Symmetry conserving configuration mixing approaches with shape and pairing fluctuations

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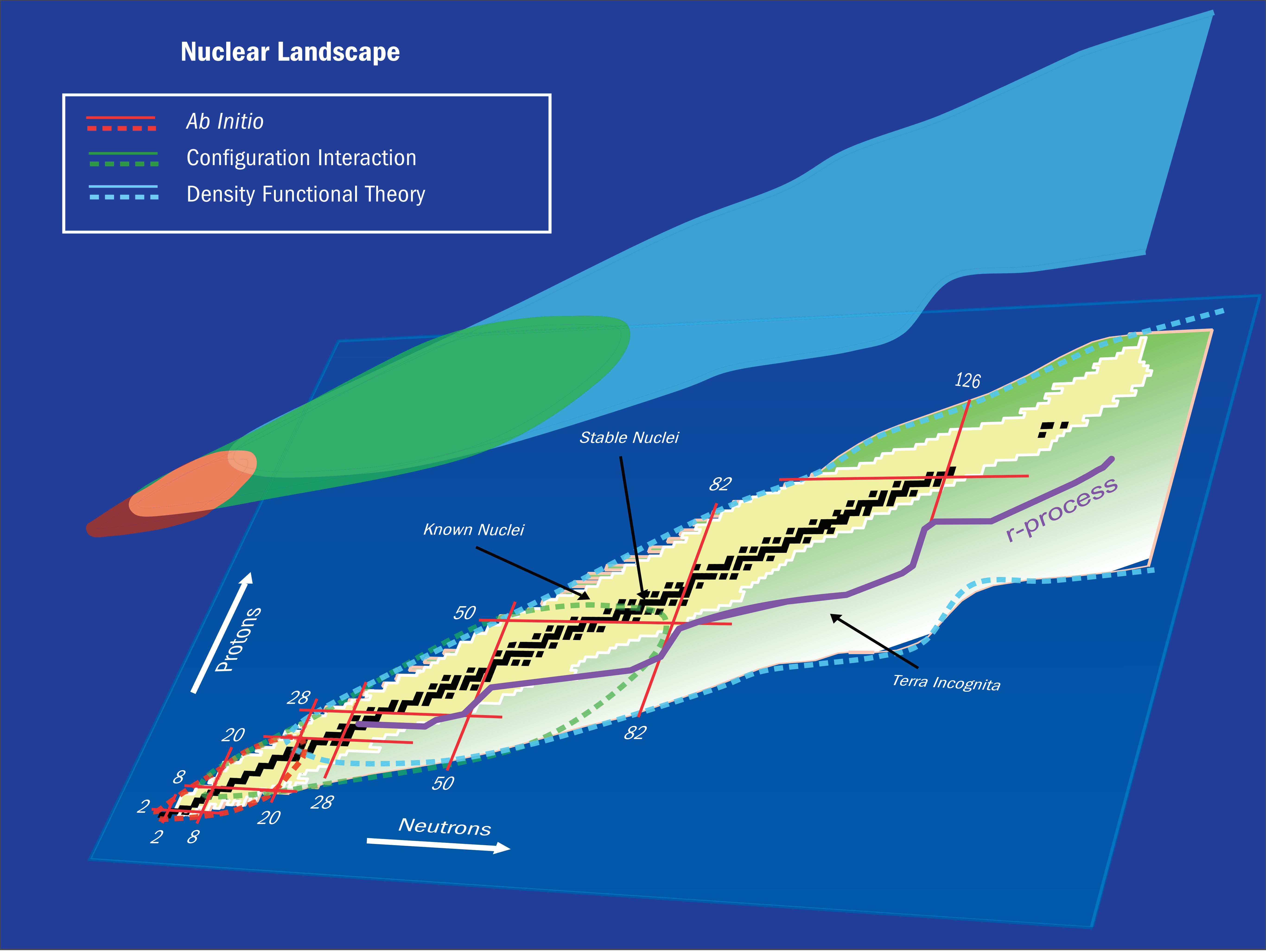
in collaboration with Tomás R. Rodriguez and Nuria López-Vaquero

YIPQS Long-term workshop

Dynamics and Correlations in Exotic Nuclei (DCEN2011)

20th September - 28th October, 2011

Yukawa Institute for Theoretical Physics, Kyoto, Japan


Nuclear Landscape
Ab Initio
Configuration Interaction
Density Functional Theory
126
Stable Nuclei
82
Known Nuclei
50
r-process
Protons
28
20
8
2
Terra Incognita
82
50
28
20
2
8
Neutrons

Outline of the talk (1)

1.- Theory

A.- Mean Field based approaches

- The Hartree-Fock-Bogoliubov (HFB) approach and the symmetry breaking mechanism.
- Symmetry Conserving mean field theory.

B.- Symmetry conserving configuration mixing approaches

- The generation of configurations in the Generator Coordinate Method:
  - -- The β-γ coordinates (triaxial shape fluctuations)
  - -- The β-Δ_π-Δ_ν coordinates (shape and pairing fluctuations)

Outline of the talk (2)

2.- Applications

A.- The ^{54}Cr nucleus.
(Ingredients: VAP-PN, AXIAL-AMP and β coordinate)

B.- The ^{24}Mg and the ^{126}Xe nuclei.
(Ingredients: VAP-PN, TRIAXIAL-AMP and β-γ coordinates)

C.- Pairing vibrations around N=30.
(Ingredients: VAP-PN, AXIAL-AMP, β and Δ_{π}-Δ_{ν} coordinates)

Mean Field approach: The HFB theory and the symmetry breaking mechanism

Let $\{c_i, c_i^\dagger\}$ be the particle operators which define the harmonic oscillator basis, and

$$\alpha_\mu = \sum_i U^*_{i\mu} c_i + \sum_i V^*_{i\mu} c_i^\dagger,$$

the most general Bogoliubov transformation.

We are looking for the coefficients U and V such that the product many-body wave function

$$|\varphi\rangle = \alpha_M \ldots \alpha_1 |-\rangle,$$

minimizes the expression

$$\delta\langle\varphi|\hat{H} - \lambda\hat{N}|\varphi\rangle = 0,$$

the parameter λ being determined by the constraint

$$\langle\varphi|\hat{N}|\varphi\rangle = N,$$

with N the number of particles of our system.

Projected Mean Field Theories

To recover the symmetries we use the many-body w.f

$$|\Psi\rangle = \hat{P}^I_M \ldots \hat{P}^N \hat{P}^Z |\varphi\rangle$$

with $\hat{P}$ a projector on the corresponding symmetry.

✷ If $|\varphi\rangle$ is determined by minimizing $E = \frac{\langle\varphi|\hat{H}|\varphi\rangle}{\langle\varphi|\varphi\rangle}$.

we refer to it as projection after the variation (PAV).

✷✷ If $|\varphi\rangle$ is determined by minimizing $E_P = \frac{\langle\varphi|\hat{H}\hat{P}^I_M \ldots \hat{P}^N \hat{P}^Z|\varphi\rangle}{\langle\varphi|\hat{P}^I_M \ldots \hat{P}^N \hat{P}^Z|\varphi\rangle}$.

we refer to it as variation after projection (VAP).

IMPORTANT: $|\varphi\rangle$ is always a product wave function.

Symmetry conserving Configuration mixing approach

In this case the the Ansatz is based in the GCM :

$$\left|\Psi_{\sigma I}^{N,Z}\right\rangle = \int dq \; f_{\sigma I}^{N,Z}(q) \; \hat{P}_M^I ... \hat{P}^N \hat{P}^Z \left|\varphi(q)\right\rangle ,$$

where $f_{\sigma I}^{N,Z}(q)$ are the collective wave functions solution of the Hill-Wheeler equation

$$\int dq' \; \mathcal{H}_I^{N,Z}(q,q') \; f_{\sigma I}^{N,Z}(q') = E_{\sigma I}^{N,Z} \int dq' \; \mathcal{N}_I^{N,Z}(q,q') \; f_{\sigma I}^{N,Z}(q'),$$

with the projected norm and Hamiltonian kernels

$$\mathcal{N}_I^{N,Z}(q,q') = \left\langle\varphi(q)\right| \hat{P}_M^I ... \hat{P}^N \hat{P}^Z \left|\varphi(q')\right\rangle ,$$

$$\mathcal{H}_I^{N,Z}(q,q') = \left\langle\varphi(q)\right| \; H \; \hat{P}_M^I ... \hat{P}^N \hat{P}^Z \left|\varphi(q')\right\rangle .$$

The calculations: 2 steps

1.- We generate a large set of highly correlated HFB wave functions $|\varphi(q_i)\rangle$ **by minimizing**

$$E^N(q_i) = \frac{\langle\varphi(q_i)|(\hat{H} - \lambda_i\hat{Q})\hat{P}^N|\varphi(q_i)\rangle}{\langle\varphi(q_i)|\hat{P}^N|\varphi(q_i)\rangle}$$

with the corresponding constraint on $\hat{Q}$ **, i.e. in the PN-VAP approach.**

2.- We perform configuration mixing calculations

$$|\Psi^{N,J}\rangle = \int f(q)\hat{P}^N\hat{P}^J|\varphi(q)\rangle\, dq,$$

diagonalizing the Hill-Wheeler equation.

We can also have a look on the diagonal matrix elements projected onto good angular momentum and particle number, i.e.,

$$E^{N,J}(q_i) = \frac{\langle\varphi(q_i)|\hat{H}\hat{P}^N\hat{P}^J|\varphi(q_i)\rangle}{\langle\varphi(q_i)|\hat{P}^N\hat{P}^J|\varphi(q_i)\rangle}$$

Details of the calculations

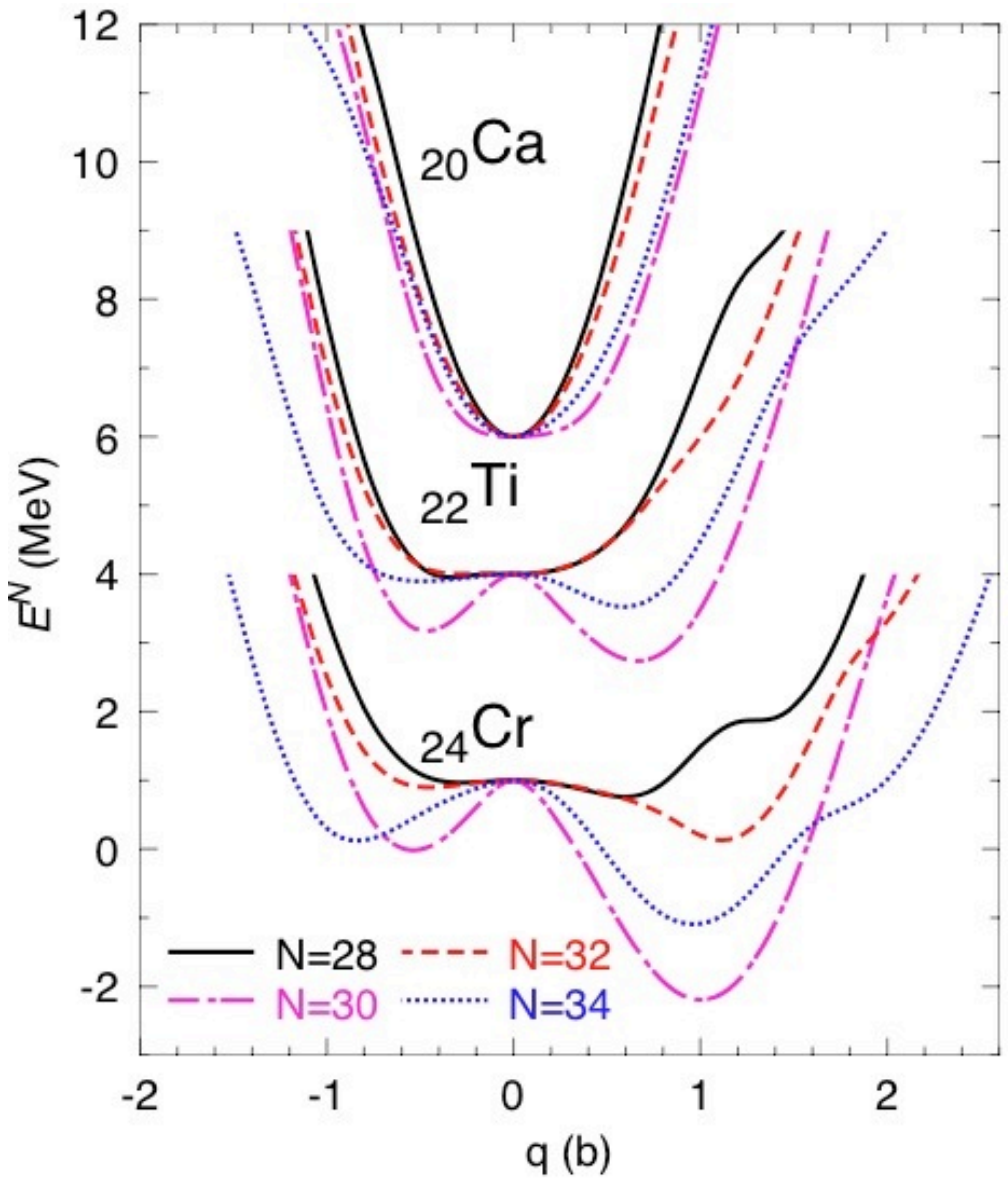
Interaction.- In the calculations the Gogny force with the D1S parametrization has been used. All exchange terms of the force are considered to avoid divergences associated with the projections.

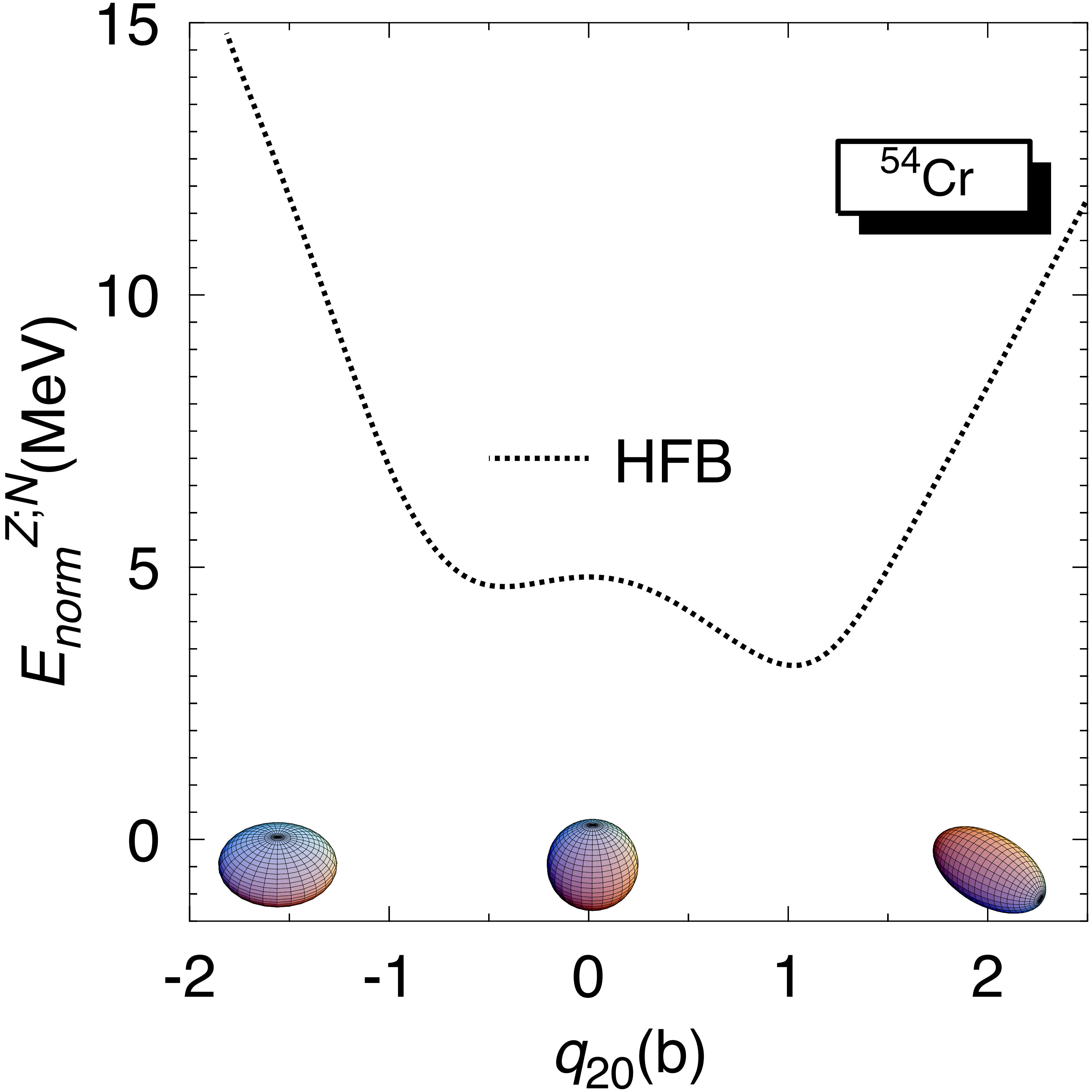
Configuration Space.- We take into account a relatively large number of major harmonic oscillator shells.

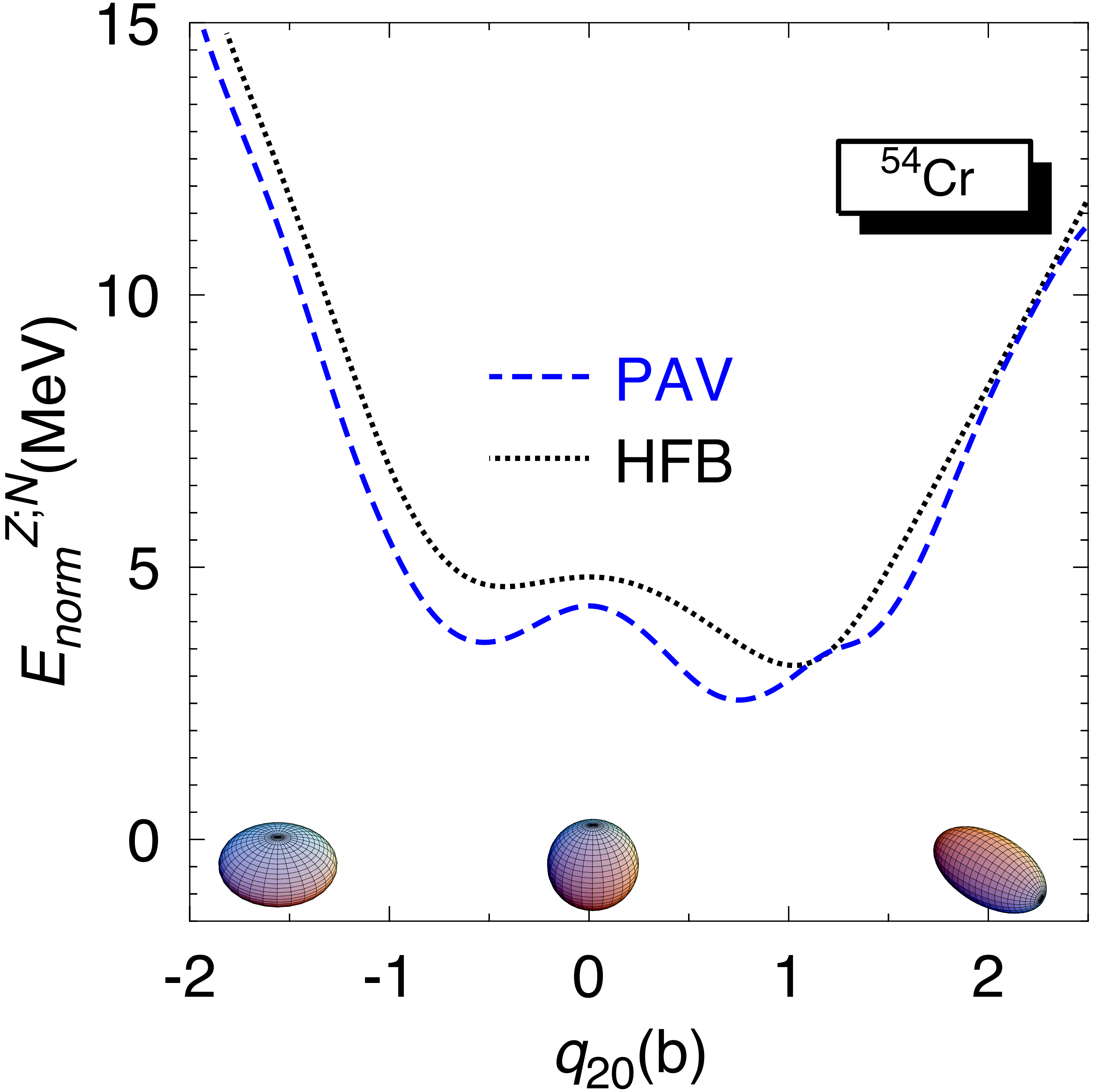
Effective charges.- NO need of effective charges in the calculations of electromagnetic properties.

The beta (q_{20}) degree of freedom in the N=30 region

Potential Energy curves in the PN-VAP approach




15
10
5
0
-2
-1
0
1
2
$E_{norm}^{Z,N}$(MeV)
q_{20}(b)
HFB
^{54}Cr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$E_{norm}^{Z;N}$(MeV)
q_{20}(b)
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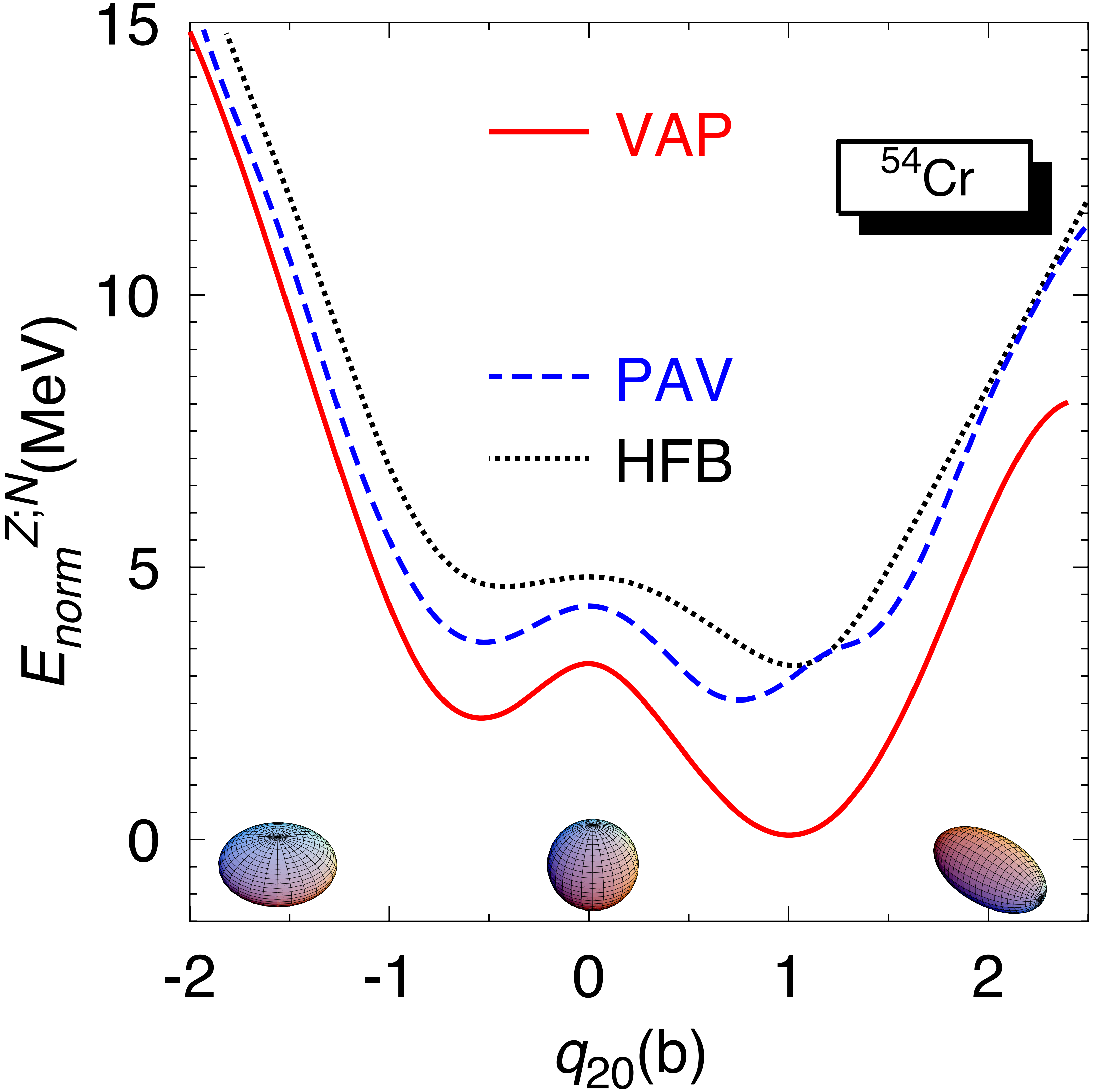
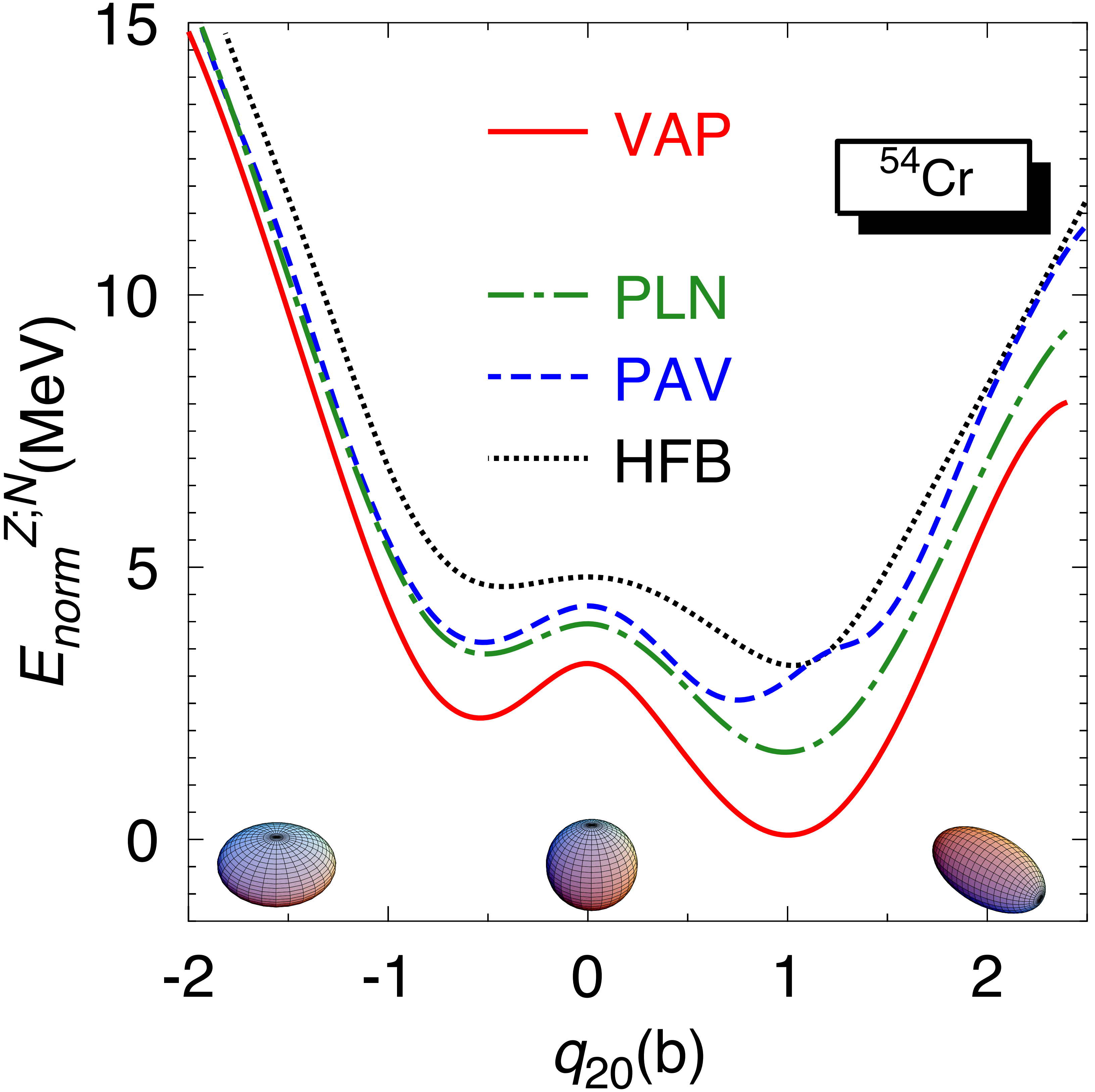
PAV
HFB



VAP
PAV
HFB
^{54}Cr
15
10
5
0
-2
-1
0
1
2
$E_{norm}^{Z;N}$(MeV)
q_{20}(b)


15
10
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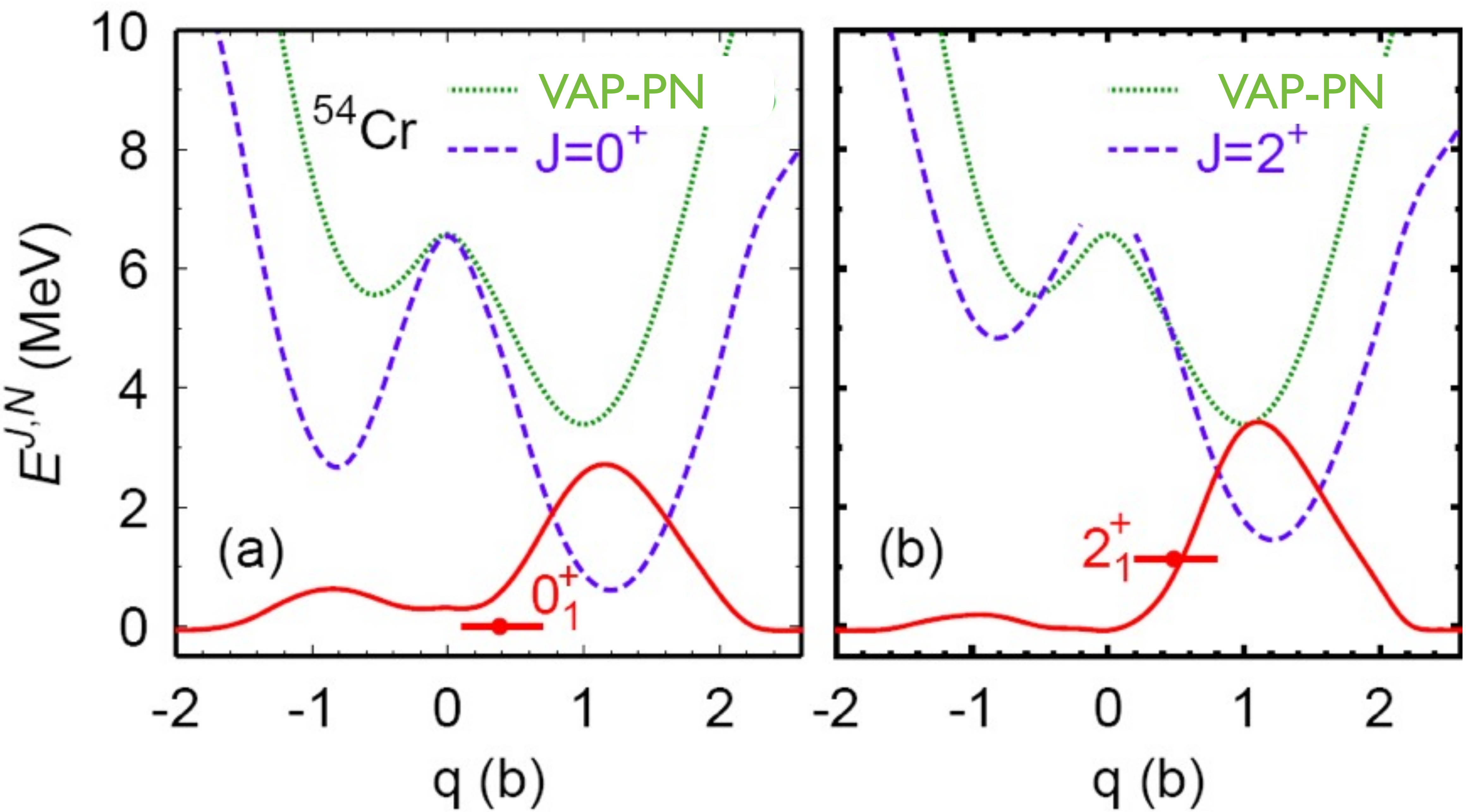
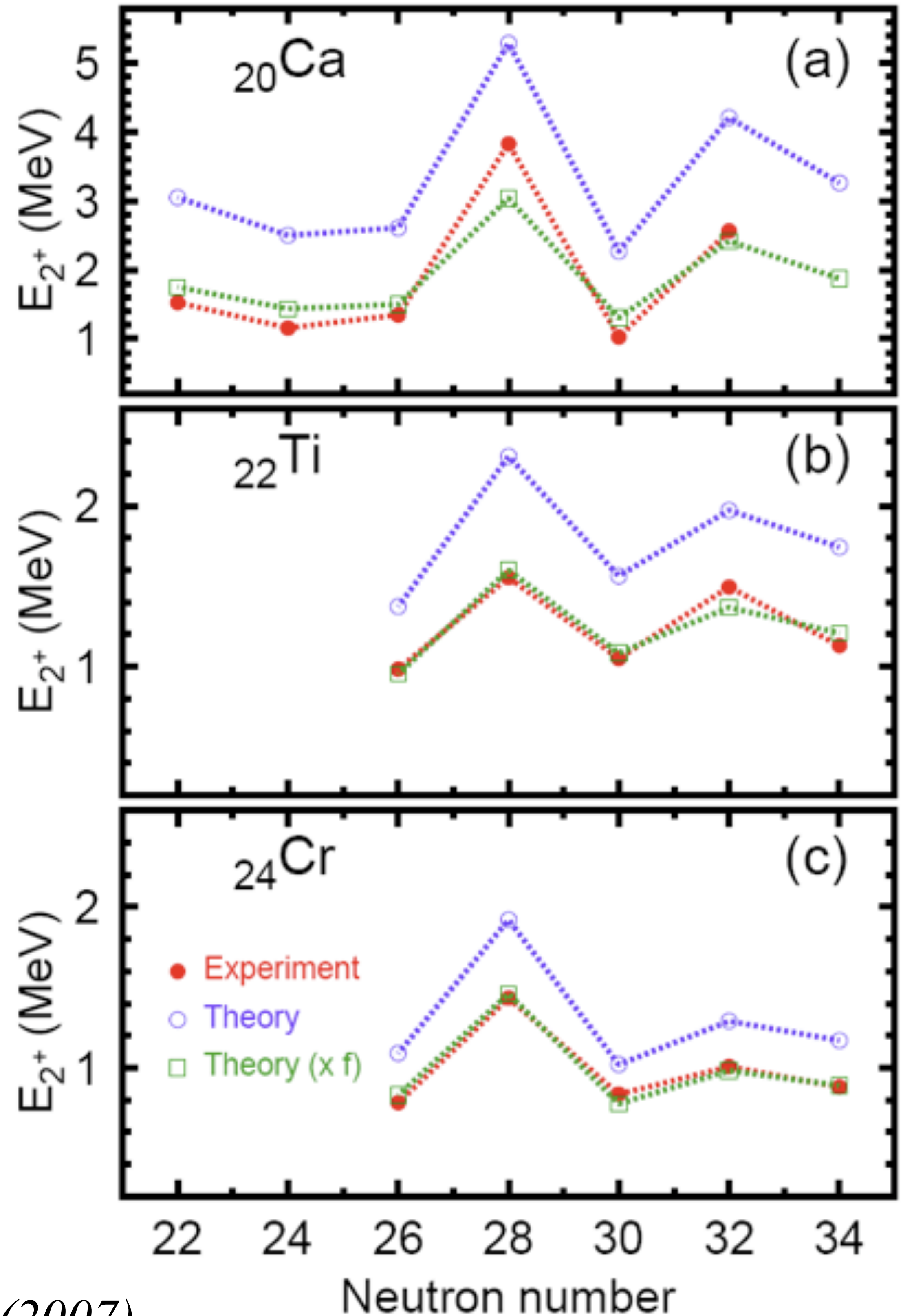
-2
-1
0
1
2
$E_{norm}^{Z,N}$(MeV)
q_{20}(b)
VAP
PLN
PAV
HFB
^{54}Cr

Examples of angular momentum PES and configuration mixing solutions





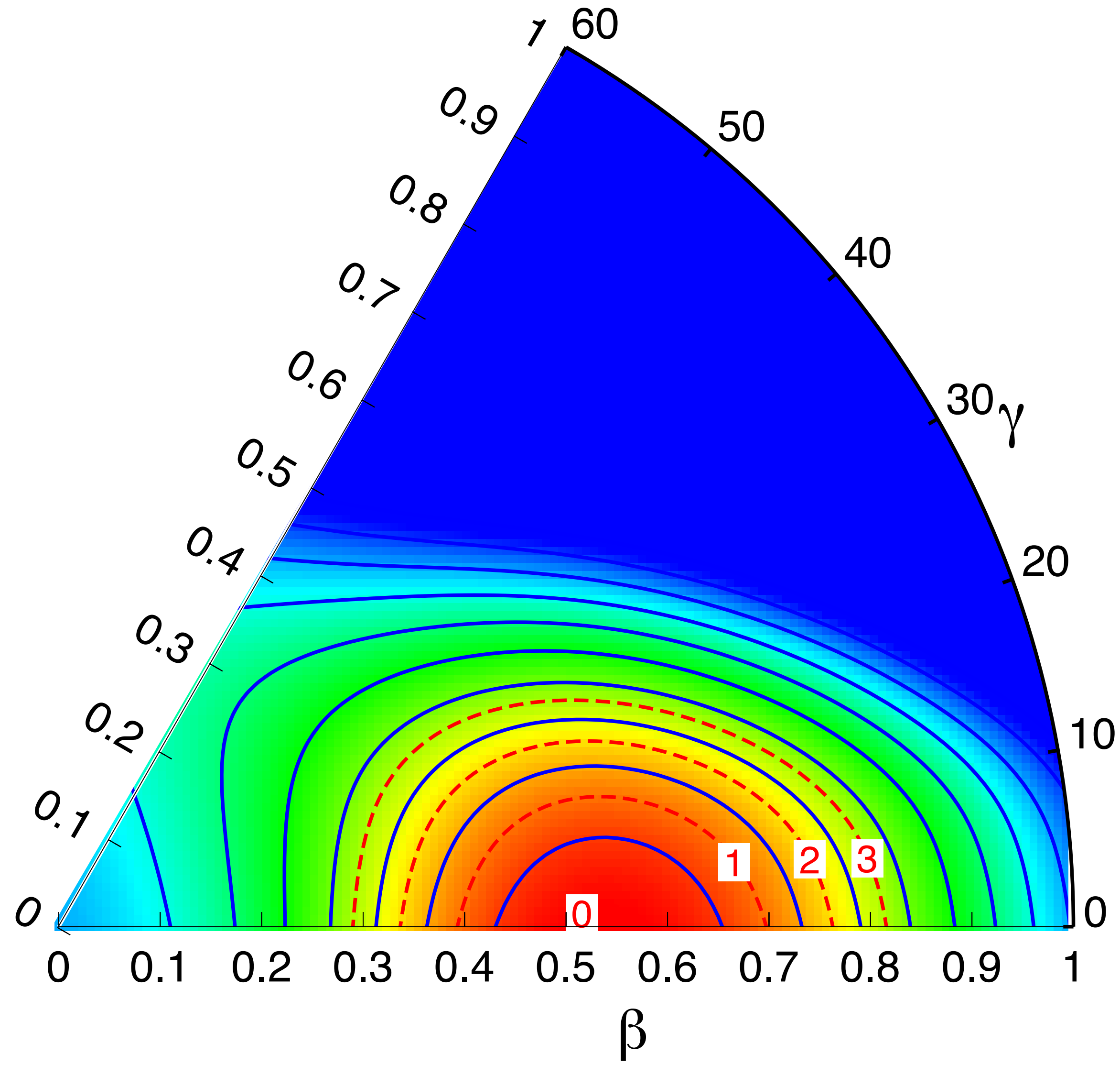
T.R. Rodriguez and J.L.E.
Phys. Rev. Lett. 99, 062501 (2007)

Particle number
and
Triaxial Angular Momentum Projection

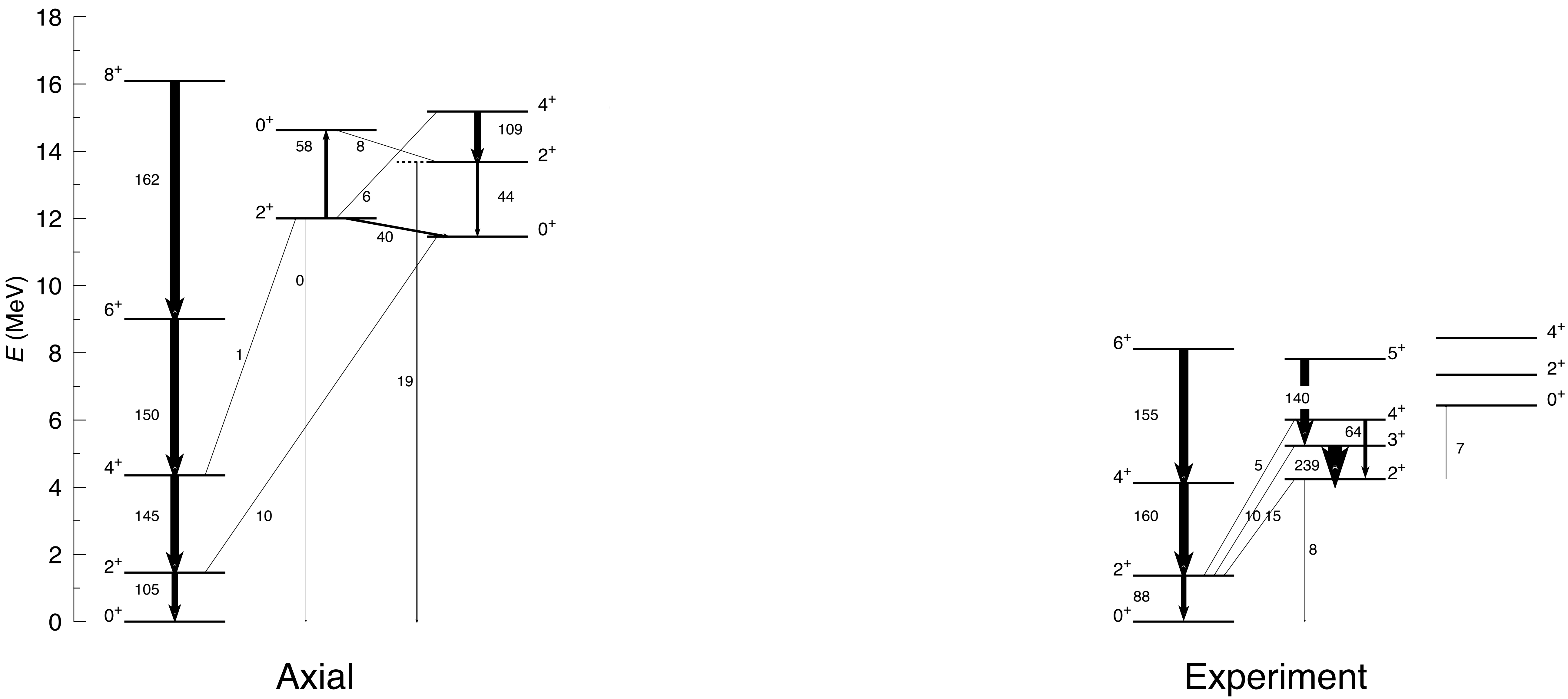
The nucleus ^{24}Mg

See also the variations of
M. Bender and P.H. Heenen, Phys. Rev. C 78, 024309(2008)
(Skyrme, LN + PNAMP)
J.M. Yao, J. Meng, P. Ring, and D. Vretener, Phys. Rev. C 81, 044311(2010)
(Relativistic, BCS+AMP)

The solution of the PN-VAP in the (β,γ) provides



^{24}Mg



18
16
14
12
10
8
6
4
2
0
E (MeV)
8+
6+
4+
2+
0+
162
150
145
105
0+
2+
58
8
6
40
0
1
10
4+
2+
0+
109
44
19
Axial
6+
4+
2+
0+
155
160
88
5+
4+
3+
2+
140
64
239
5
10 15
8
4+
2+
0+
7
Experiment

Projection of a mean field wave function |ϕ(β,γ)>

The projected wave function is given by

$$|IM;N,Z,\beta\gamma\rangle = \sum_K g^I_K P^I_{MK} P^N P^Z |\Phi(\beta,\gamma)\rangle \equiv \sum_K g^I_K \; |IMK;N,Z,\beta\gamma\rangle$$

with the projectors

$$P^I_{MK} = \frac{2I+1}{8\pi^2}\int \mathrm{d}\Omega \mathcal{D}^{I*}_{MK}(\Omega)\hat{R}(\Omega) \qquad P^N = \frac{1}{2\pi}\int_0^{2\pi} e^{i\varphi(\hat{N}-N)} d\varphi$$

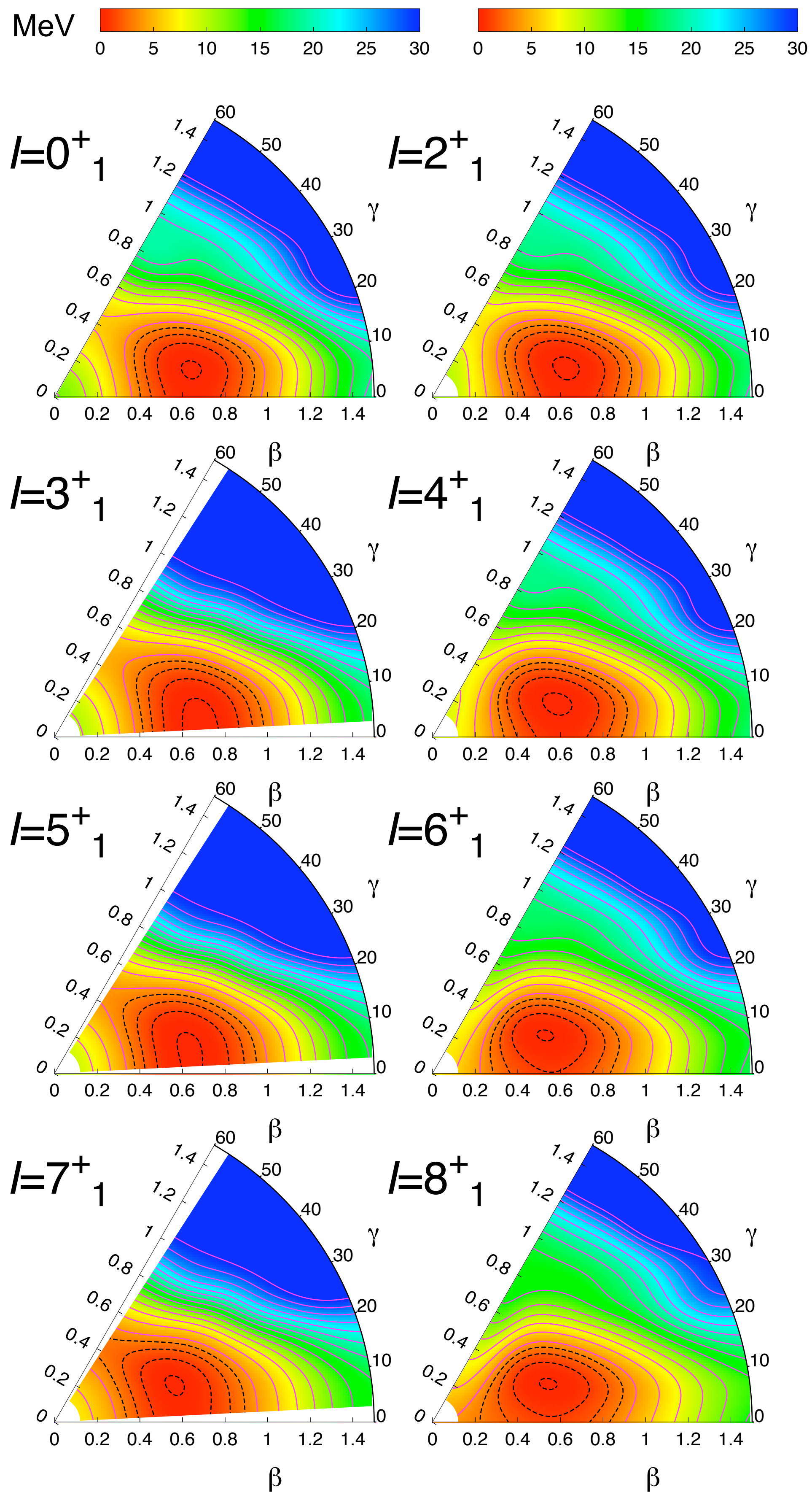
Variation with respect to the coefficients g^I_K provides

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

with the matrix elements

$$\begin{aligned} O^I_{KK'}(\beta\gamma,\beta\gamma) &= \langle\Phi(\beta\gamma)|\hat{O} P^I_{KK'} P^N P^Z|\Phi(\beta\gamma)\rangle \\ &= \frac{2I+1}{8\pi^2}\int d\Omega \mathcal{D}^{I*}_{KK'}(\Omega)\langle\Phi(\beta\gamma)|\hat{O}\hat{R}(\Omega)P^N P^Z|\Phi(\beta\gamma)\rangle \end{aligned}$$

Projected energies in the (β,γ) plane



Projected Generator Coordinate Theories

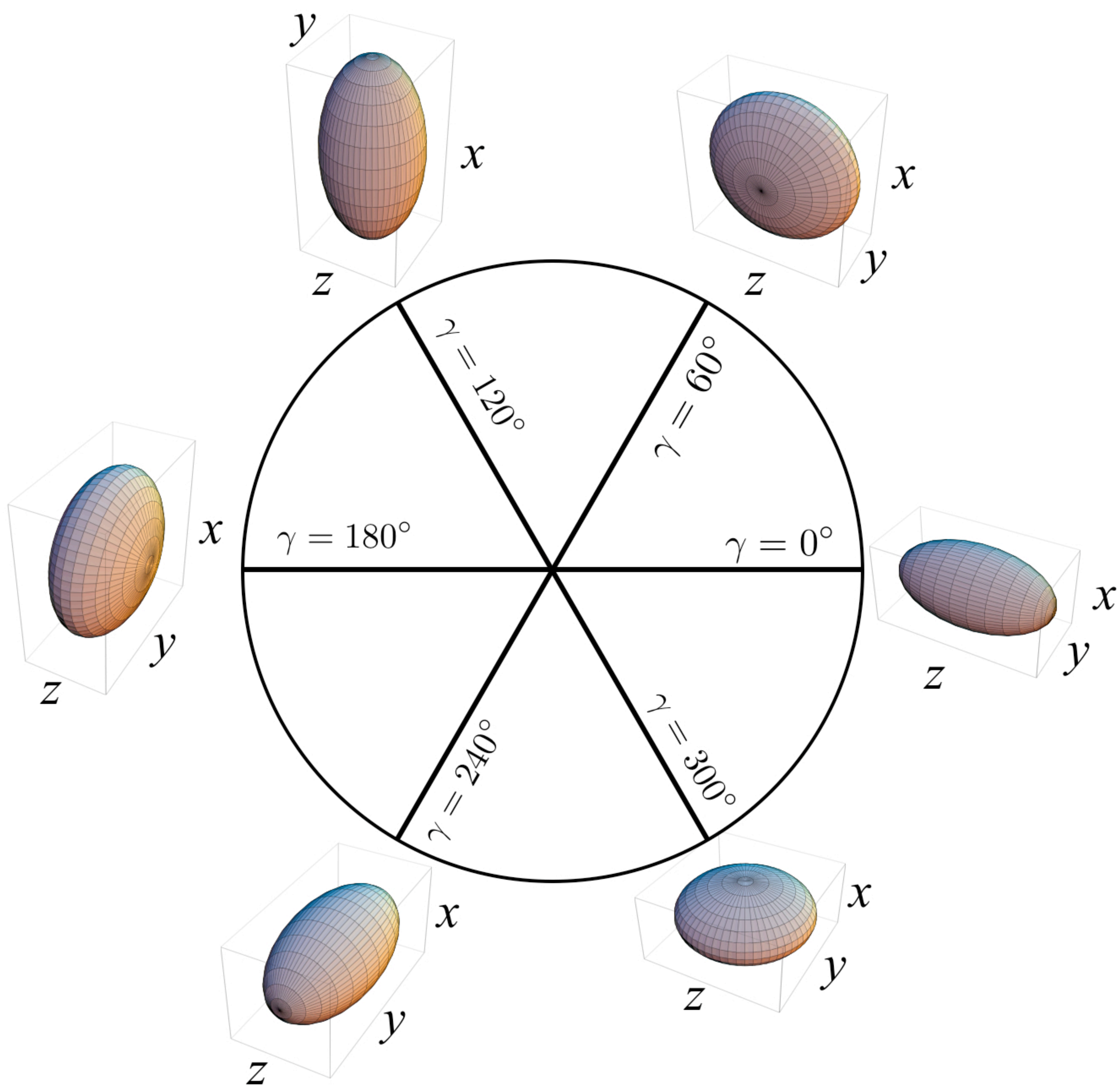
Ansatz : $$|IM;NZ\sigma\rangle = \sum_{K\beta\gamma} f^{I;NZ,\sigma}_{K\beta\gamma} |IMK;NZ;\beta\gamma\rangle$$

with : $$|IMK;NZ;\beta\gamma\rangle = \frac{2I+1}{8\pi^2}\int \mathcal{D}^{I*}_{MK}(\Omega)\hat{R}(\Omega)P^N P^Z|\Phi(\beta,\gamma)\rangle d\Omega$$

The variational principle provides the HW equation:

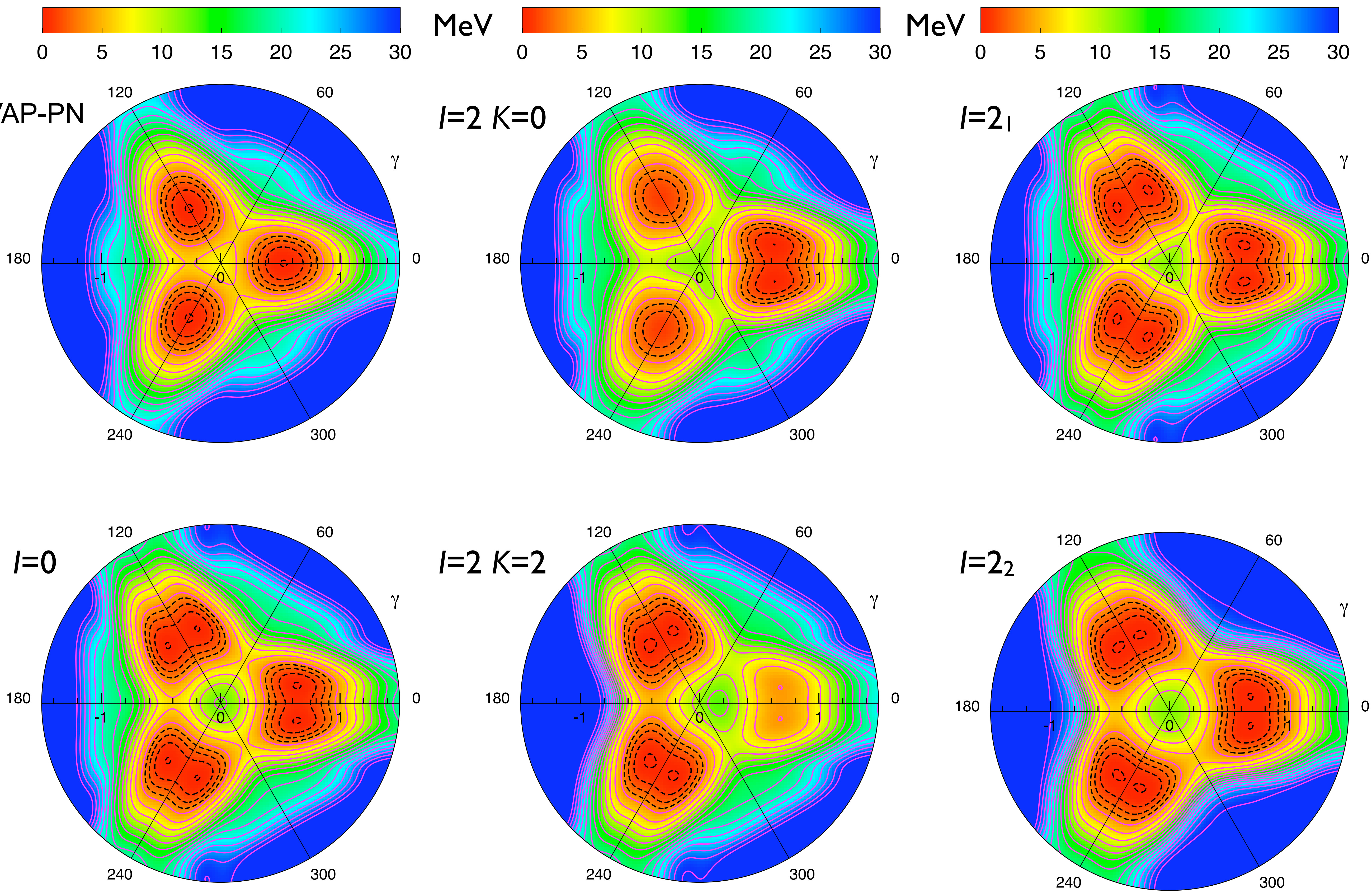
$$\sum_{K'\beta'\gamma'}\left(\mathcal{H}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} - E^{I;NZ;\sigma}\mathcal{N}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'}\right) f^{I;NZ;\sigma}_{K'\beta'\gamma'} = 0$$

with : $$\mathcal{O}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \equiv \langle IMK;NZ;\beta\gamma|\hat{O}|IMK';NZ;\beta'\gamma'\rangle =$$
$$\frac{2I+1}{8\pi^2}\int \mathcal{D}^{I*}_{KK'}(\Omega)\langle\Phi(\beta,\gamma)|\hat{O}\hat{R}(\Omega)P^N P^Z|\Phi(\beta',\gamma')\rangle d\Omega$$


$\gamma = 0°$
$\gamma = 60°$
$\gamma = 120°$
$\gamma = 180°$
$\gamma = 240°$
$\gamma = 300°$
x
y
z

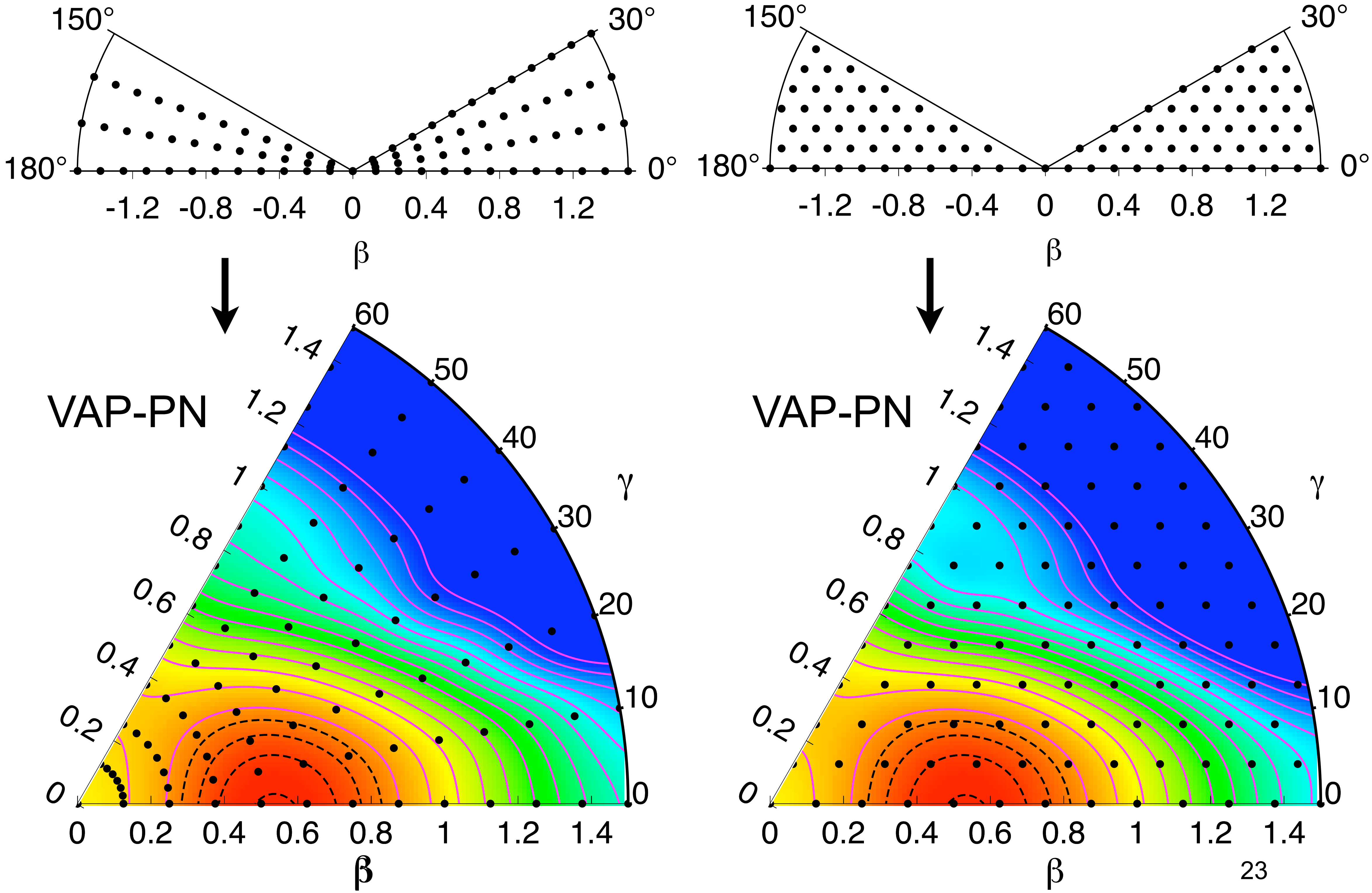
Energy contour plots in the (β,γ) plane

$$|IM;NZ;\beta\gamma\rangle = \sum_K g_K |IMK,NZ;\beta\gamma\rangle$$

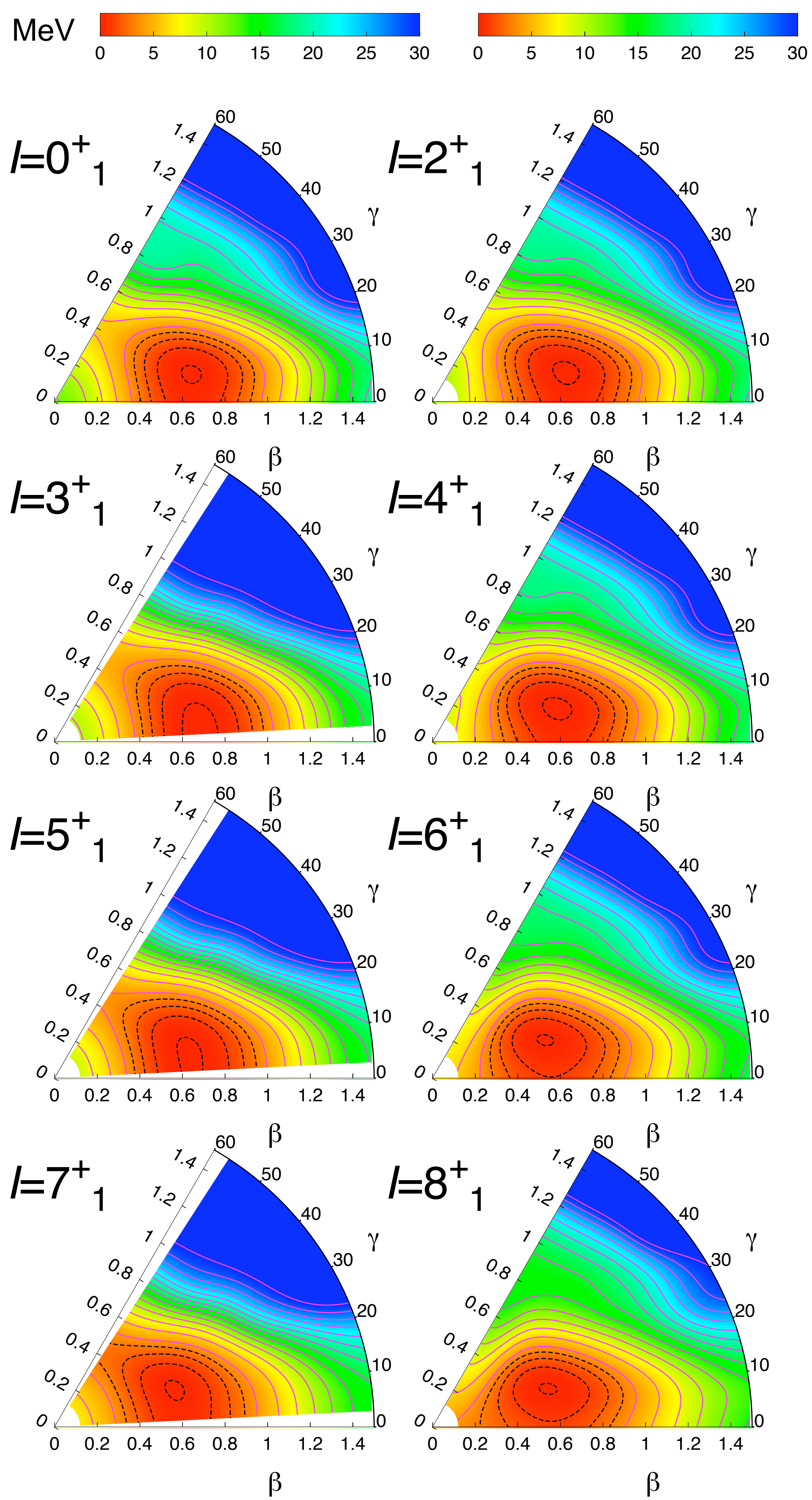


$$|IMK;NZ;\beta\gamma\rangle = P^I_{MK} P^N P^Z |\Phi(\beta,\gamma)\rangle$$

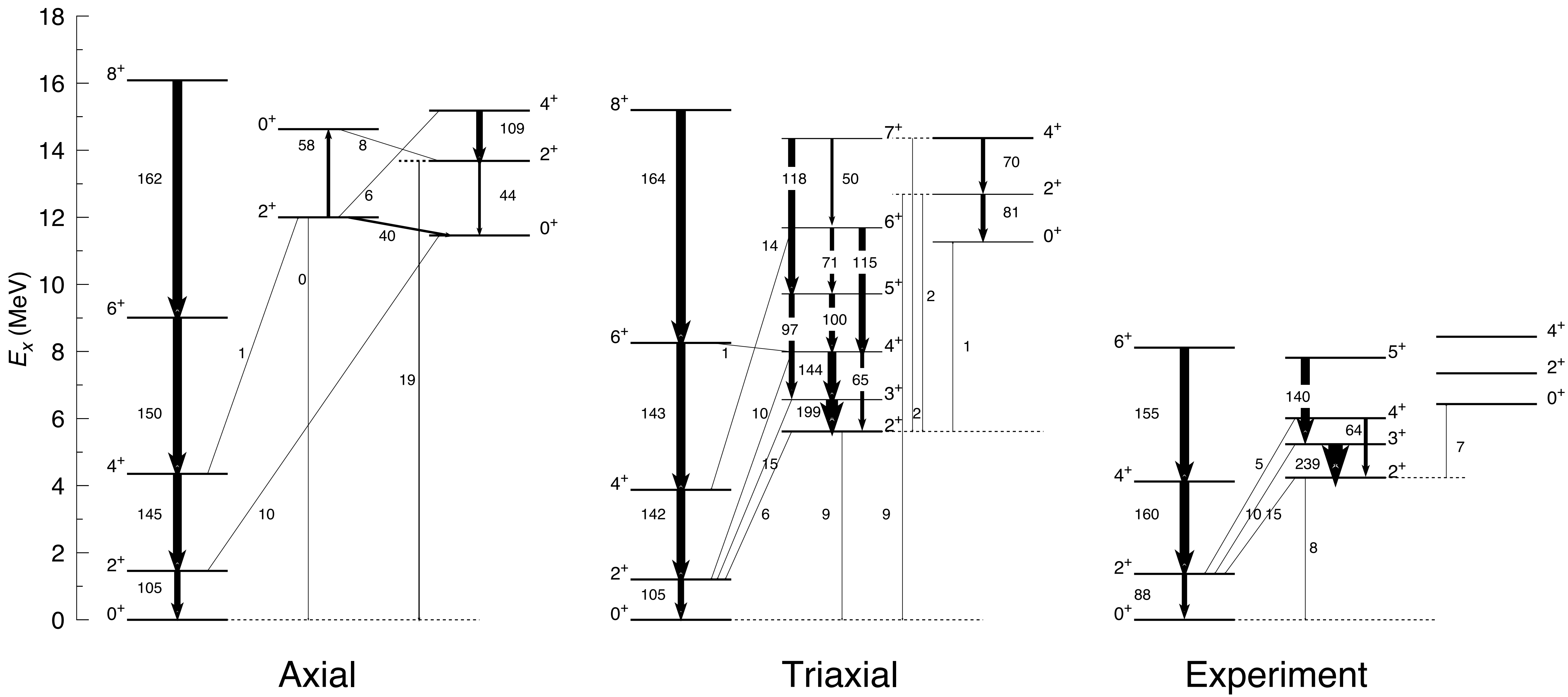
Choice of sextant and grid in (β,γ) plane



Projected energies in the (β,γ) plane

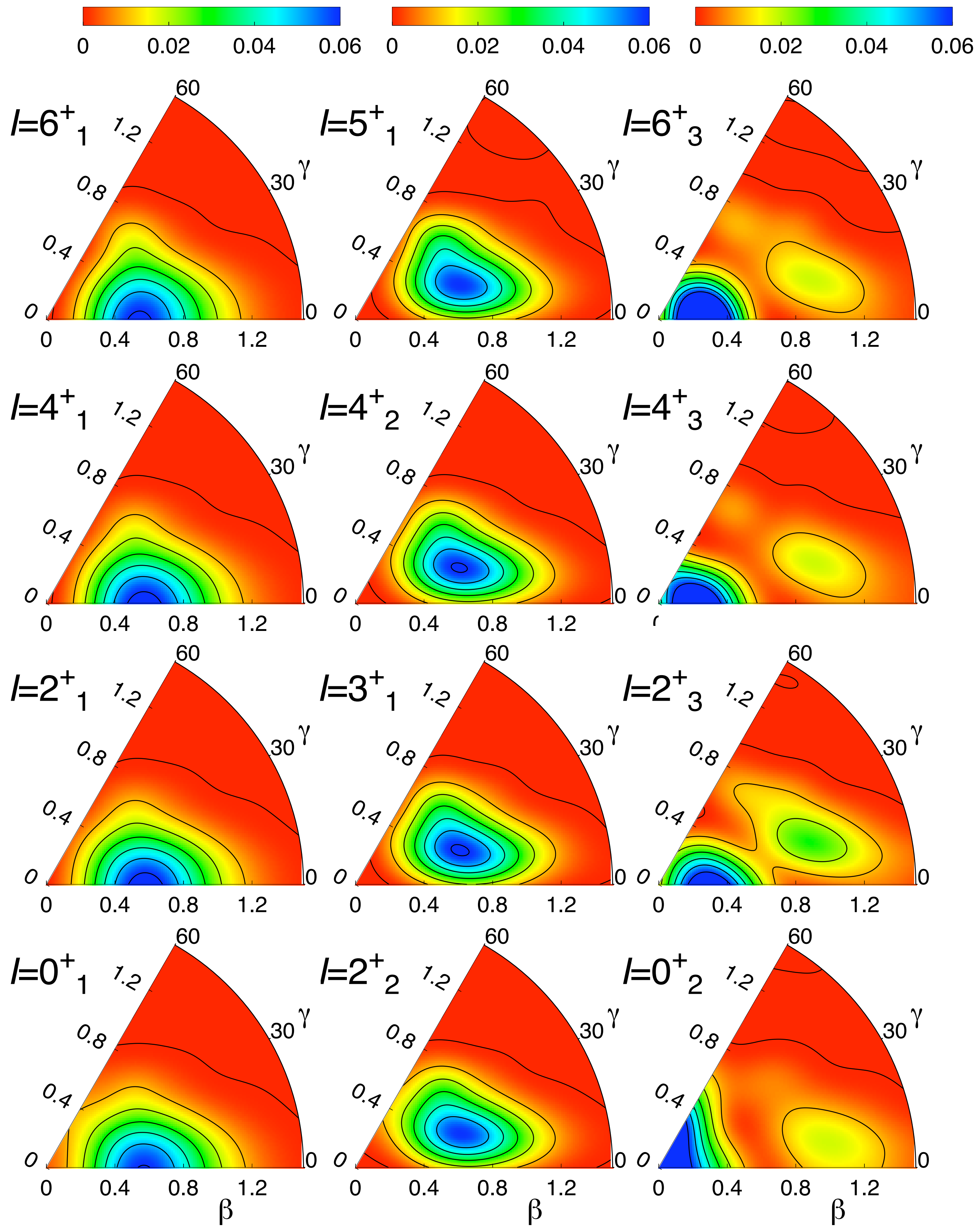


^{24}Mg



T. R. Rodriguez and J.L.E., Phys. Rev. **C81**, 064323(2010)

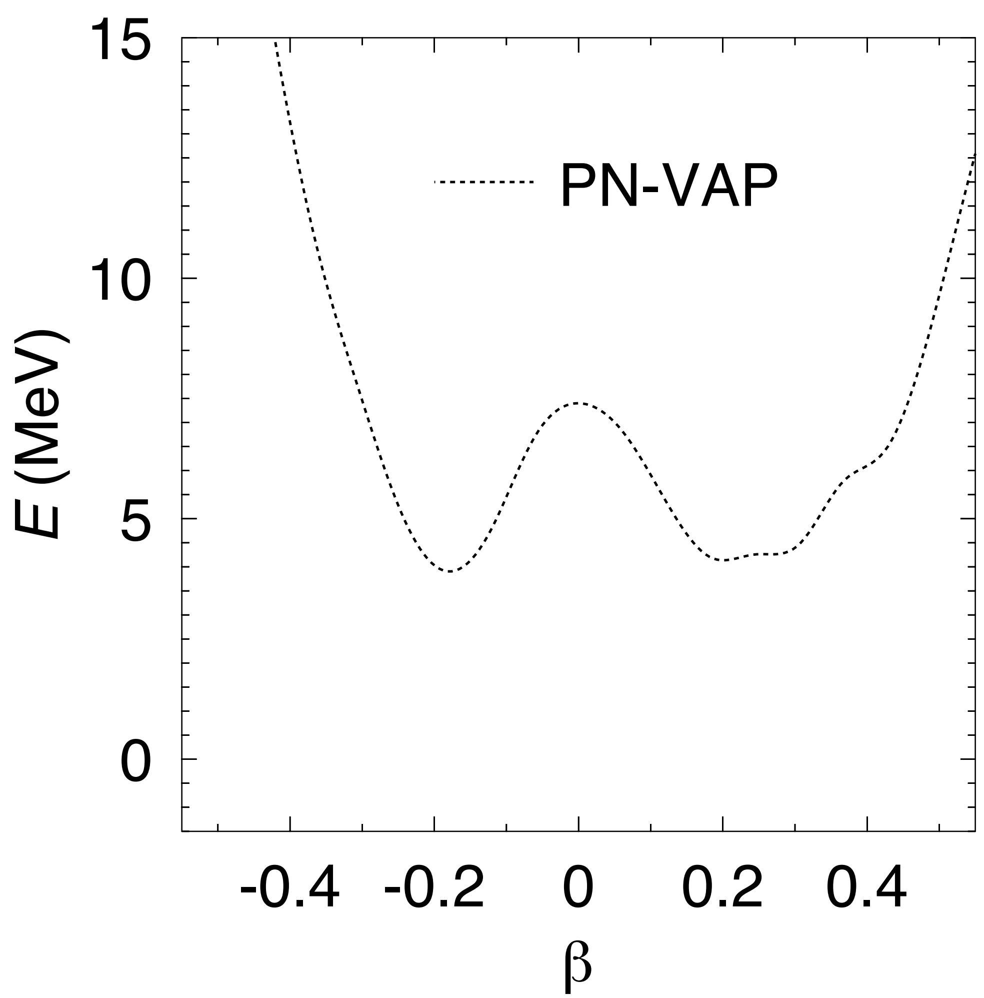
Collective wave functions in the (β,γ) plane



The need of triaxiality:

^{126}Xe as an example

Axial calculations ^{126}Xe



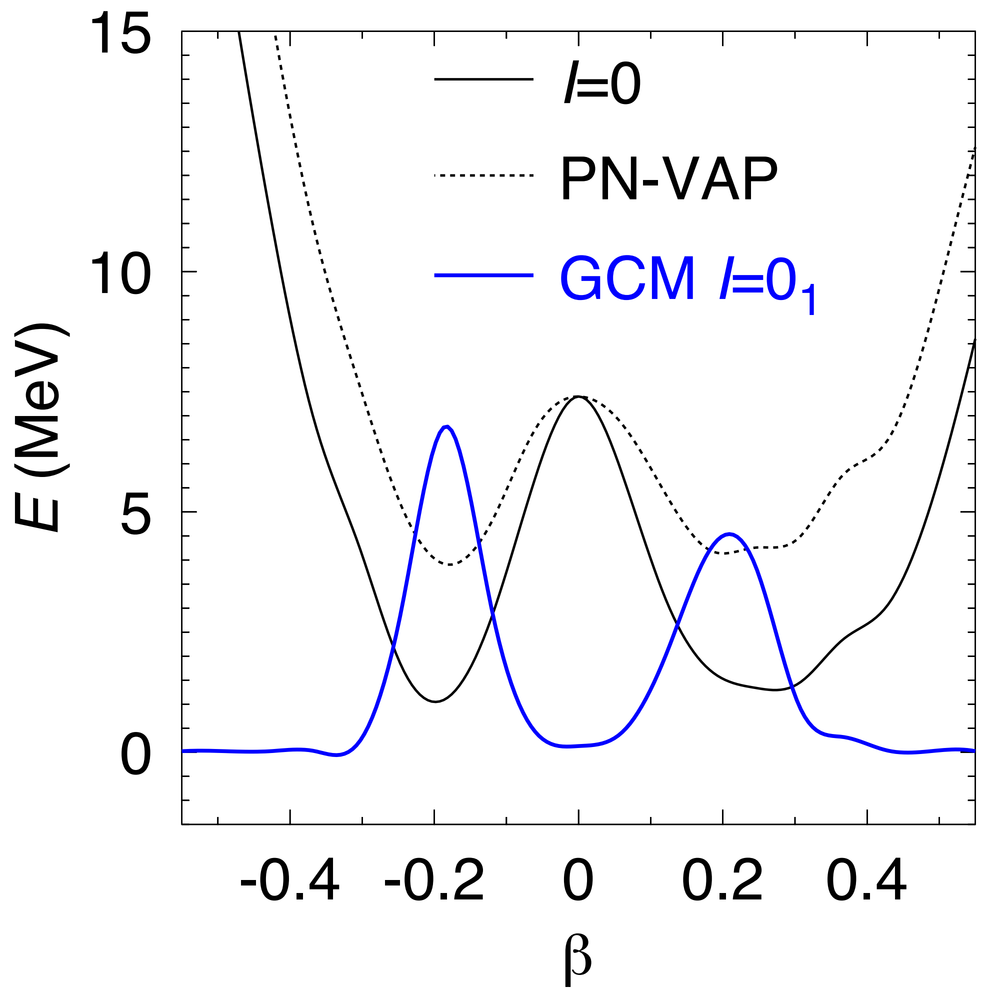
✓ AXIAL calculations

✓ Two minima almost degenerated in the potential energy surface

✓ The collective wave function of the ground state is distributed in these two minima (shape coexistence)

✓ TRIAXIAL calculations?

Axial calculations ^{126}Xe



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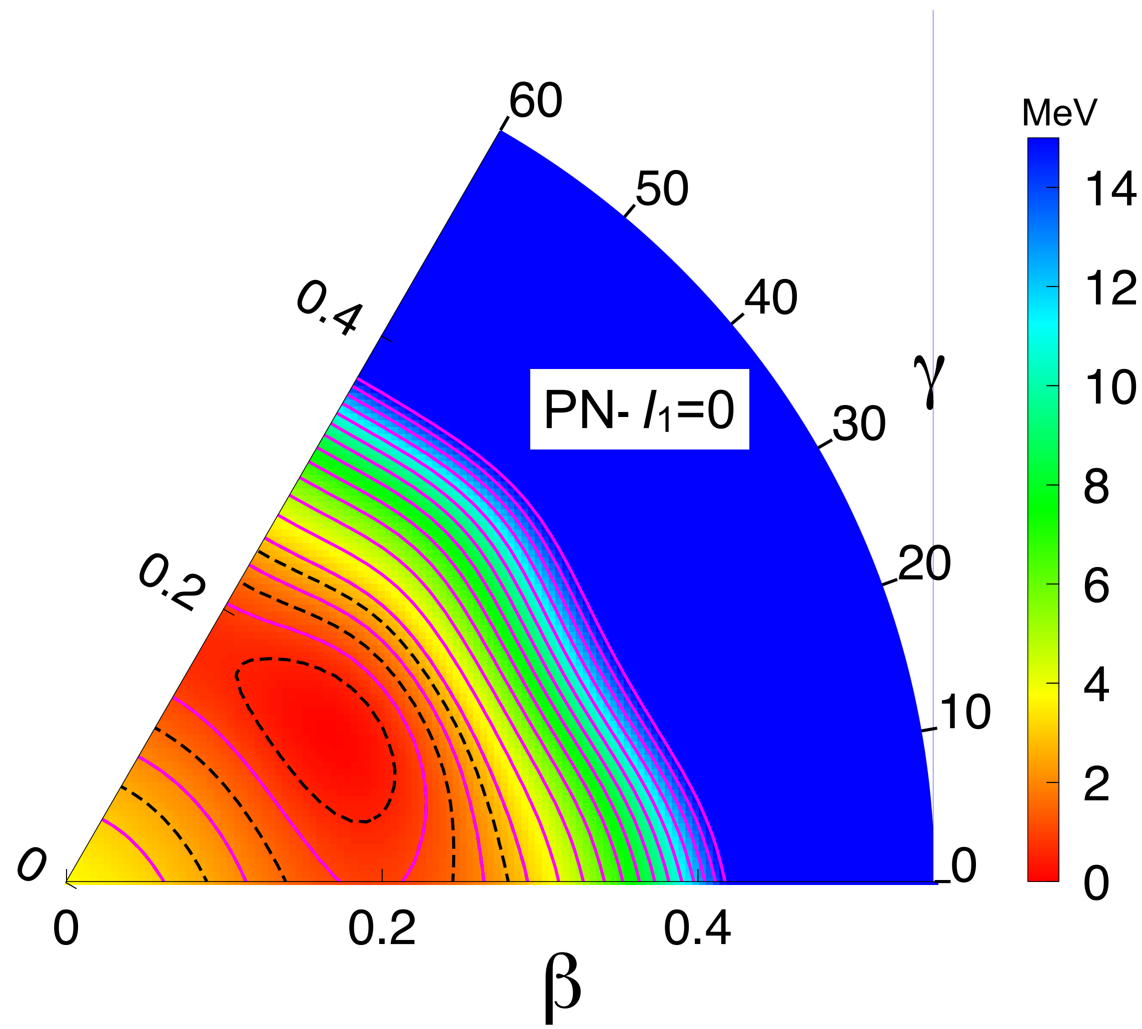
Triaxial calculations ^{126}Xe in a reduced configuration space (seven shells)

T.R.Rodriguez and J.L. Egido, Journal of Physics: Conference Series (2011)



✓ TRIAXIAL calculations

✓ One single minimum in γ=30° and saddle points in the axial configurations

✓ PES very soft in the γ degree of freedom

✓ After GCM, there is not coexistence of prolate and oblate configurations for the ground state, just a triaxial state.

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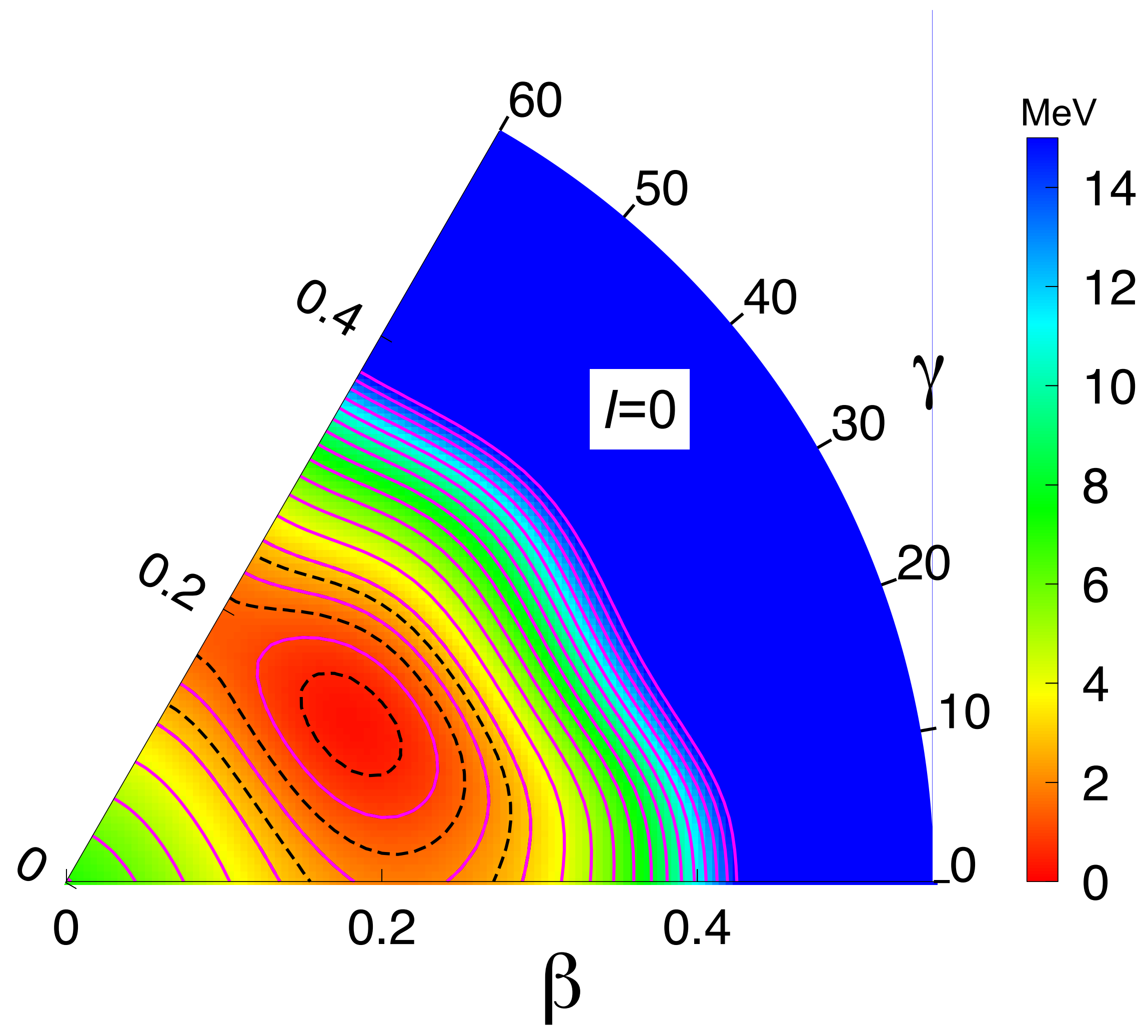

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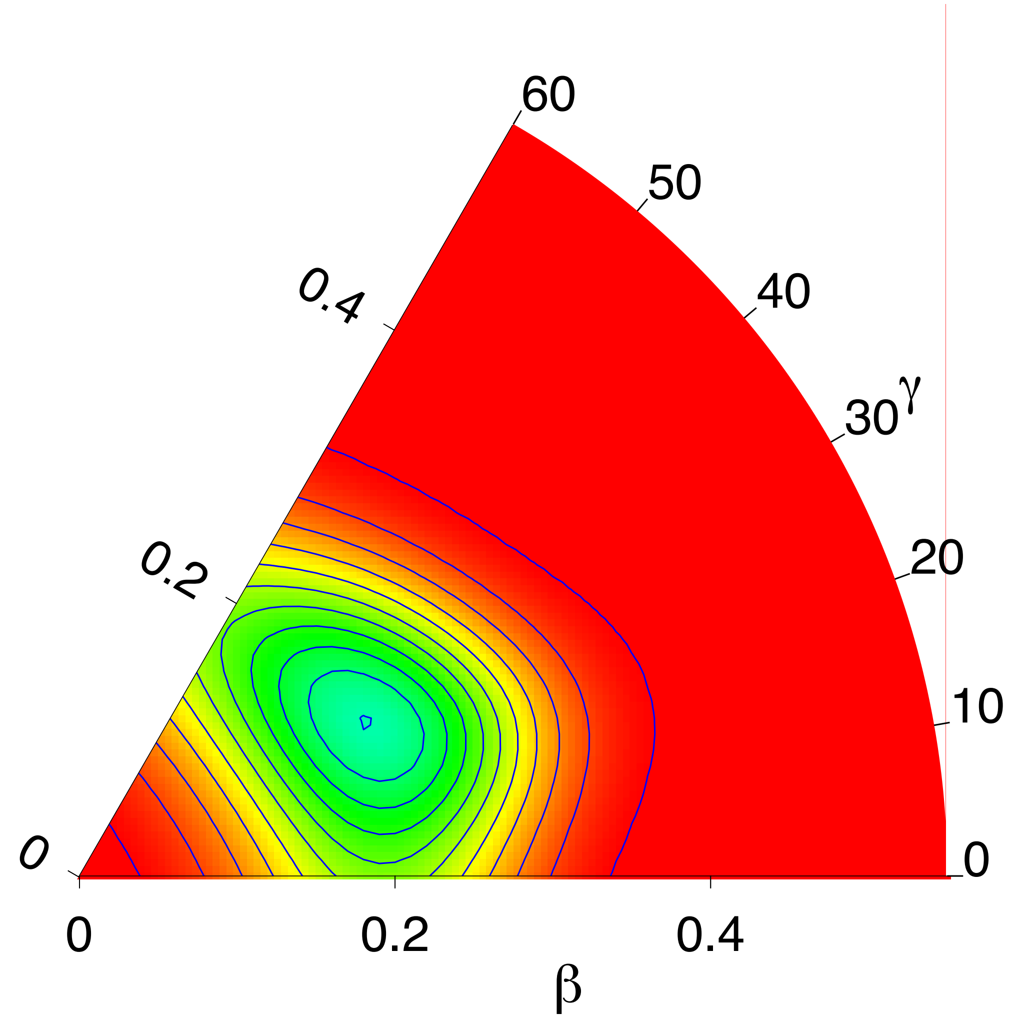

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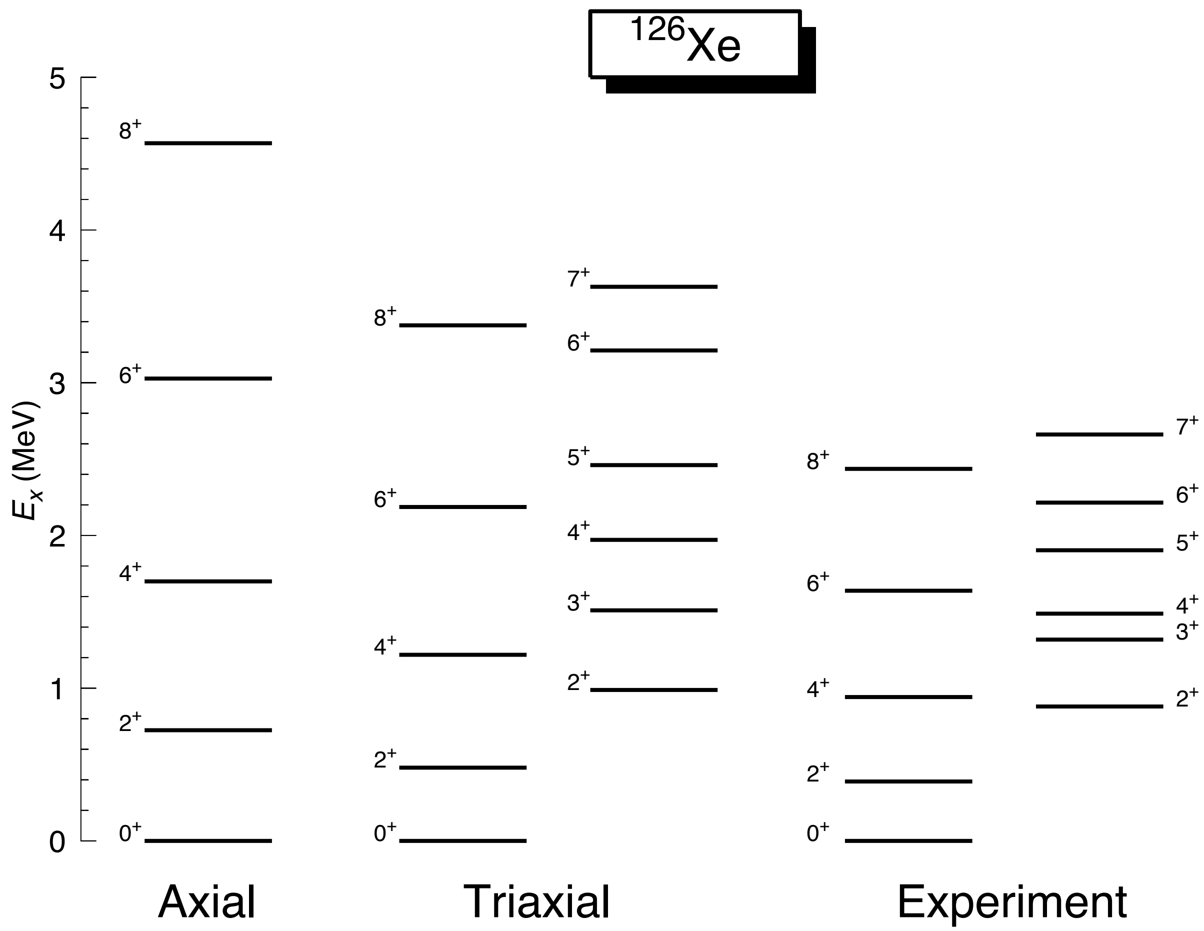
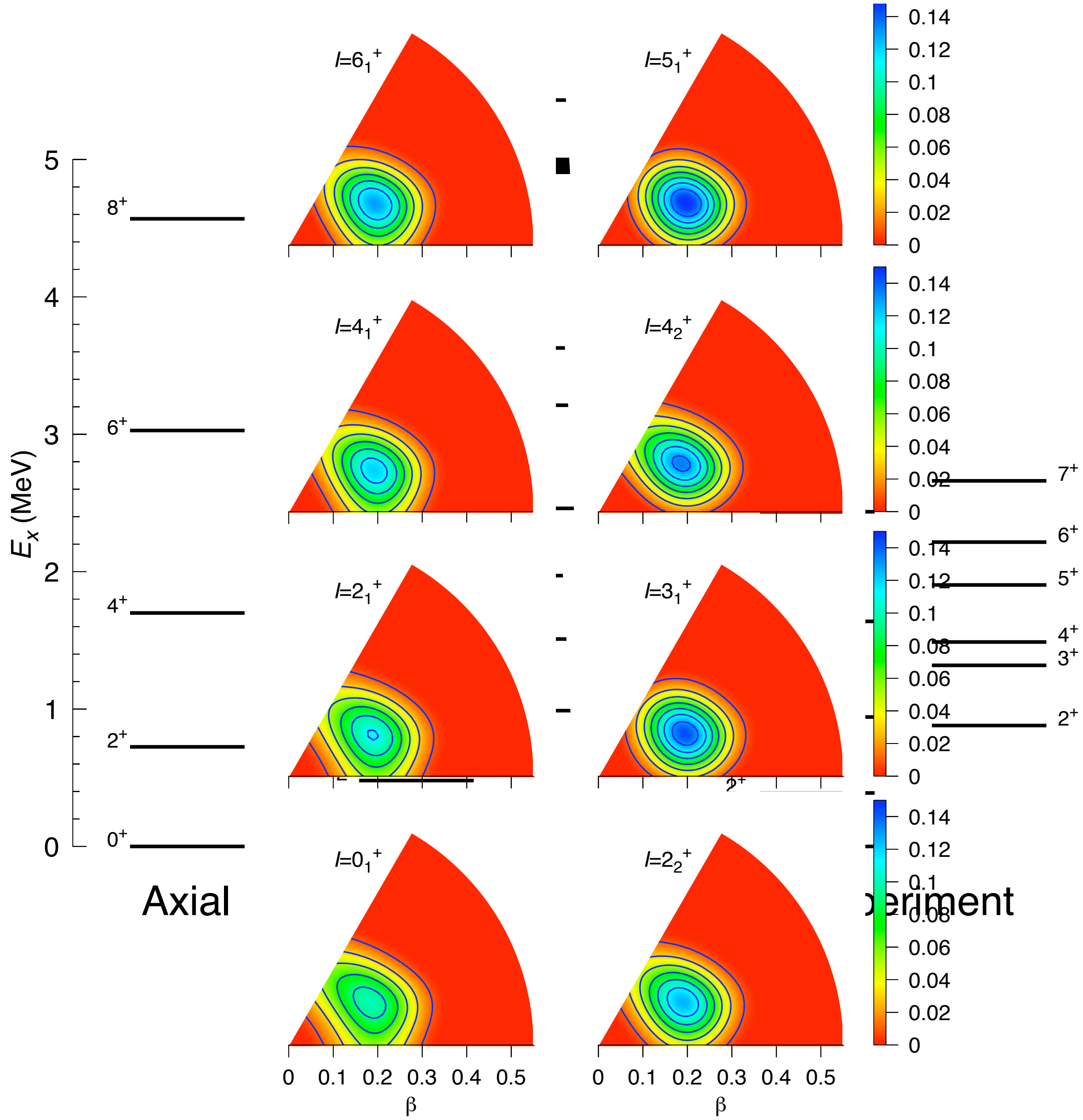


- ✓ TRIAXIAL calculations
  - ✓ Triaxial calculations are able to describe qualitatively the experimental data
  - ✓ Branching ratios for the B(E2) nicely reproduced.

$I_i \to I_f$	Exp.	Theory
$2_2^+ \to 2_1^+$	100.	100.
$2_2^+ \to 0_1^+$	1.5 $\pm$0.4	0.001
$3_1^+ \to 4_1^+$	$35.^{+10}_{-34}$	40.48
$3_1^+ \to 2_2^+$	100.	100.
$3_1^+ \to 2_1^+$	$2.0^{+0.6}_{-1.7}$	0.000
$4_2^+ \to 4_1^+$	76. $\pm$22	80.6
$4_2^+ \to 2_2^+$	100.	100.
$4_2^+ \to 2_1^+$	0.4$\pm$0.1	0.007
$5_1^+ \to 6_1^+$	75. $\pm$23	59.6
$5_1^+ \to 4_2^+$	76. $\pm$21	90.6
$5_1^+ \to 3_1^+$	100.	100.
$5_1^+ \to 4_1^+$	2.9 $\pm$0.8	0.02
$6_2^+ \to 6_1^+$	$34.^{+15}_{-23}$	27.1
$6_2^+ \to 4_2^+$	100.	100.
$6_2^+ \to 4_1^+$	0.49 $\pm$0.15	0.003
$7_1^+ \to 6_2^+$	40. $\pm$26	45.11
$7_1^+ \to 5_1^+$	100.	100.

Triaxial calculations ^{126}Xe



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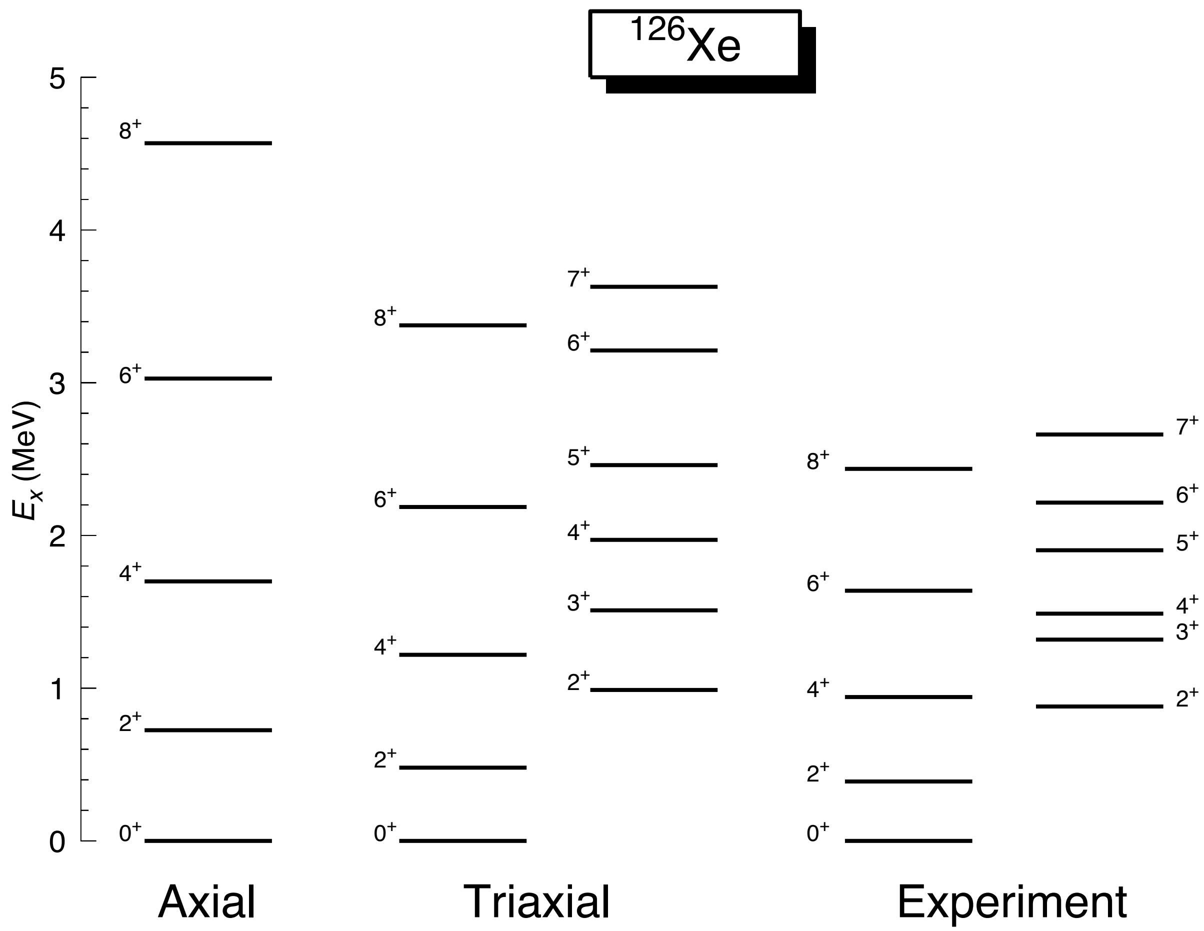

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Interplay of fluctuations in deformation and pairing in the GCM framework

Preliminary considerations

How to constraint pairing degrees of freedom ? In the case of space deformation we use (β, γ)

For a pure monopole pairing force, one has state independent gap and the obvious choice is the pairing gap Δ

Which is the simplest choice for the Gogny force? We can have a hint from the monopole pairing case, in this case (Ring-Schuck)

$$\langle (\Delta \hat{N})^2 \rangle = 4 \sum_{k>0} u_k^2 v_k^2 = \Delta^2 \sum_{k>0} \frac{1}{E_k^2} \propto \Delta^2 \propto E_{PAIRING}$$

We will use as a constraint with Gogny force the quantity

$$\delta = \langle (\Delta \hat{N})^2 \rangle^{1/2} \propto (E_{PAIRING})^{1/2} (?)$$

Variational Equations (I)

We proceed in two steps. In the first one we determine the intrinsic wave functions by the minimalization principle

$$\delta E'^{N}[\phi(q,\delta)] = 0,$$

the constrained energy being given by

$$E'^{N} = \frac{\langle\Phi|\hat{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} - \lambda_q \langle\phi|\hat{Q}_{20}|\phi\rangle - \lambda_\delta \langle\phi|(\Delta\hat{N})^2|\phi\rangle^{1/2},$$

with

$$|\Phi\rangle = P^N P^Z|\phi\rangle \;\; (\mathrm{VAP}) \quad \text{or} \quad |\Phi\rangle = |\phi\rangle \quad \text{and} \quad |\phi\rangle = |HFB\rangle$$

and the Lagrange multipliers determined by the conditions:

$$\langle\phi|\hat{Q}_{20}|\phi\rangle = q, \qquad \langle\phi|(\Delta\hat{N})^2|\phi\rangle^{1/2} = \delta.$$

Variational Equations (II)

In the second step we perform the configuration mixing calculations

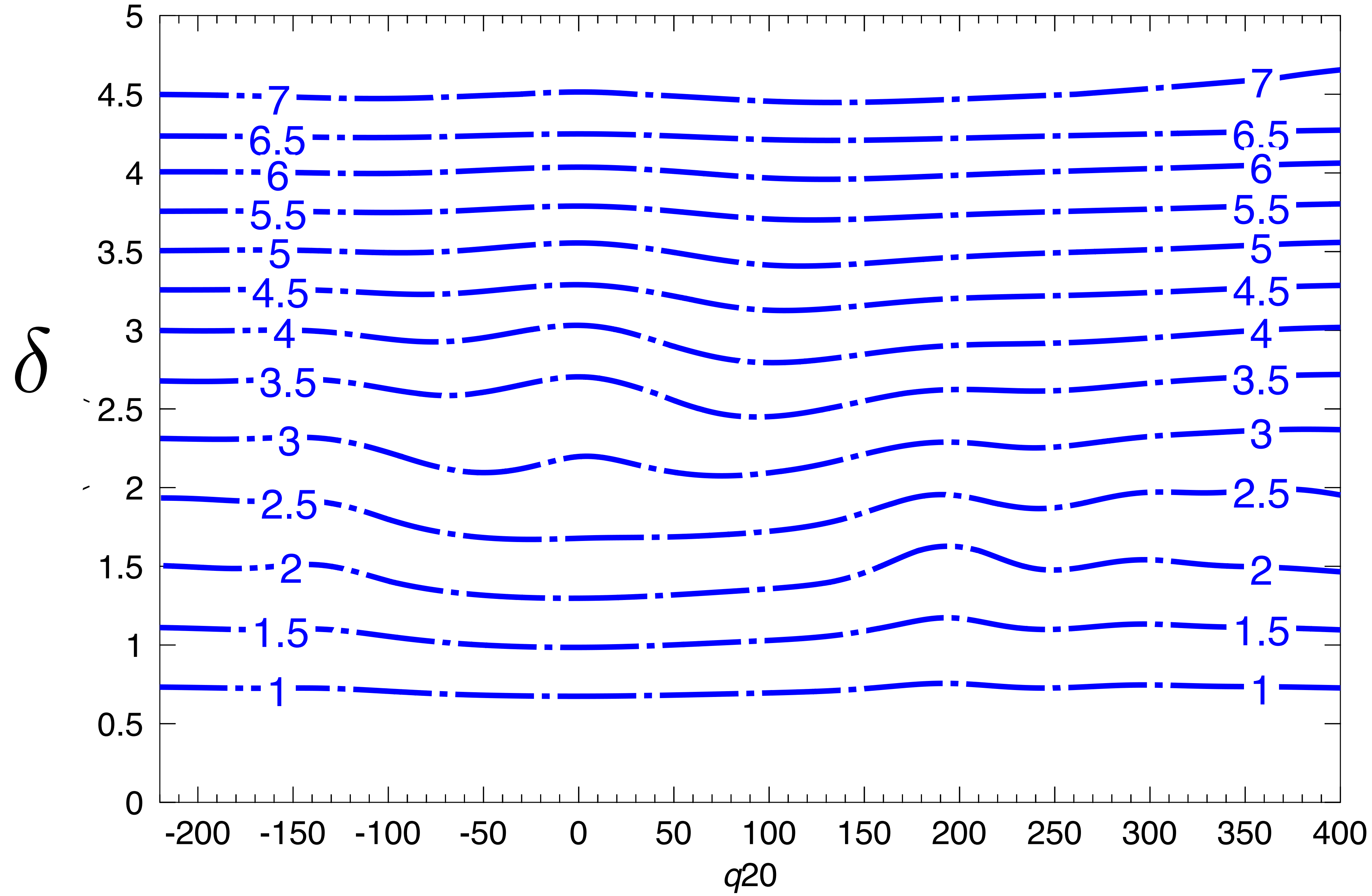
$$|\Psi^{N,I,\sigma}\rangle = \int f^{N,I,\sigma}(q,\delta)\ \hat{P}^I \hat{P}^N \hat{P}^Z\ |\phi(q,\delta)\rangle dq d\delta.$$

The mixing coefficients being determined by the Hill-Wheeler equation

$$\int \left(\mathcal{H}^{N,Z,I}(q\delta, q'\delta') - E^{N,Z,I,\sigma}\mathcal{N}^{N,Z,I}(q\delta, q'\delta')\right) f^{N,Z,I,\sigma}(q'\delta')dq'd\delta' = 0,$$

Pairing energies vs. particle # fluctuations

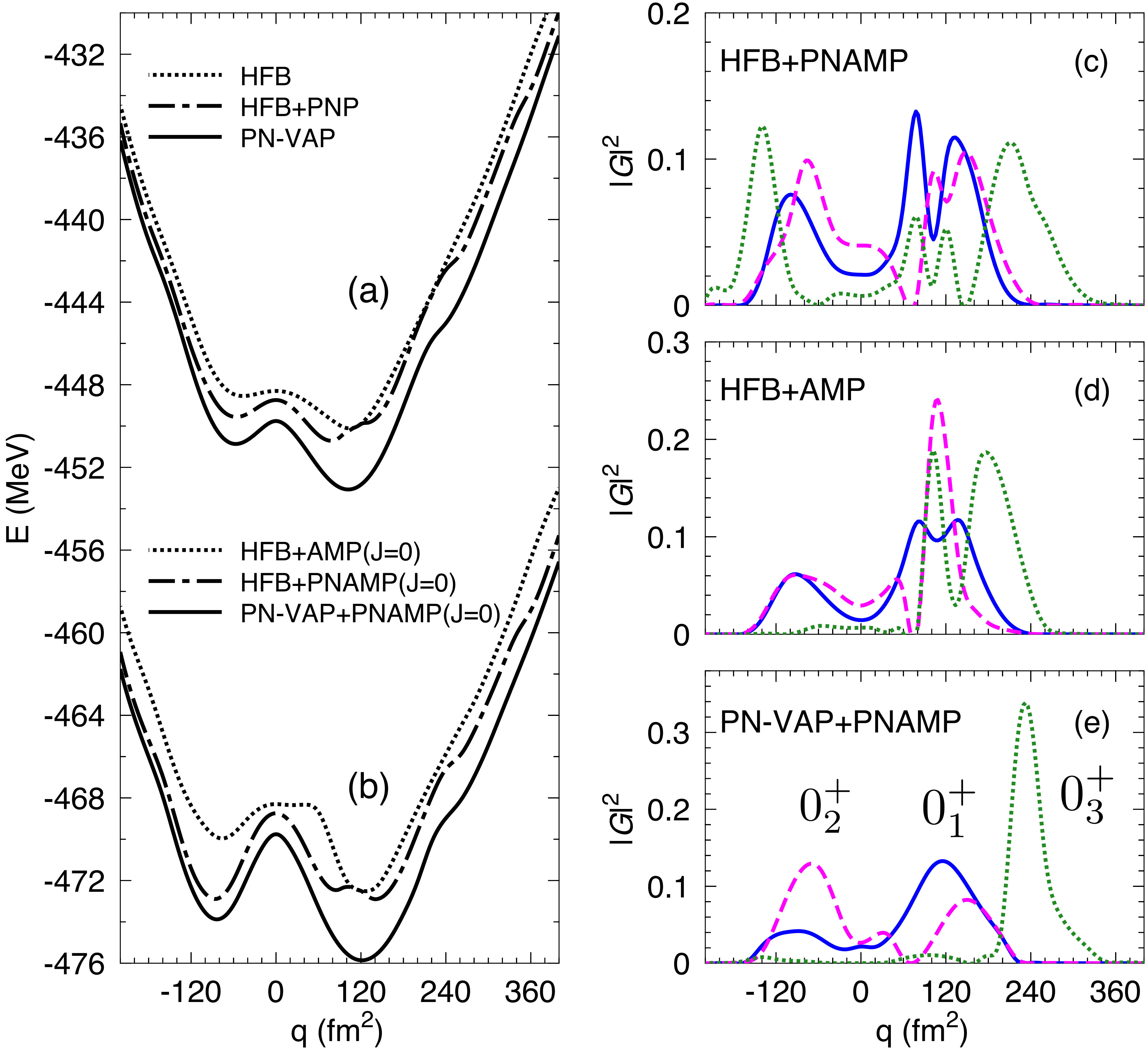
We have seen that $\delta = \langle (\Delta N)^2 \rangle^{1/2} \propto \Delta \propto (-E_{PAIRING})^{1/2}$



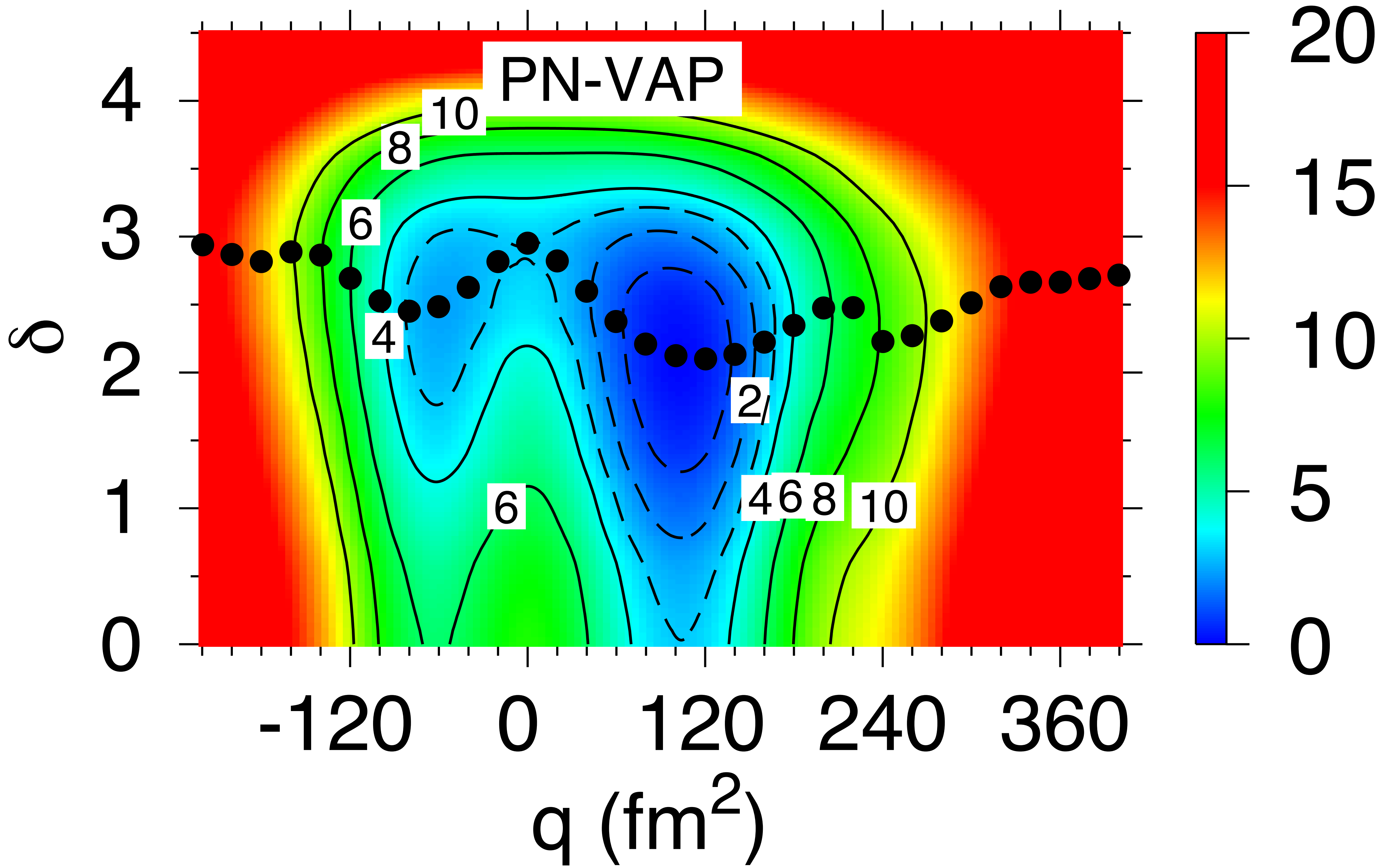
$^{54}\mathrm{Cr}$

Contour curves of the square root of the pairing energies in the plane (q_{20}, δ) with wave functions $P^{I=0} P^Z P^N |\Phi\rangle_{VAP}$

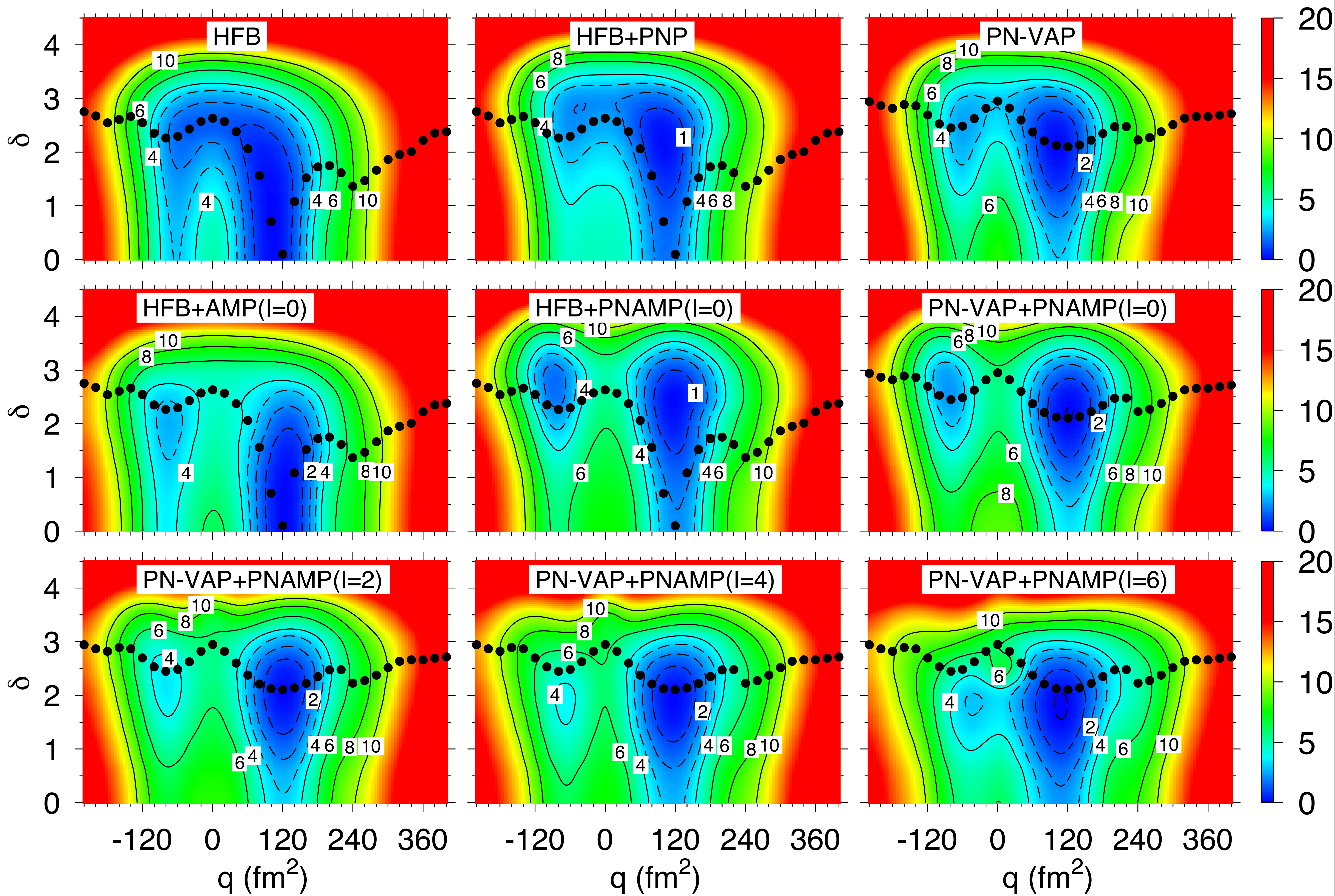
One dimensional calculations for ^{54}Cr



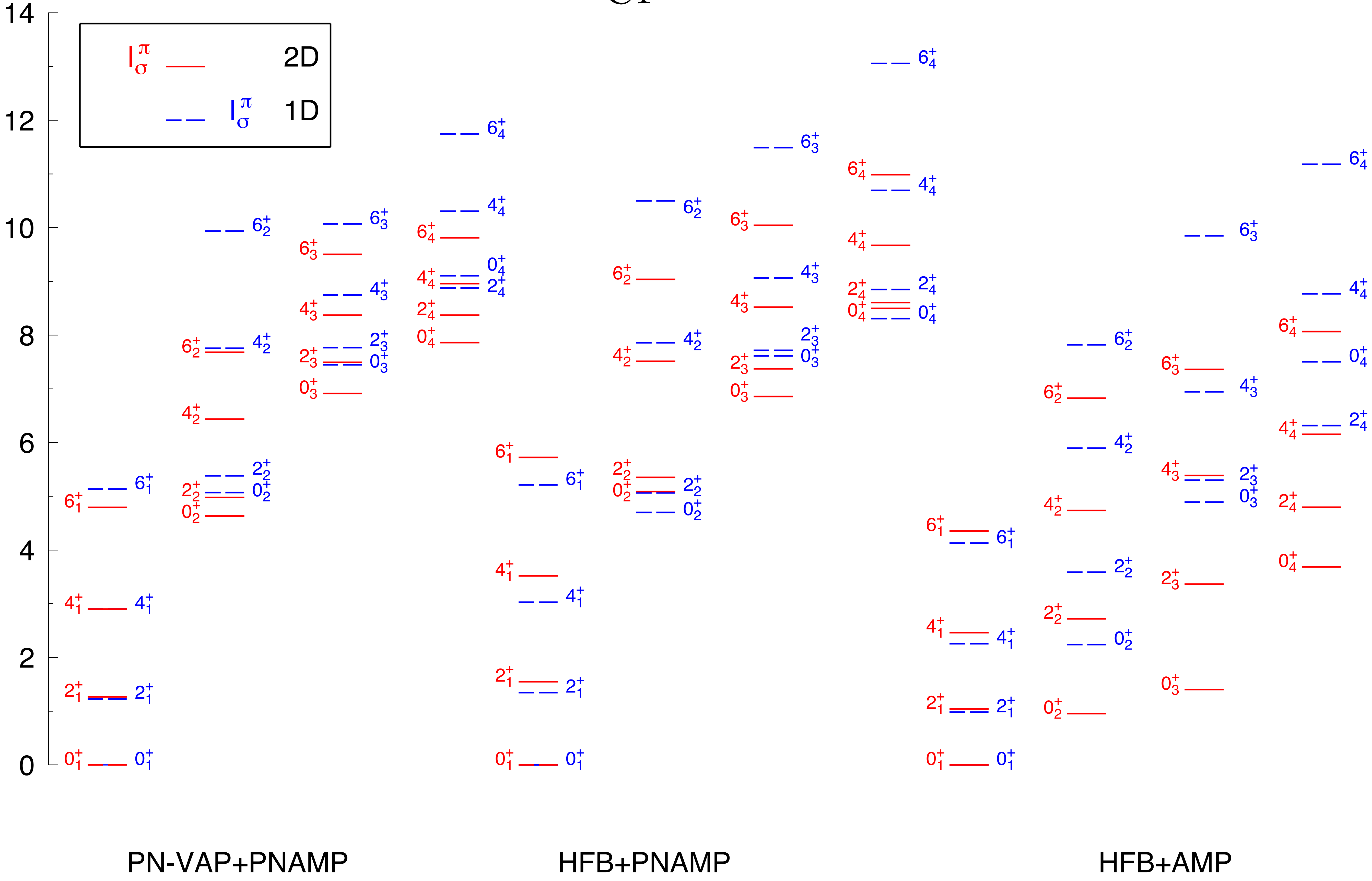
Two dimensional calculations for ^{54}Cr



Potential Energy Surfaces for ^{54}Cr in 2D

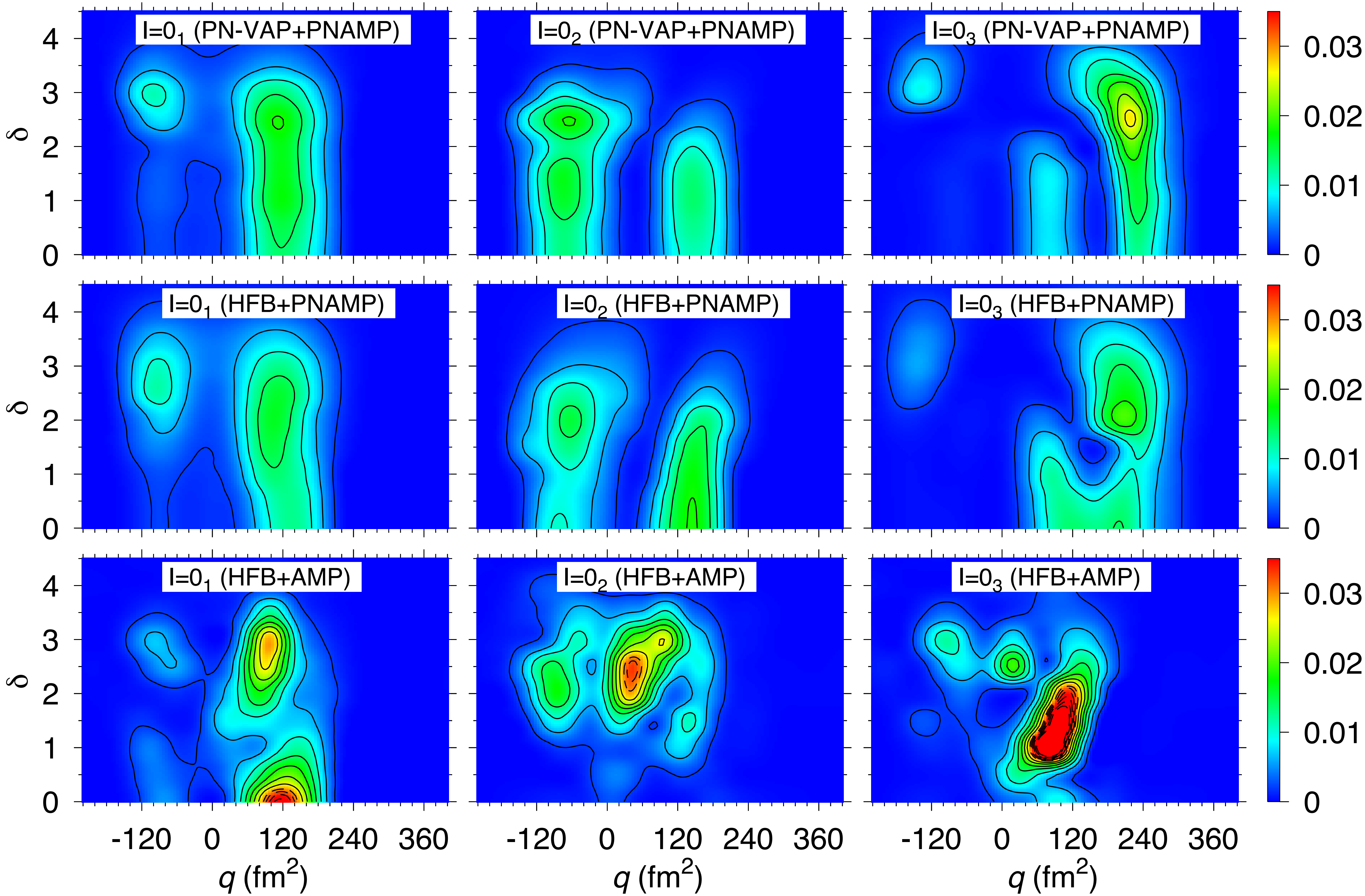


^{54}Cr



(N. Lopez-Vaquero, T.R. Rodriguez and J.L.E, Phys. Lett. B, in press)

Wave functions in various approaches



Pairing energies of the lowest 0^+ states

		0_1^+	0_2^+	0_3^+
HFB+PNAMP (1D)	$\mathrm{E}_P(Z,N)$	$-2.183,\ -2.227$	$-1.994,\ -2.639$	$-2.555,\ -3.339$
HFB+PNAMP(2D)	$\mathrm{E}_P(Z,N)$	$-3.604,\ -5.009$	$-2.484,\ -2.837$	$-2.884,\ -5.709$
HFB+AMP(1D)	$\mathrm{E}_P(Z,N)$	$-1.274,\ -1.977$	$-1.751,\ -1.686$	$-0.151,\ -3.165$
HFB+AMP(2D)	$\mathrm{E}_P(Z,N))$	$-1.723,\ -2.989$	$-3.321,\ -4.073$	$-2.881,\ -5.466$
VAP+PNAMP(1D)	$\mathrm{E}_P(Z,N)$	$-4.756,\ -5.396$	$-4.848,\ -4.871$	$-4.404,\ -5.509$
VAP+PNAMP(2D)	$\mathrm{E}_P(Z,N)$	$-4.888,\ -5.613$	$-4.144,\ -3.942$	$-4.787,\ -6.939$

Energy convergence of the ground state

Approach	$^{54}\mathrm{Cr}$ Energy (MeV)	$^{52}\mathrm{Ti}$ Energy (MeV)
HFB	-470.097	-448.234
PN_VAP	-473.066 (-2.97)	-450.534 (-2.30)
+AMP (I=0)	-475.805 (-2.74)	-453.180 (-2.65)
+beta_fluc	-476.636 (-0.83)	-454.136 (-0.96)
+pair_fluc	-476.865 (-0.23)	-454.275 (-0.14)

Conclusions and outlook

- **Symmetry Conserving Configuration Mixing calculations provide a general and, at the same time, detailed description of atomic nuclei.**

- **Pairing fluctuations play a fundamental role in the description of excited states.**

- **The small collectivity of the pairing correlations makes necessary the PN-VAP approach for the configuration mixing calculations.**

- **At least for the nuclei considered in this work the pairing vibrations are strongly damped by the deformation degree of freedom.**

- **The ground state energy seems to have converged with the included terms (the GCM contributions for additional degrees is negligible).**

- **The breaking of the time reversal symmetry as well as two-quasiparticle admixtures will improve the quality of the calculations.**

- **A fine tuning of the Gogny interaction for SCCM calculations would be desirable**