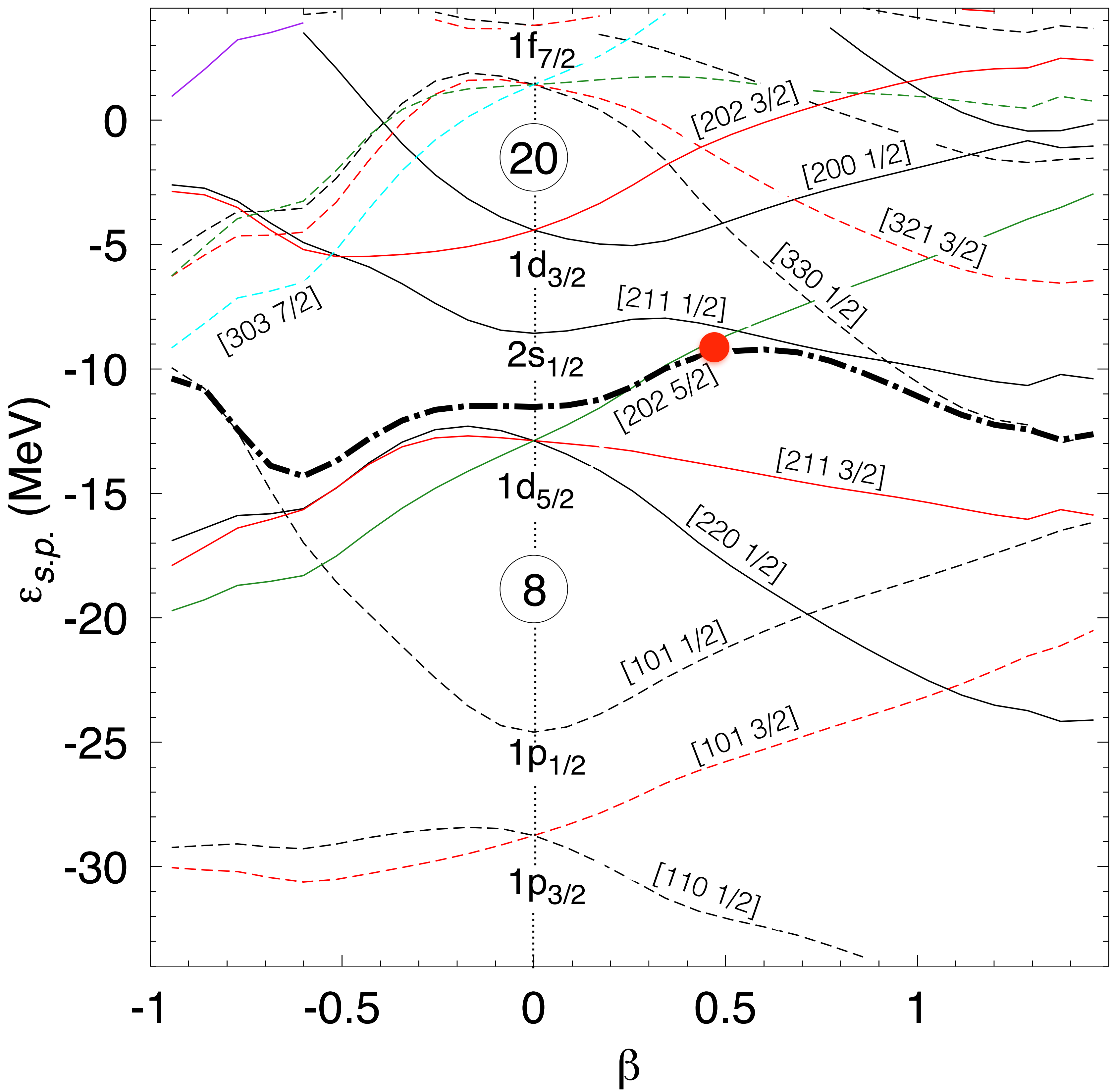


rot. band on [202 5/2]

Nilsson neutron s.p.e. levels in ^{25}Mg

$^{25}Mg_{13}$



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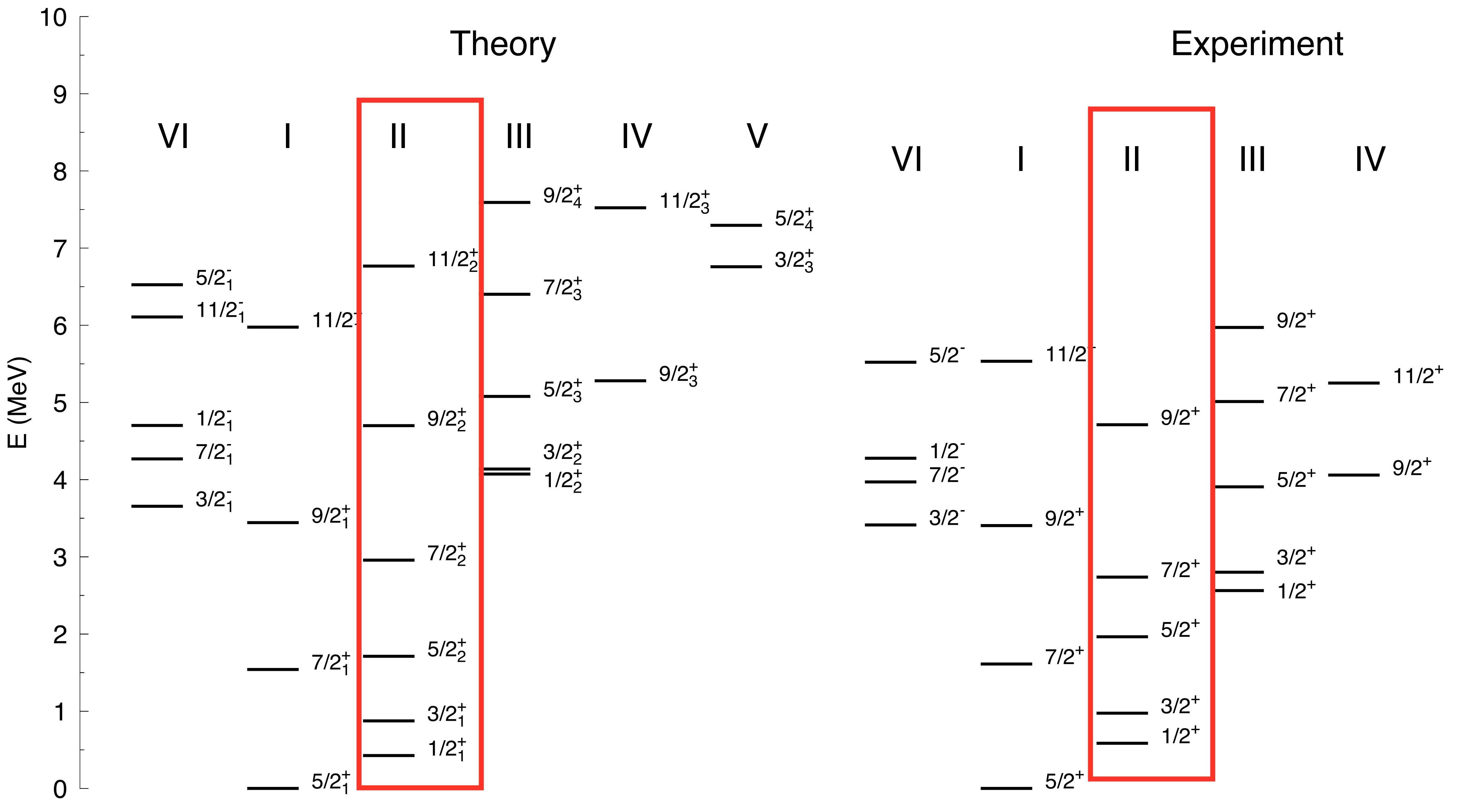

[rot. band on [211 1/2]]

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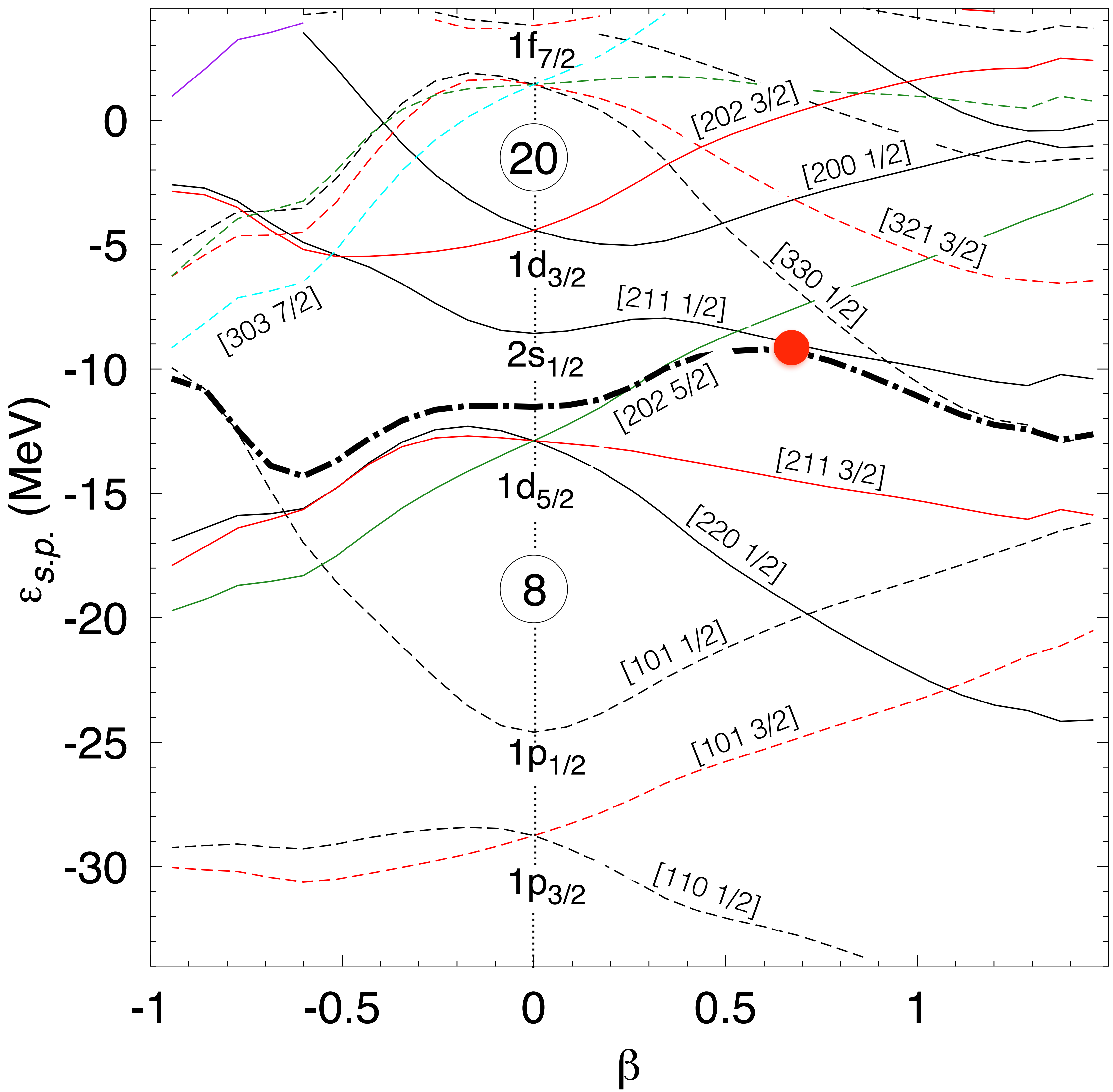

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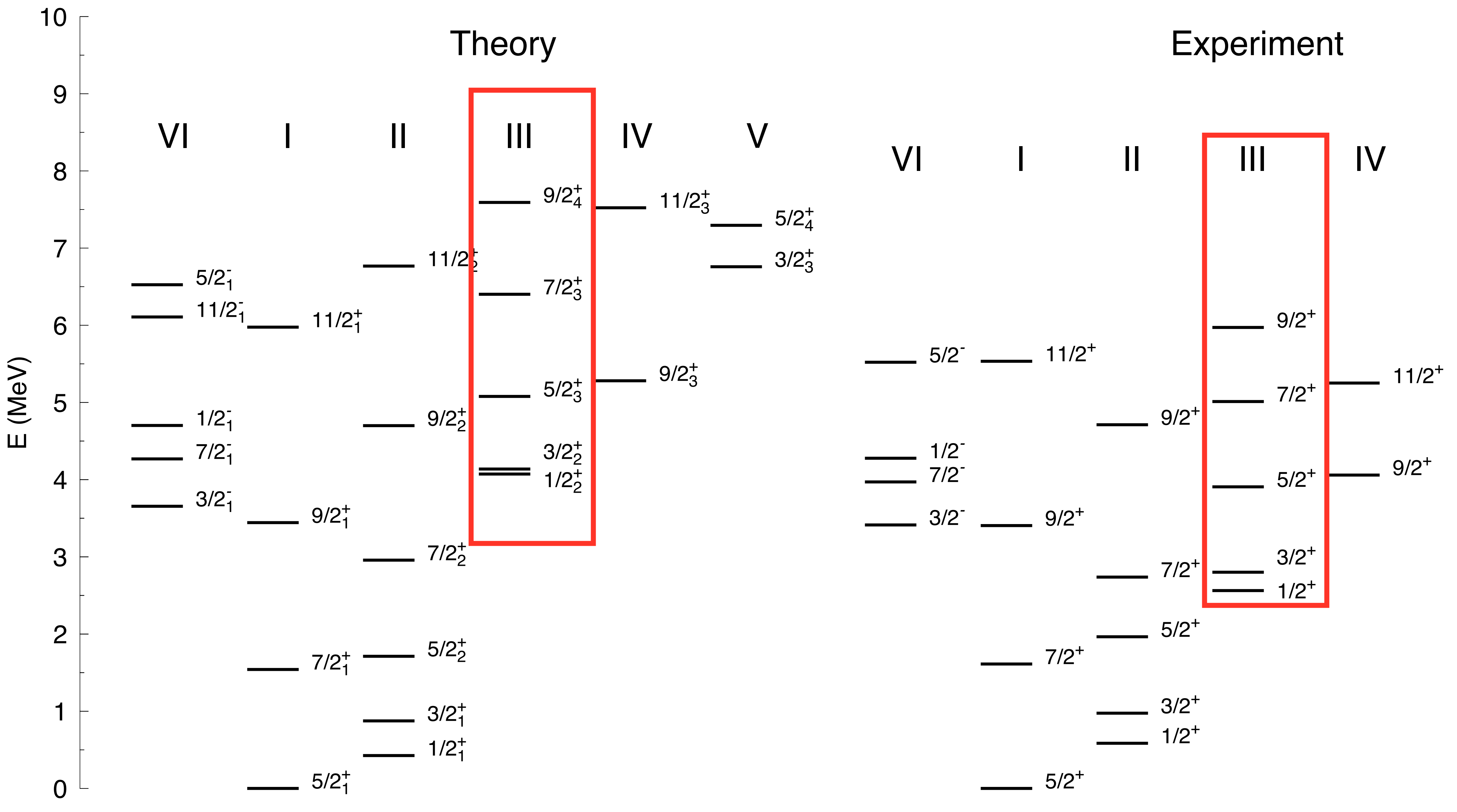

$n\gamma=1$ vibration on the [211 1/2]

M. Borrajo, J.L. E., to be published

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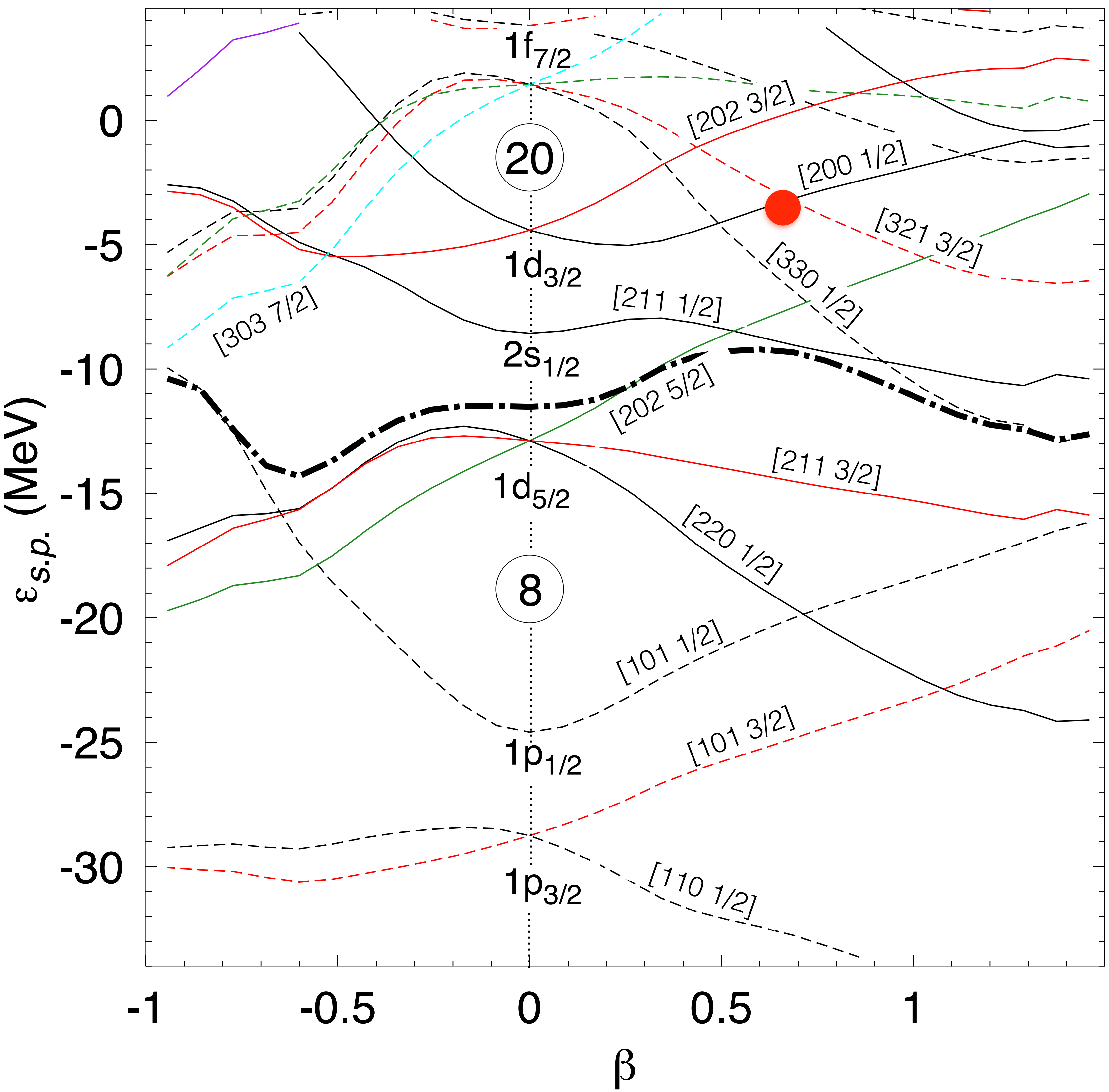

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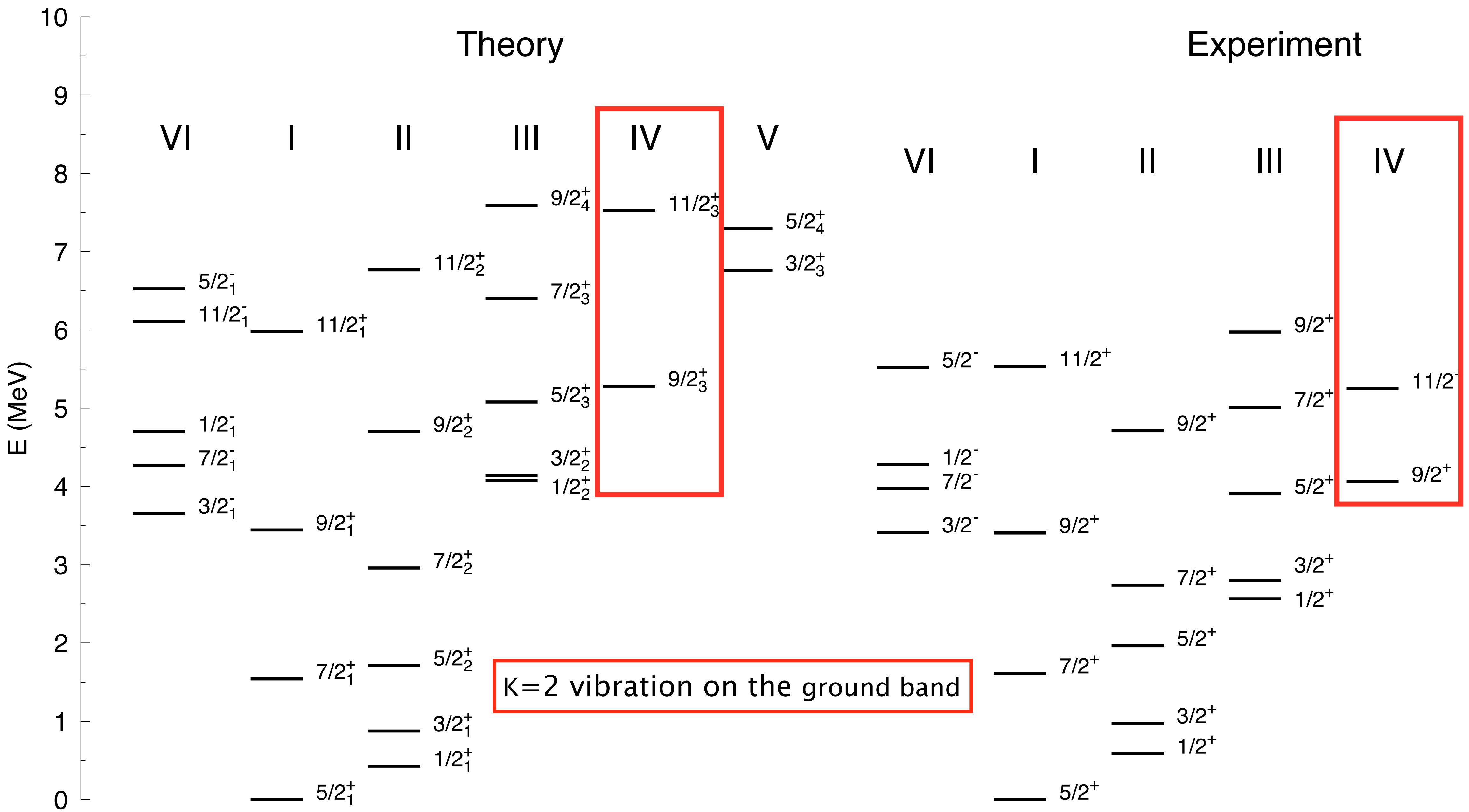

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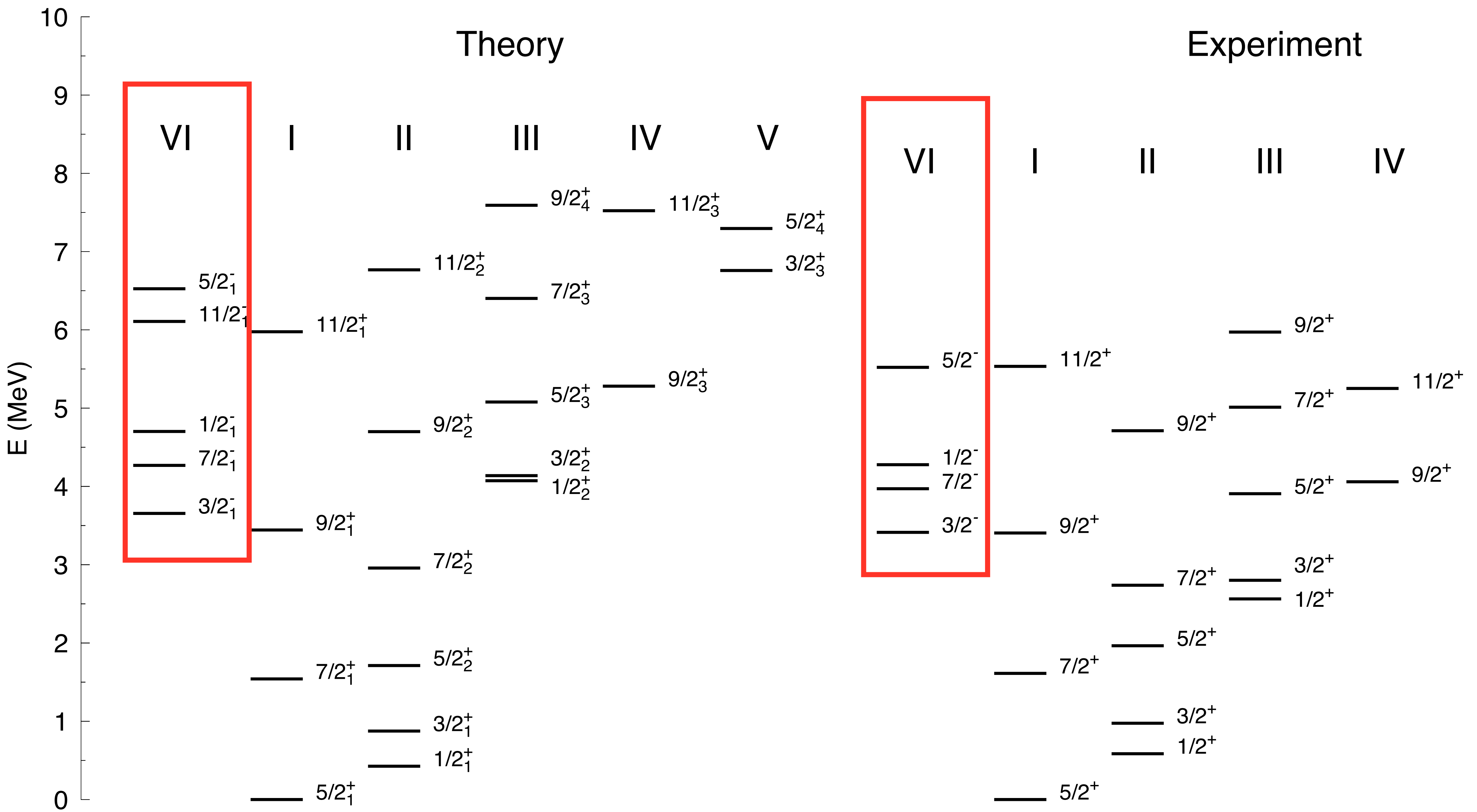
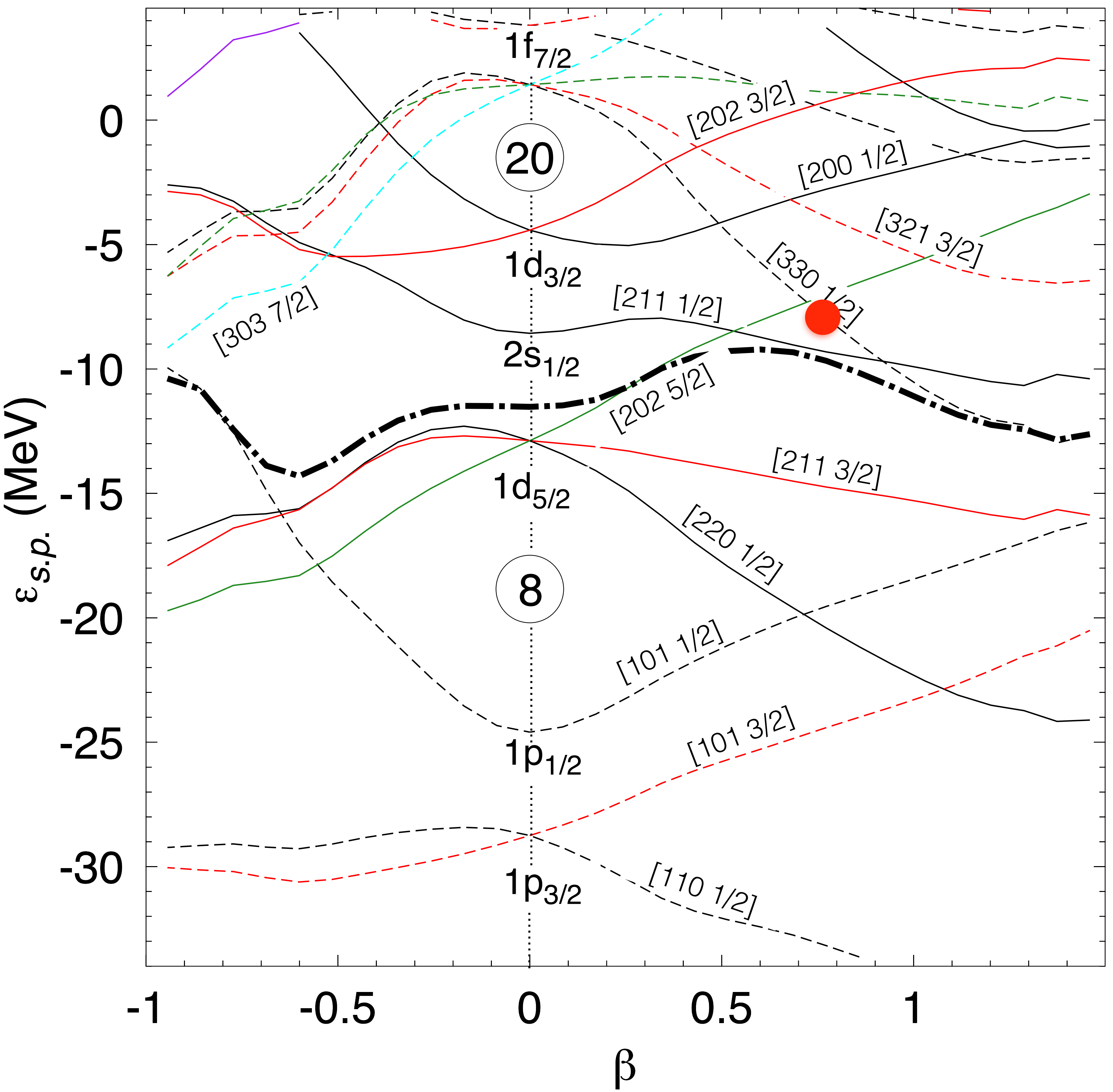


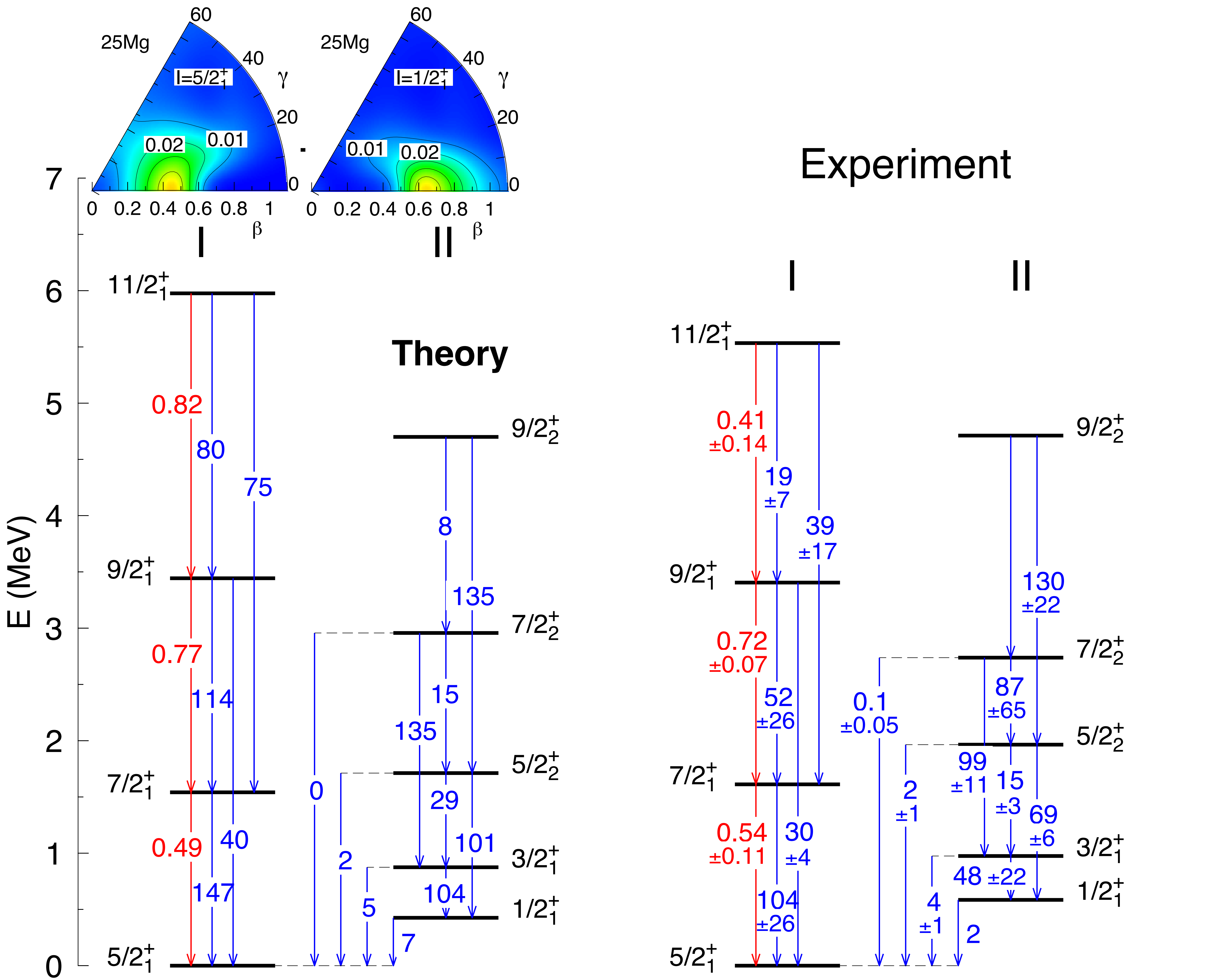
K=1/2 rot. band on [330 1/2]

Nilsson neutron s.p.e. levels in ^{25}Mg

$^{25}Mg_{13}$



Transition Probabilities: Theory vs. Experiment



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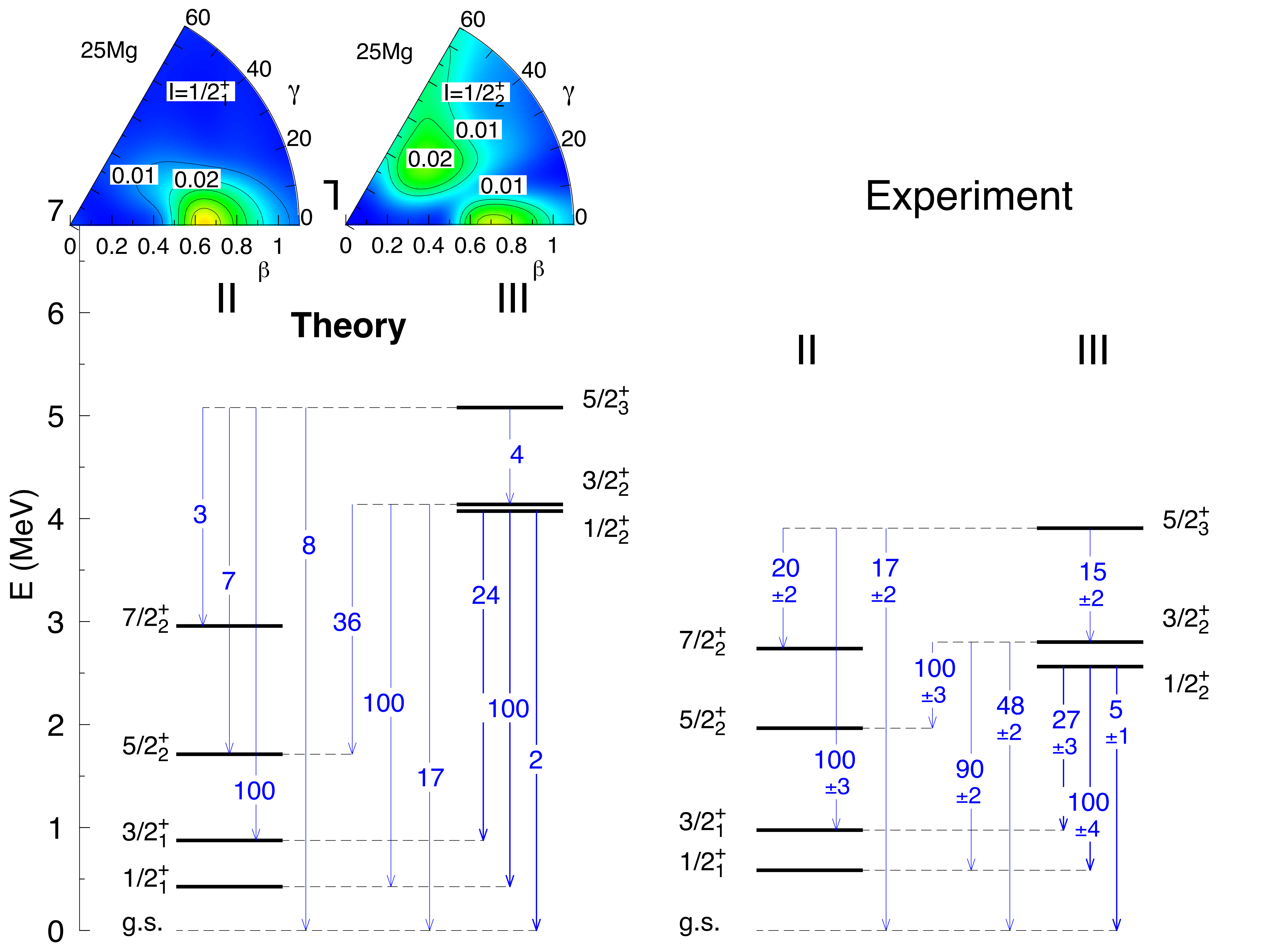
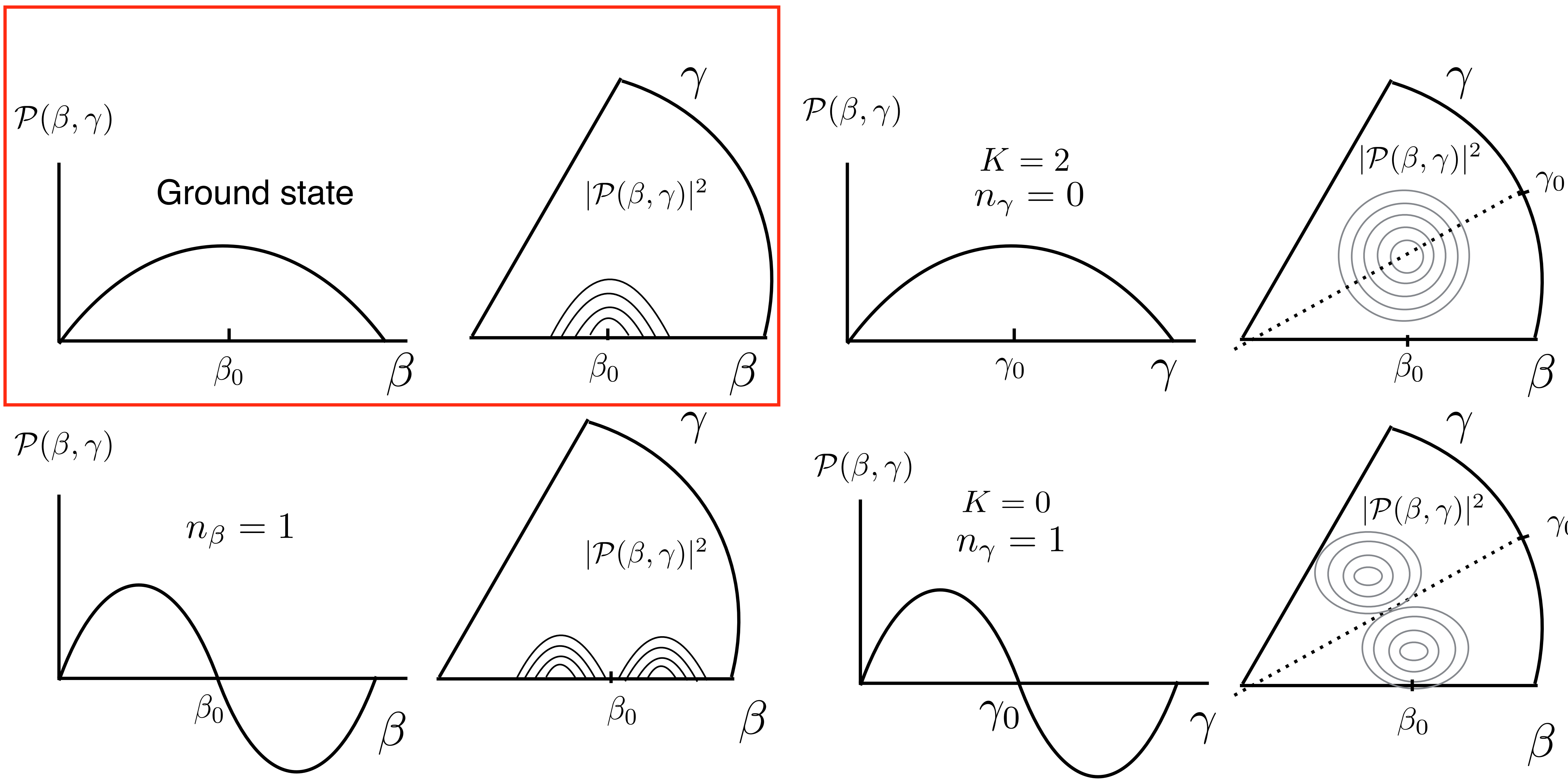


Schematic representation of some wave functions in the collective model



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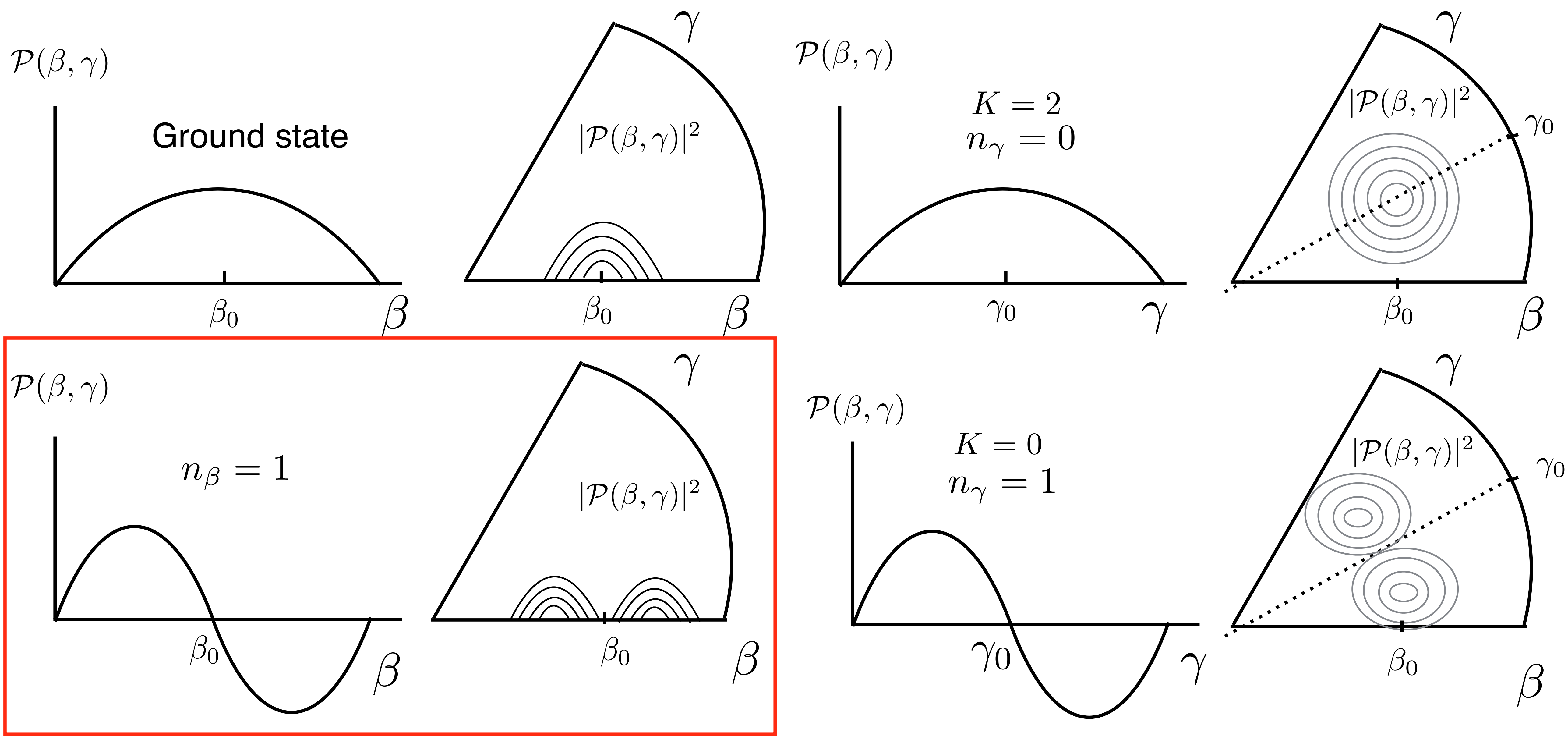

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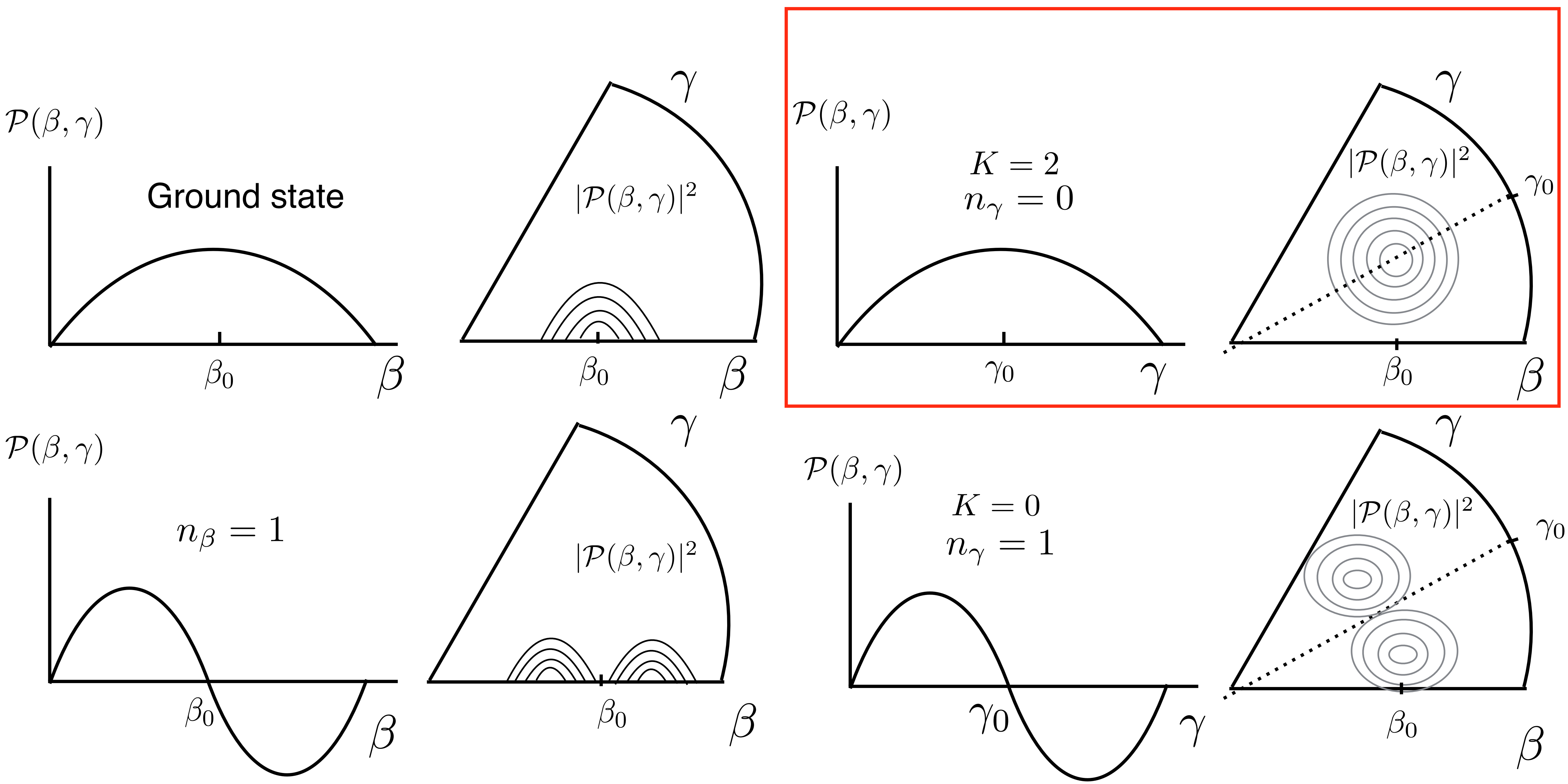

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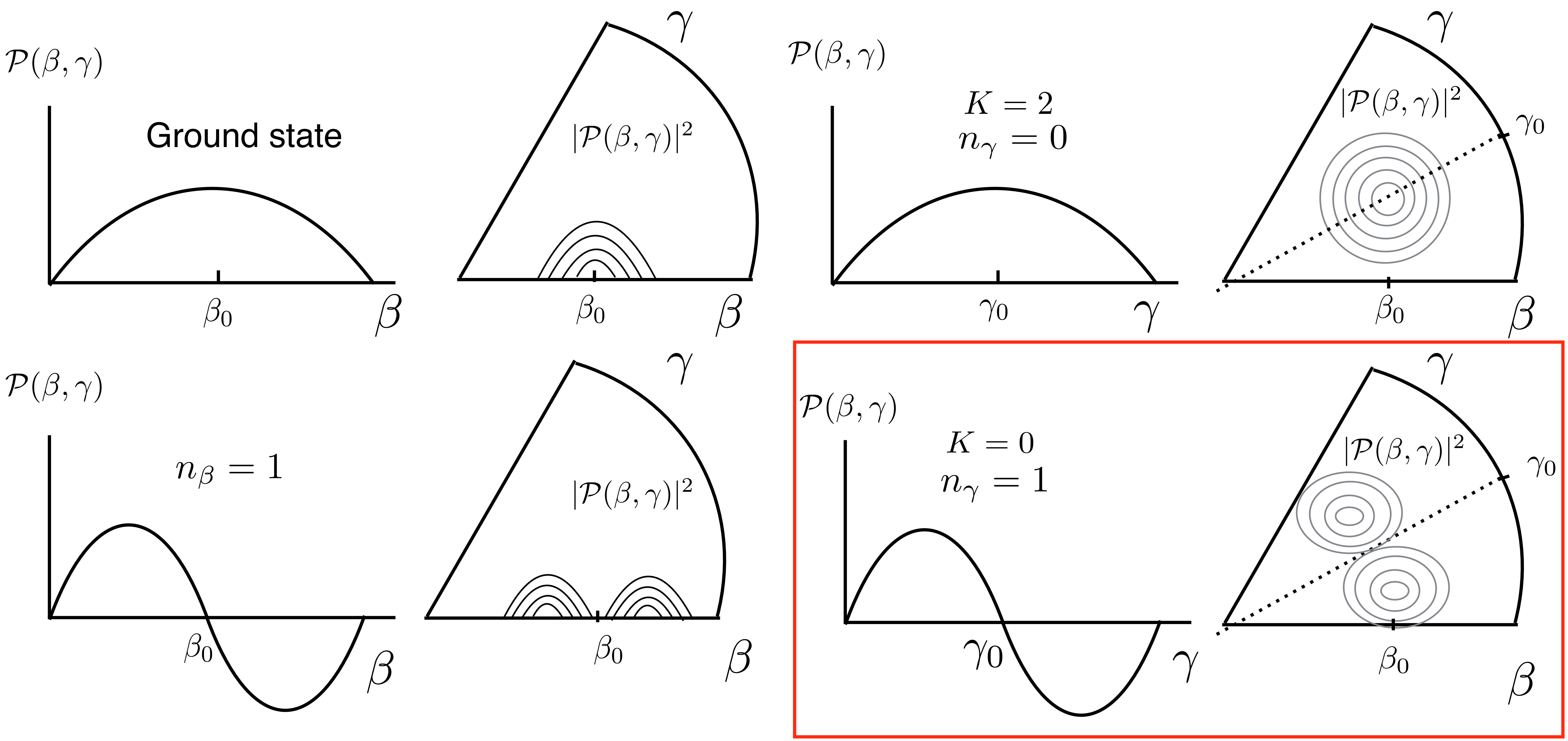
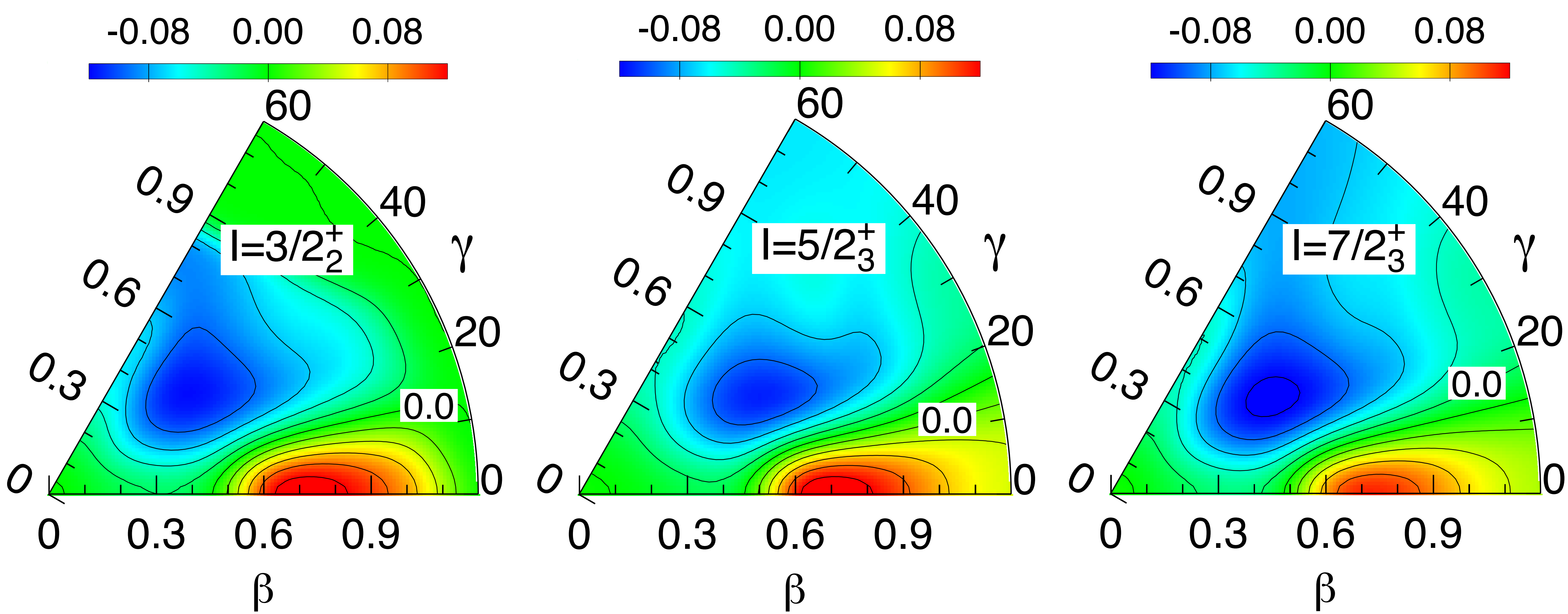
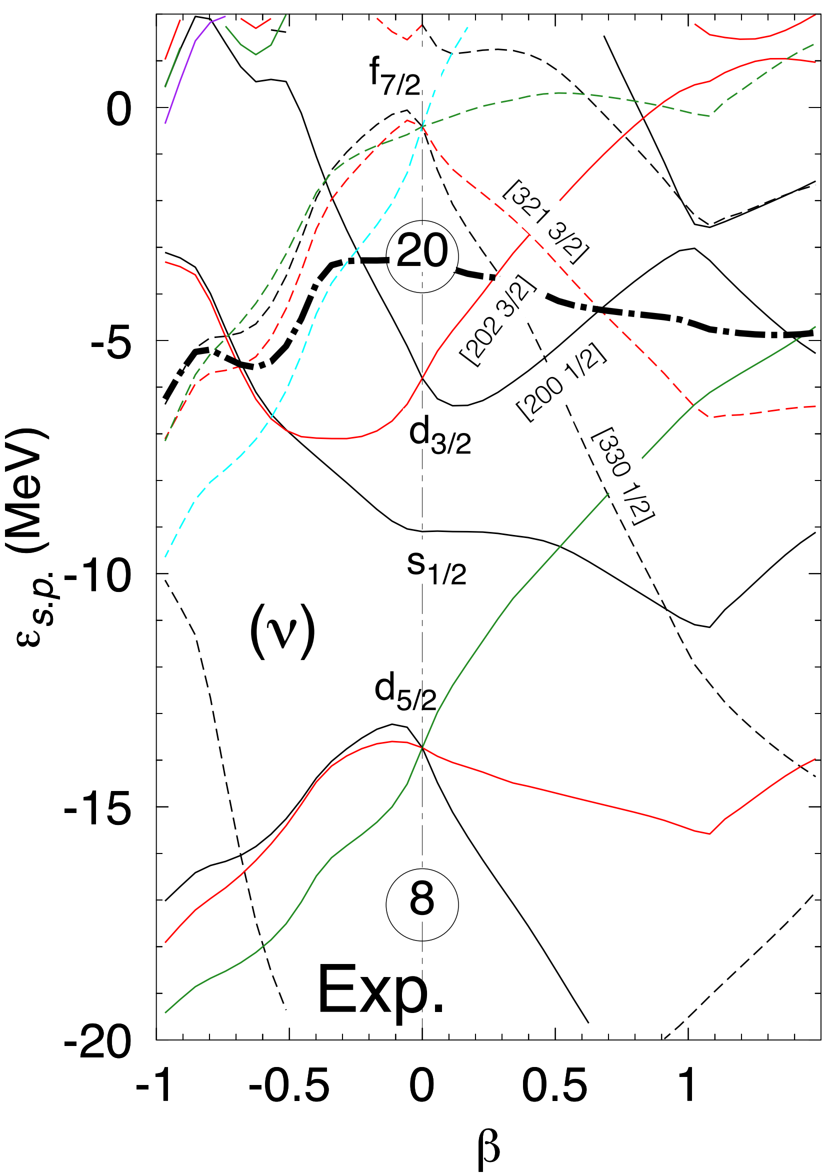


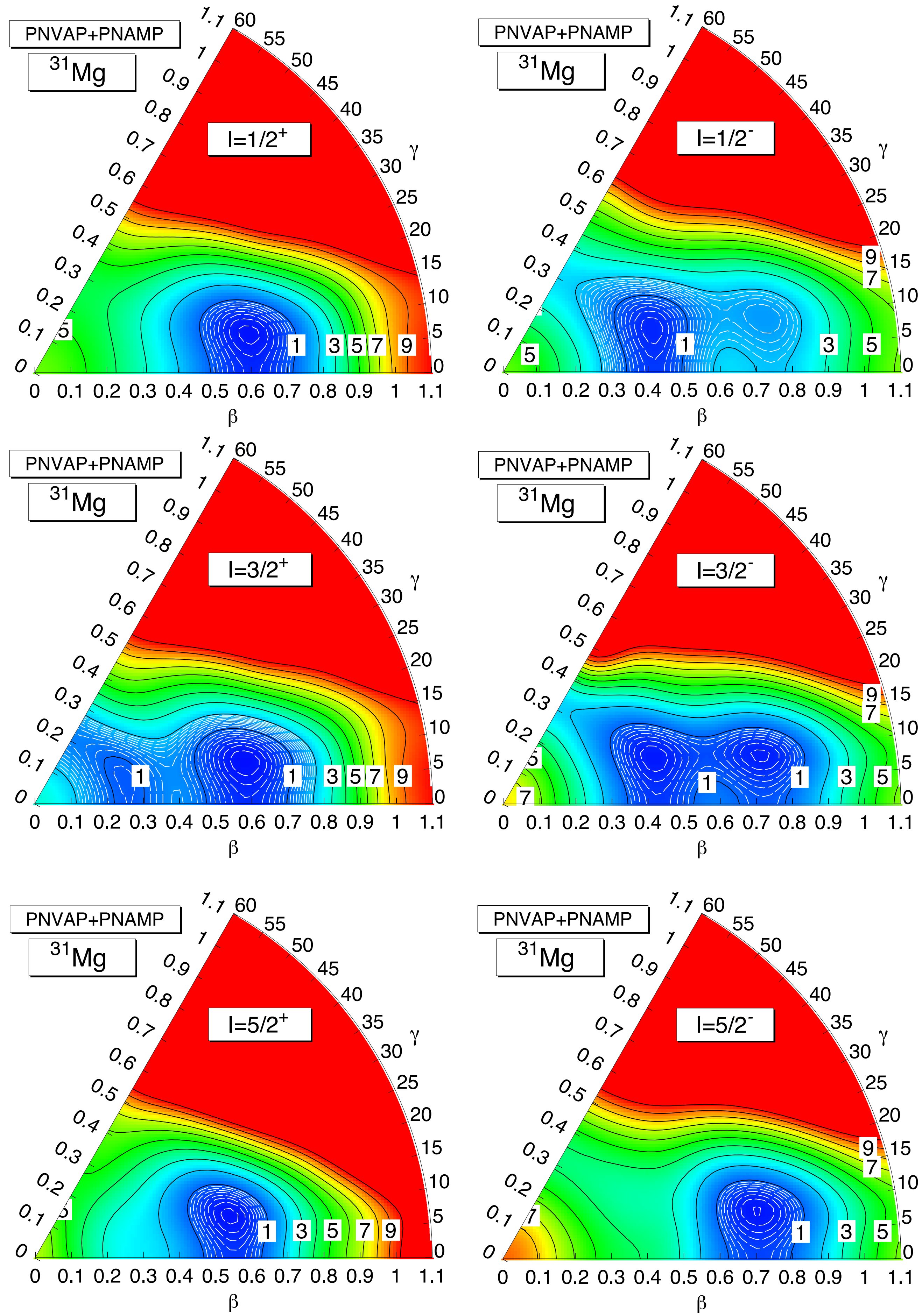
Collective wave functions of band III

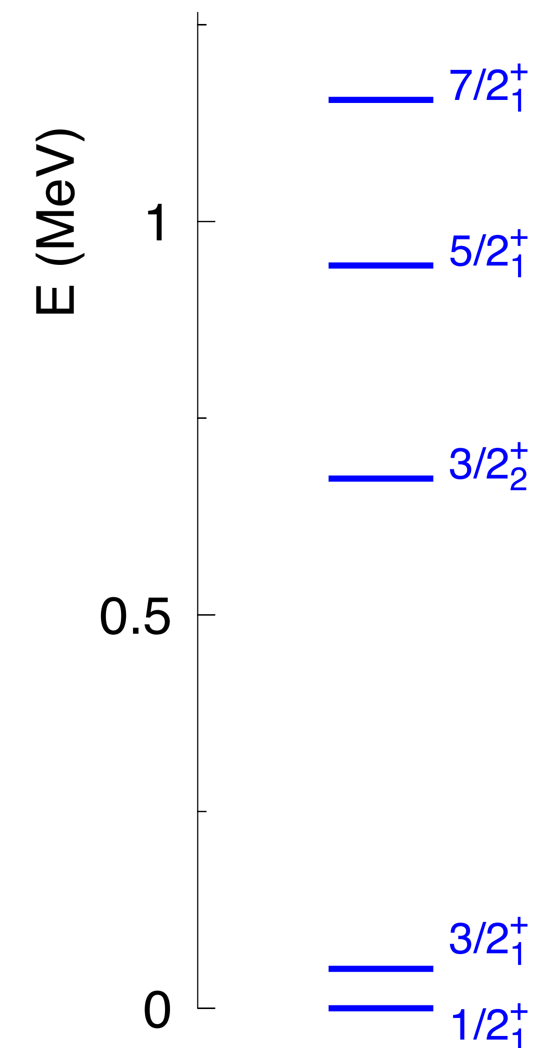


Some comments
about
shape coexistence

Shape coexistence in ^{31}Mg







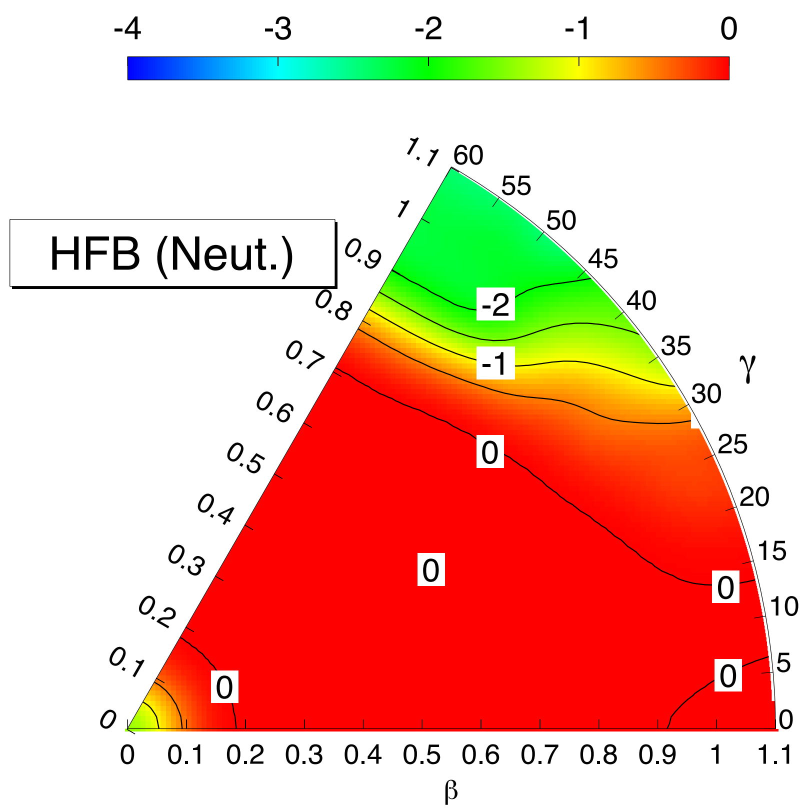
M. Borrajo & J.L. E.

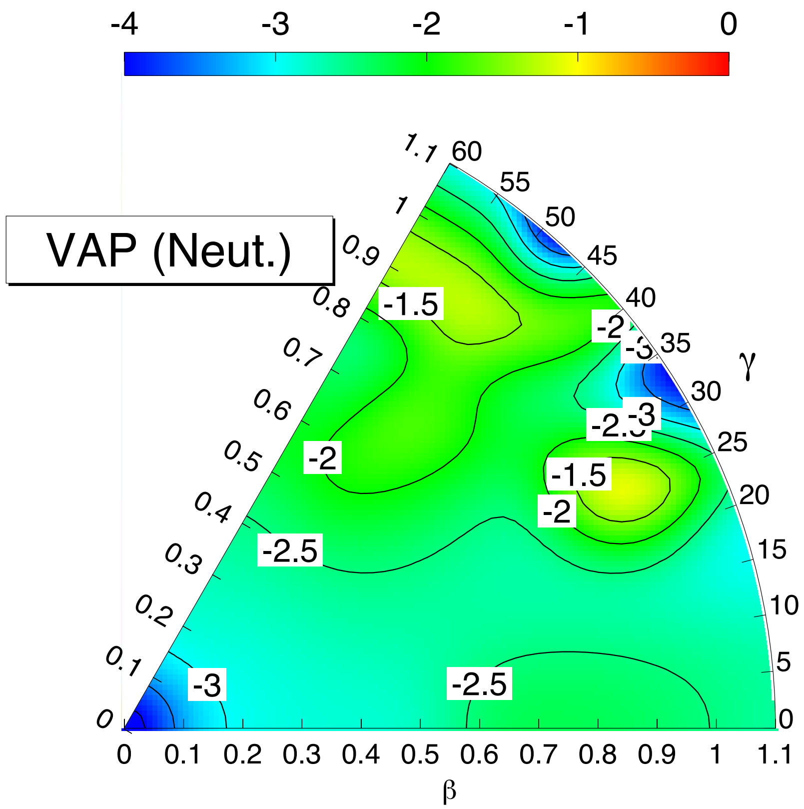
Eur. Phys. J. A (2016) 52: 277

A few words about pairing transitions

Pairing energies (MeV) in the HFB and in the Particle Number Projected approaches (VAP)

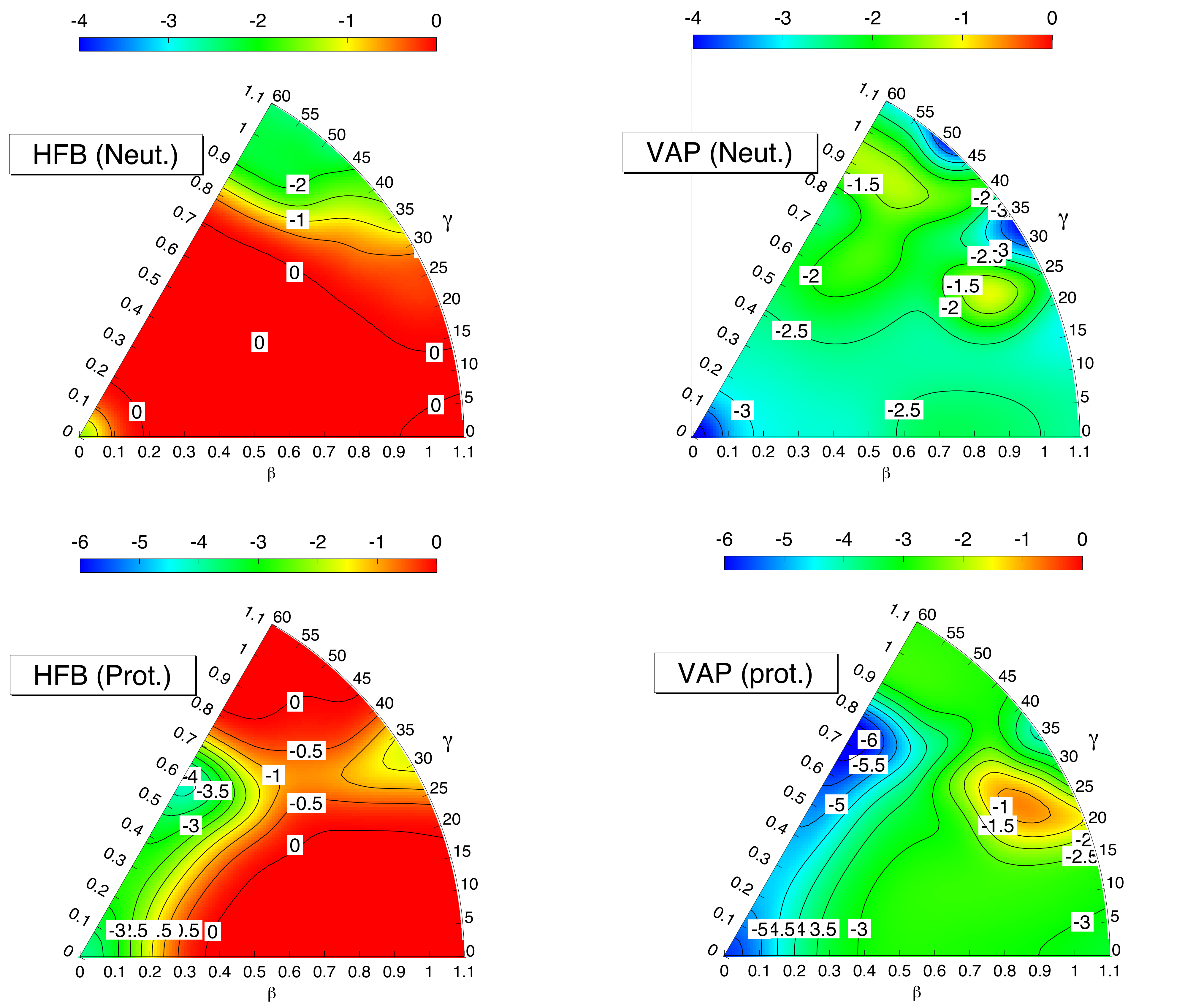
^{25}Mg





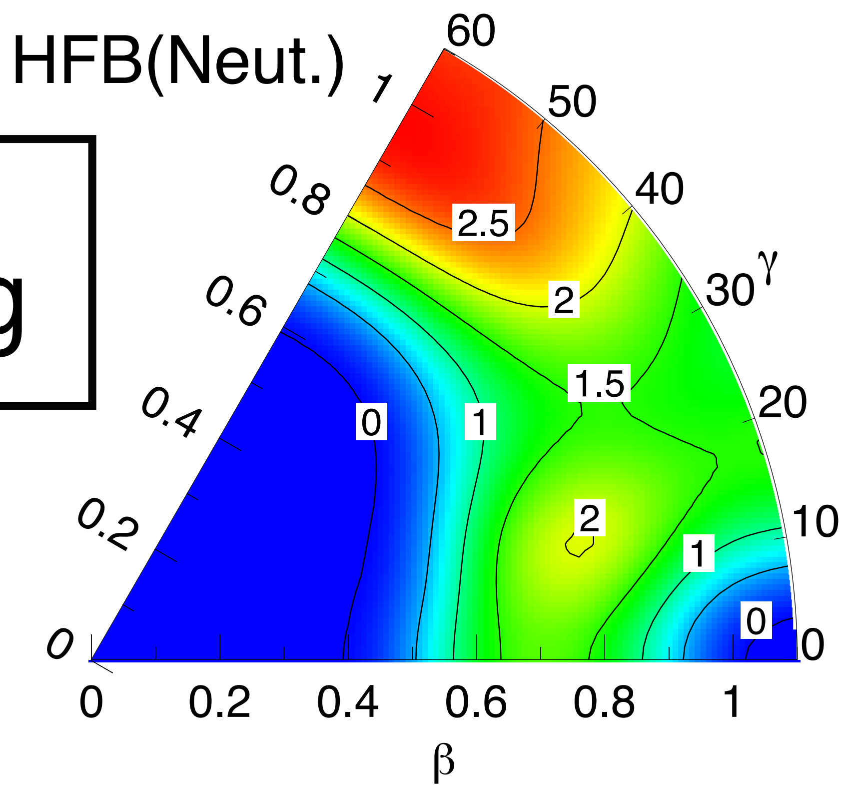
Pairing energies (MeV) in the HFB and in the Particle Number Projected approaches (VAP)

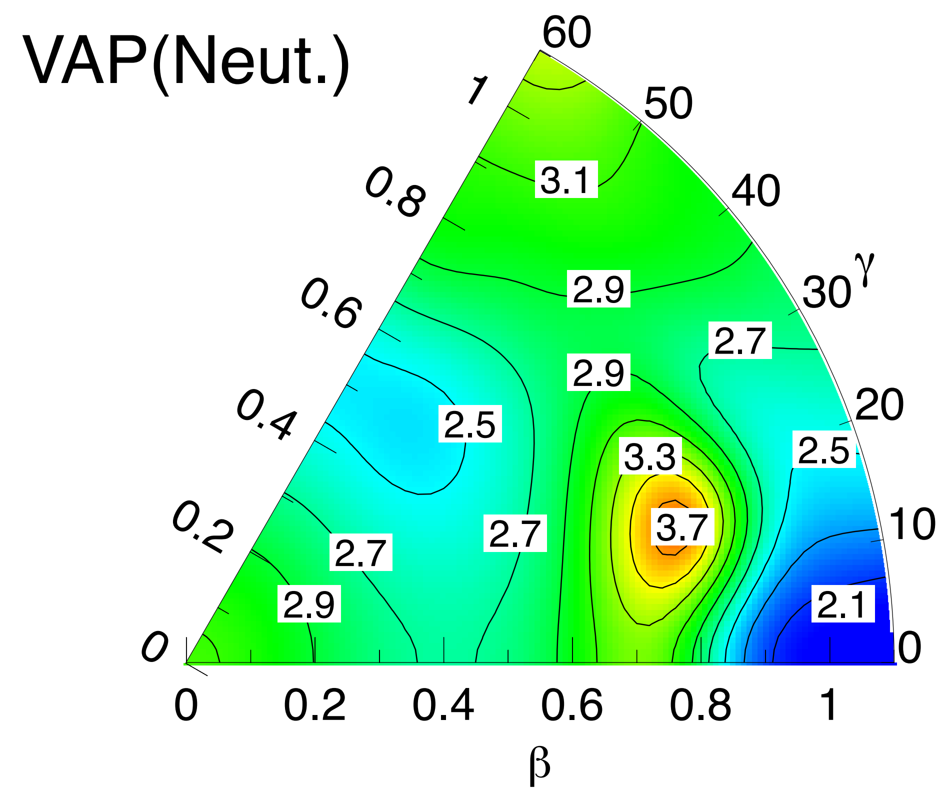
^{25}Mg



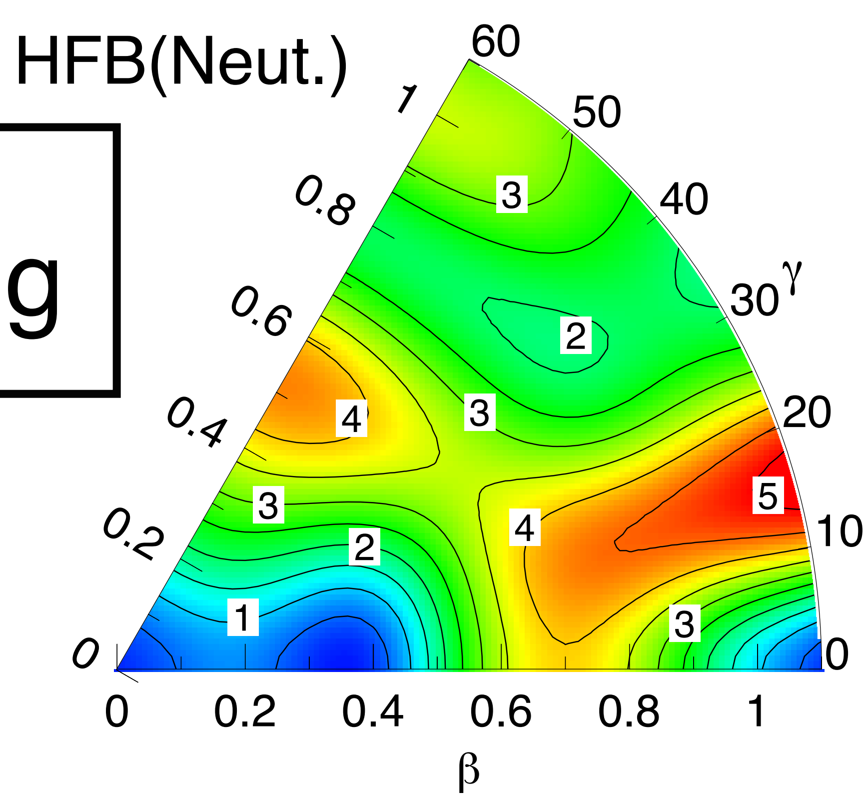
Neutron Pairing energies for ^{27}Mg and ^{28}Mg

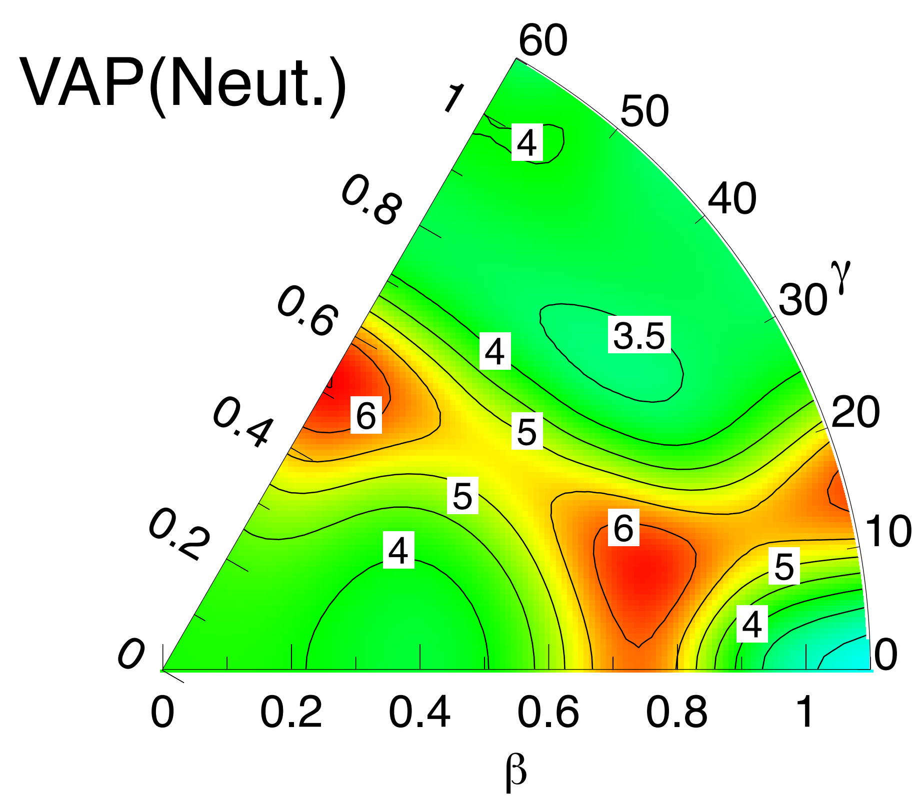
^{27}Mg



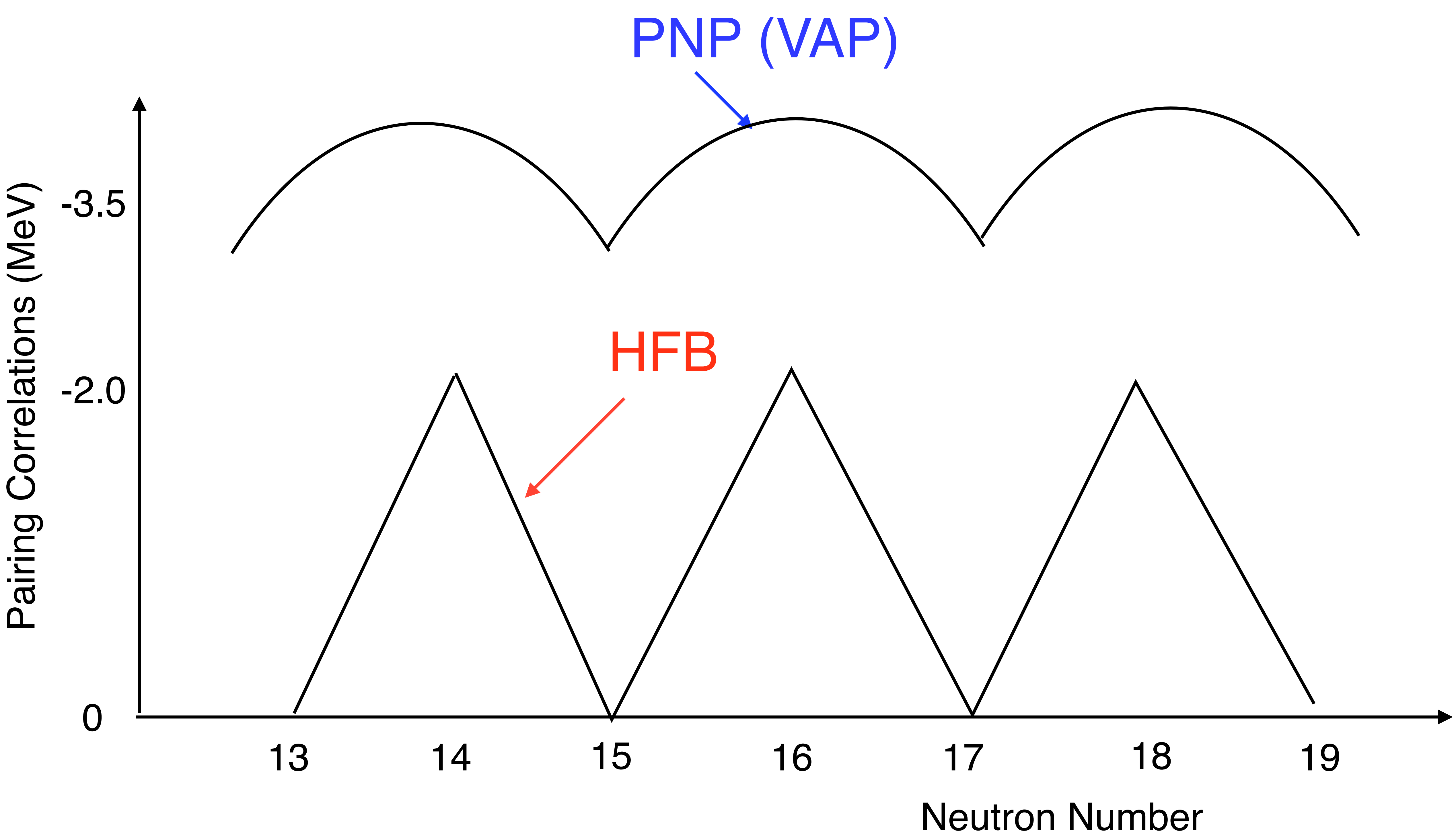


^{28}Mg



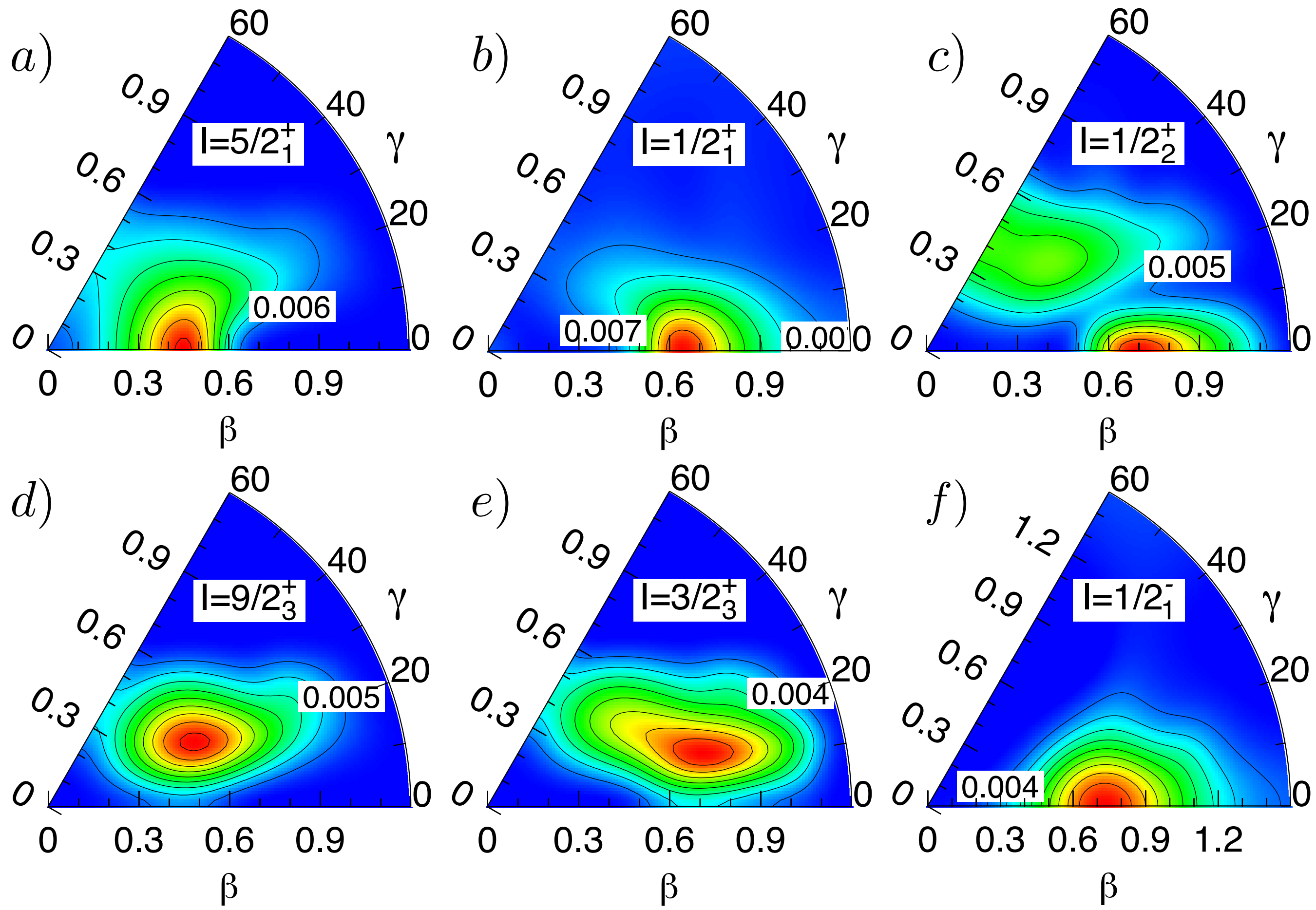


Schematic odd-even effect on the pairing correlations



Conclusions

- As with even-even nuclei, state-of-the-art symmetry conserving configuration mixing calculations provide high quality nuclear spectroscopy of odd-even nuclei, both energies and transition probabilities.
- We have to add the bonus of providing at the same time a good description of the global properties, like masses, radii, etc.
- Furthermore, the predicting power of the Finite Range Density dependent Gogny force will be of valuable help to the experimentalists. Notice that there is not adjustable parameters nor effective charges.
- One goal is to perform calculations in odd-odd and heavier nuclei.
- To improve the description of excited states one could consider additional one quasiparticle states in the description of odd nuclei.


a)
I=5/2$^+_1$
0.006
b)
I=1/2$^+_1$
0.007
c)
I=1/2$^+_2$
0.005
d)
I=9/2$^+_3$
0.005
e)
I=3/2$^+_3$
0.004
f)
I=1/2$^-_1$
0.004
β
γ