On the impact of pairing fluctuation on nuclear spectra

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

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On the ocassion of the 70th Birthday of Peter Ring, Primosten

Outline of the talk (1)

1.- Theory

A.- Mean Field based approaches

- The Hartree-Fock-Bogoliubov 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 (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 nucleus .
(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)

MFA: The Hartree-Fock-Bogoliubov Theory

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 GCM

In this case the the Ansatz for the AMPGCM is

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

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

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

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

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 $\hat{Q}$.

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.,

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

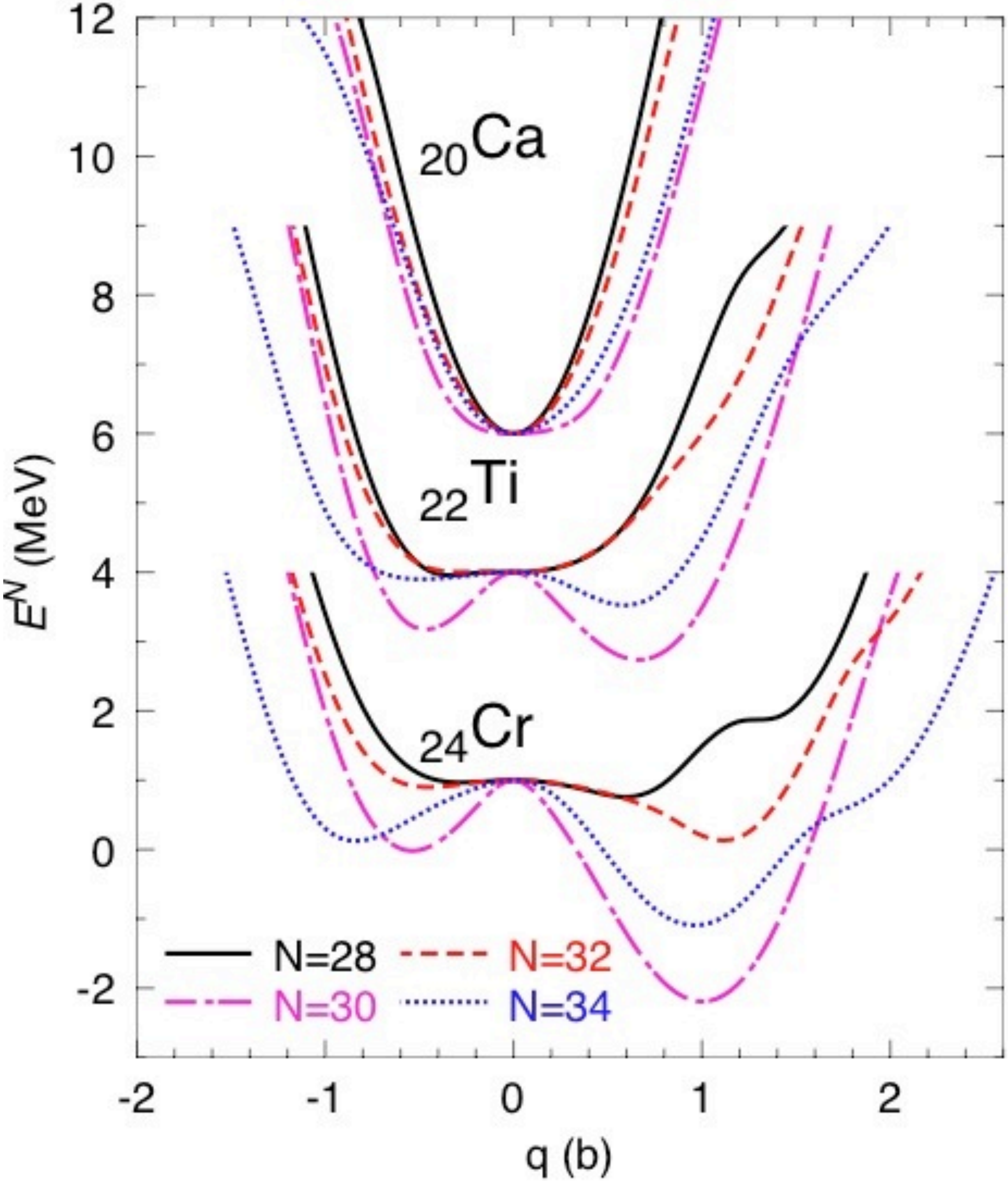
Details of the calculations

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.

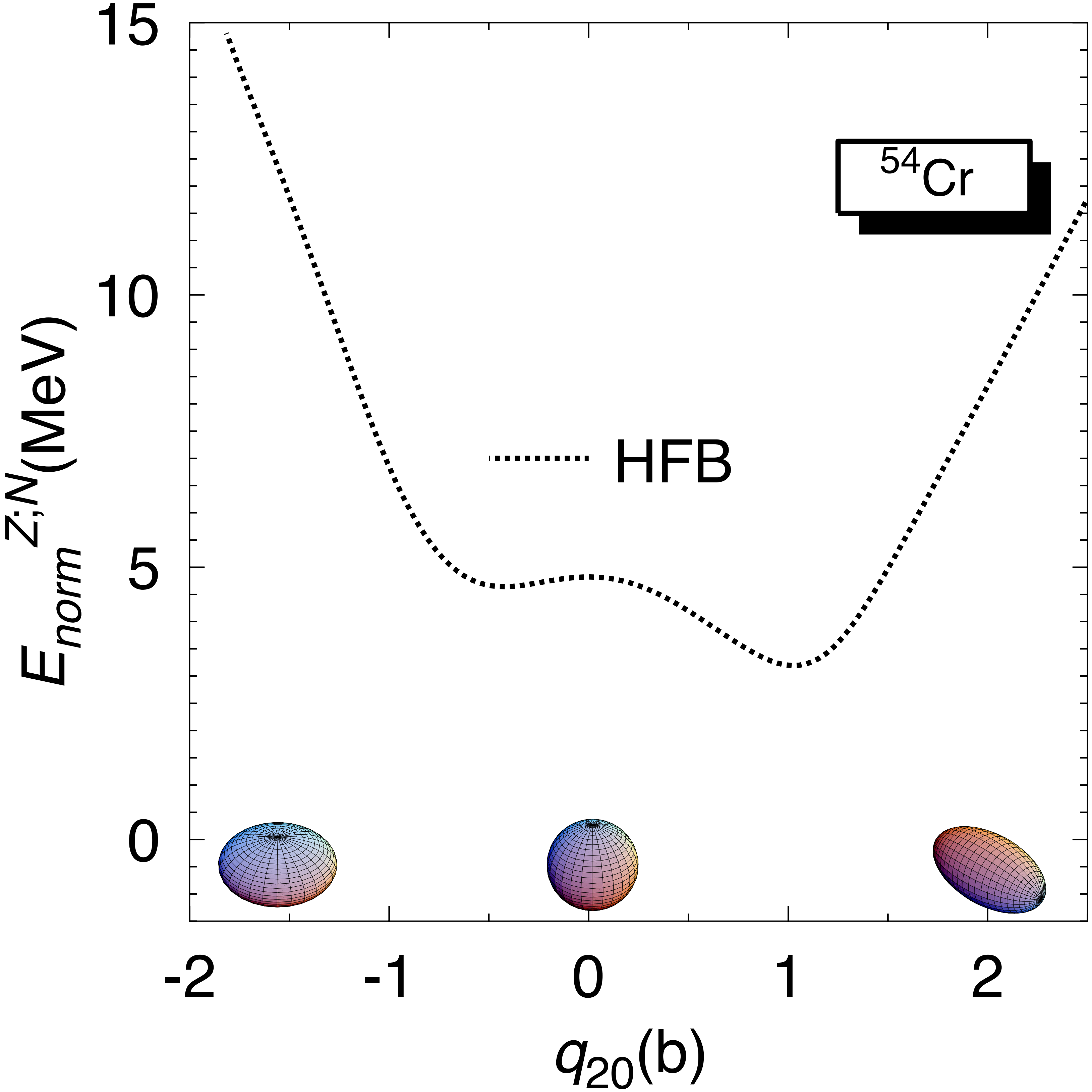
Configuration Space.- We take into account a large number of major harmonic oscillator shells.

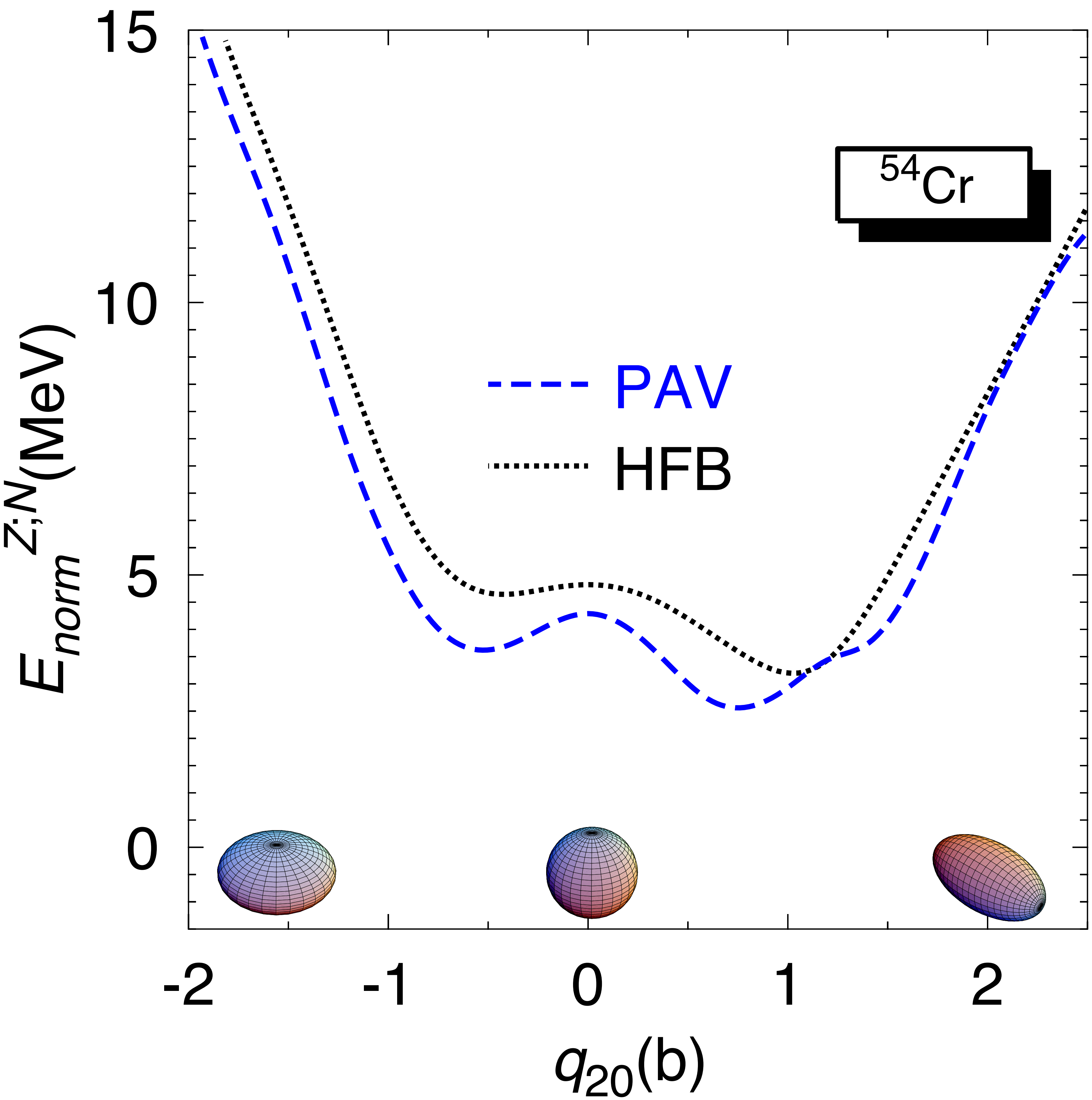
Effective charges.- NO need of effective charges in the calculations of electromagnetic properties.

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



$_{20}$Ca
$_{22}$Ti
$_{24}$Cr
N=28
N=32
N=30
N=34
E^N (MeV)
q (b)


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


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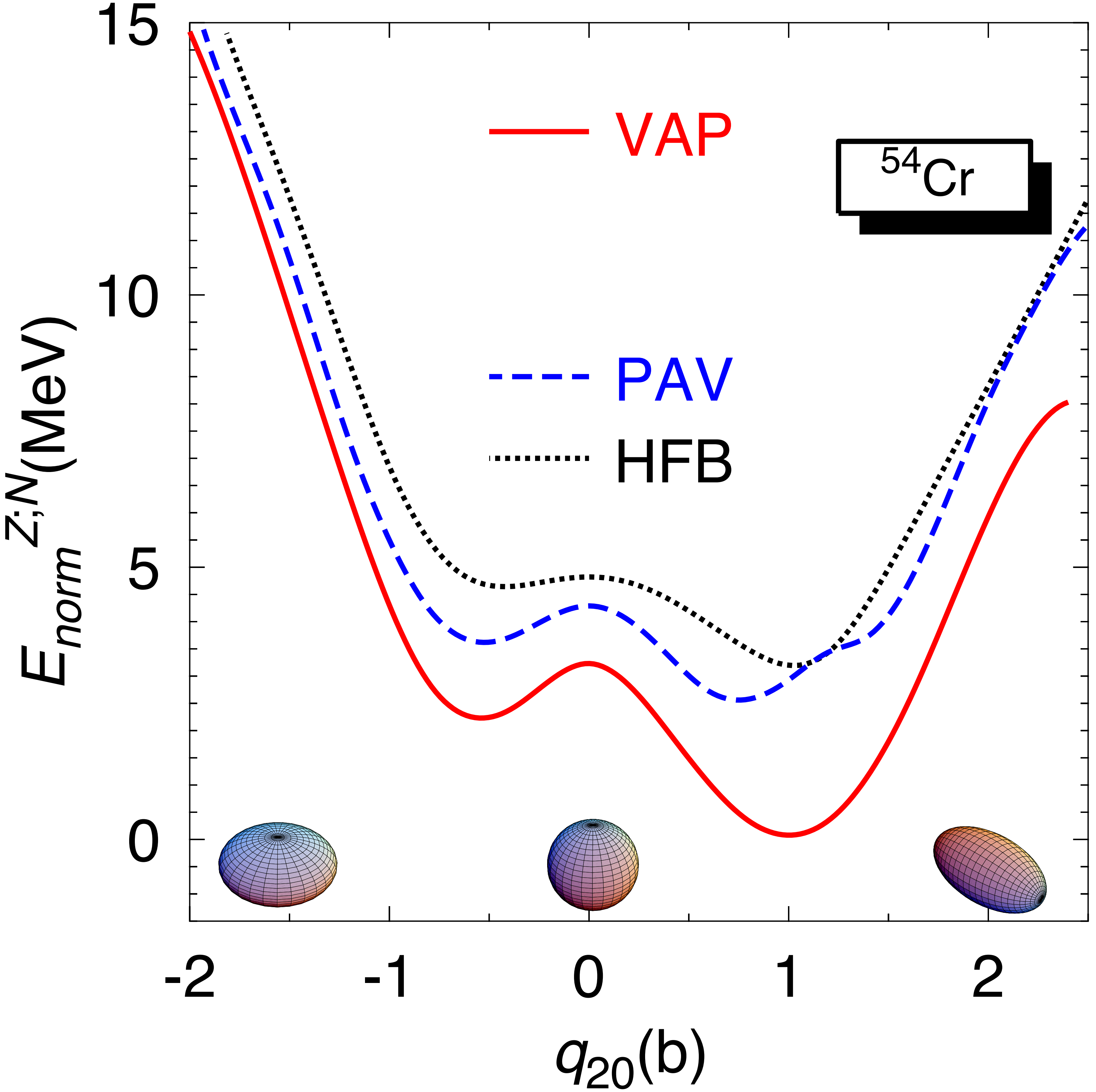
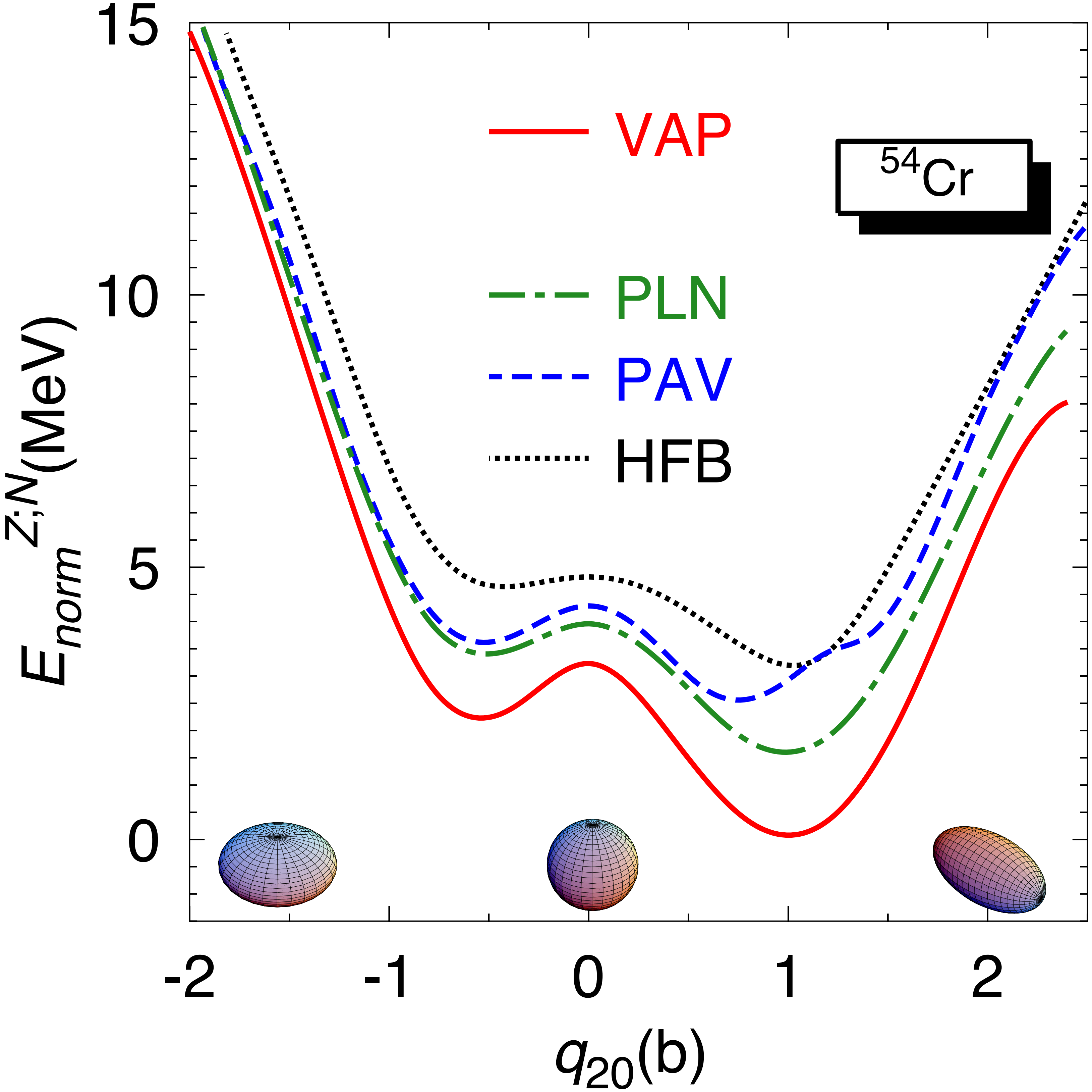
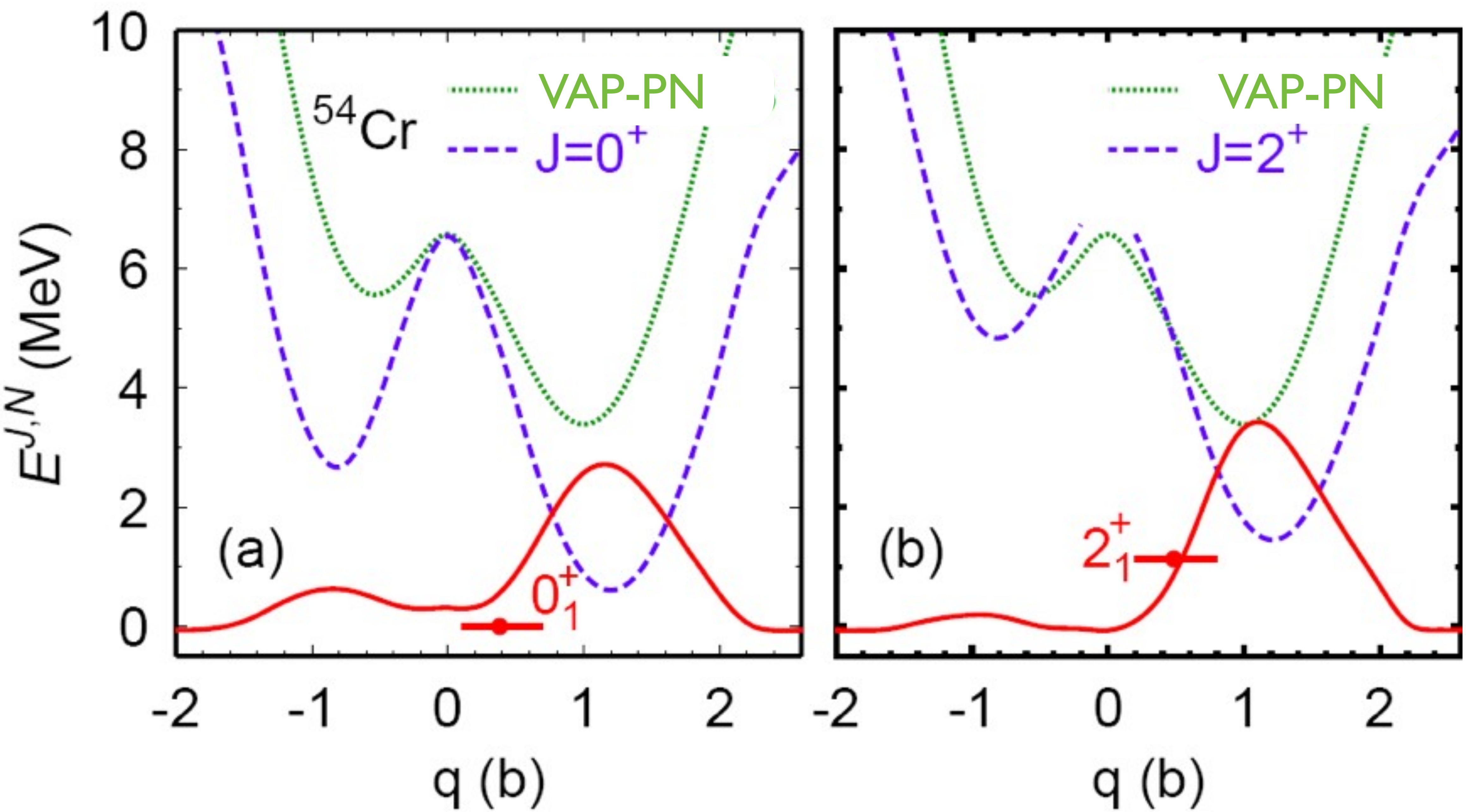
0
-2
-1
0
1
2
$E_{norm}^{Z;N}$(MeV)
q_{20}(b)
^{54}Cr
PAV
HFB

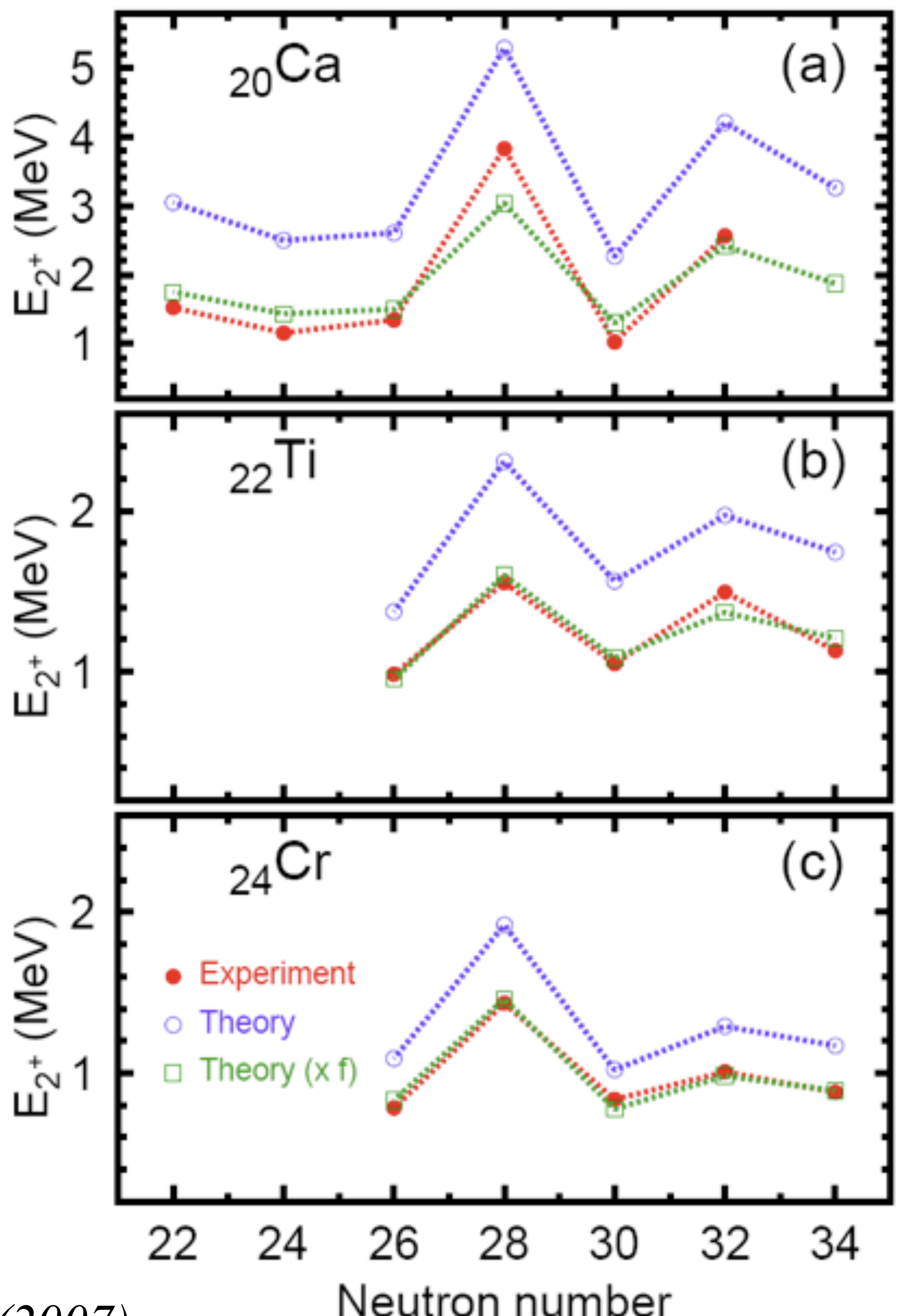

15
10
5
0
-2
-1
0
1
2
$E_{norm}^{Z;N}$(MeV)
q_{20}(b)
VAP
PAV
HFB
^{54}Cr



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

Examples of the angular momentum PEC and configuration mixing solutions



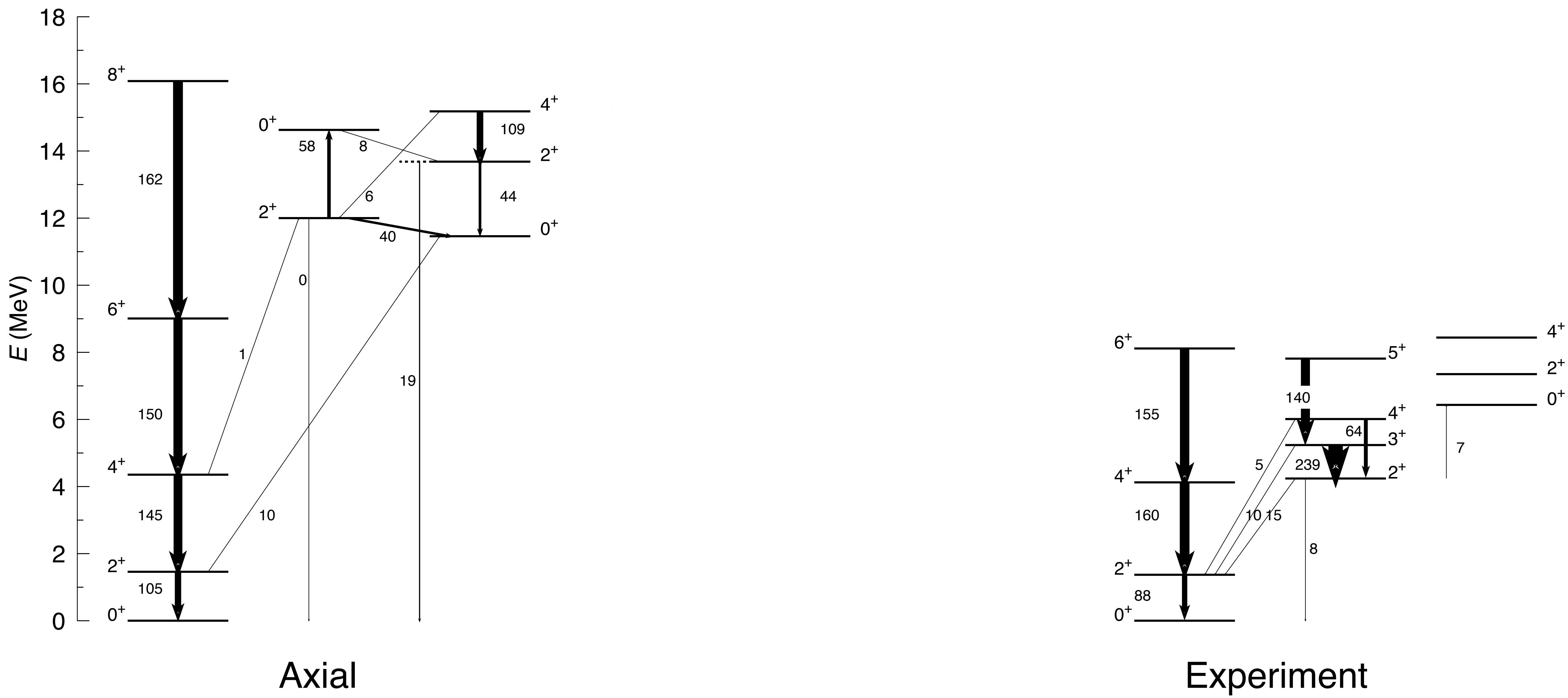


T.R. Rodriguez and J.L.E.
Phys. Rev. Lett. 99, 062501 (2007)

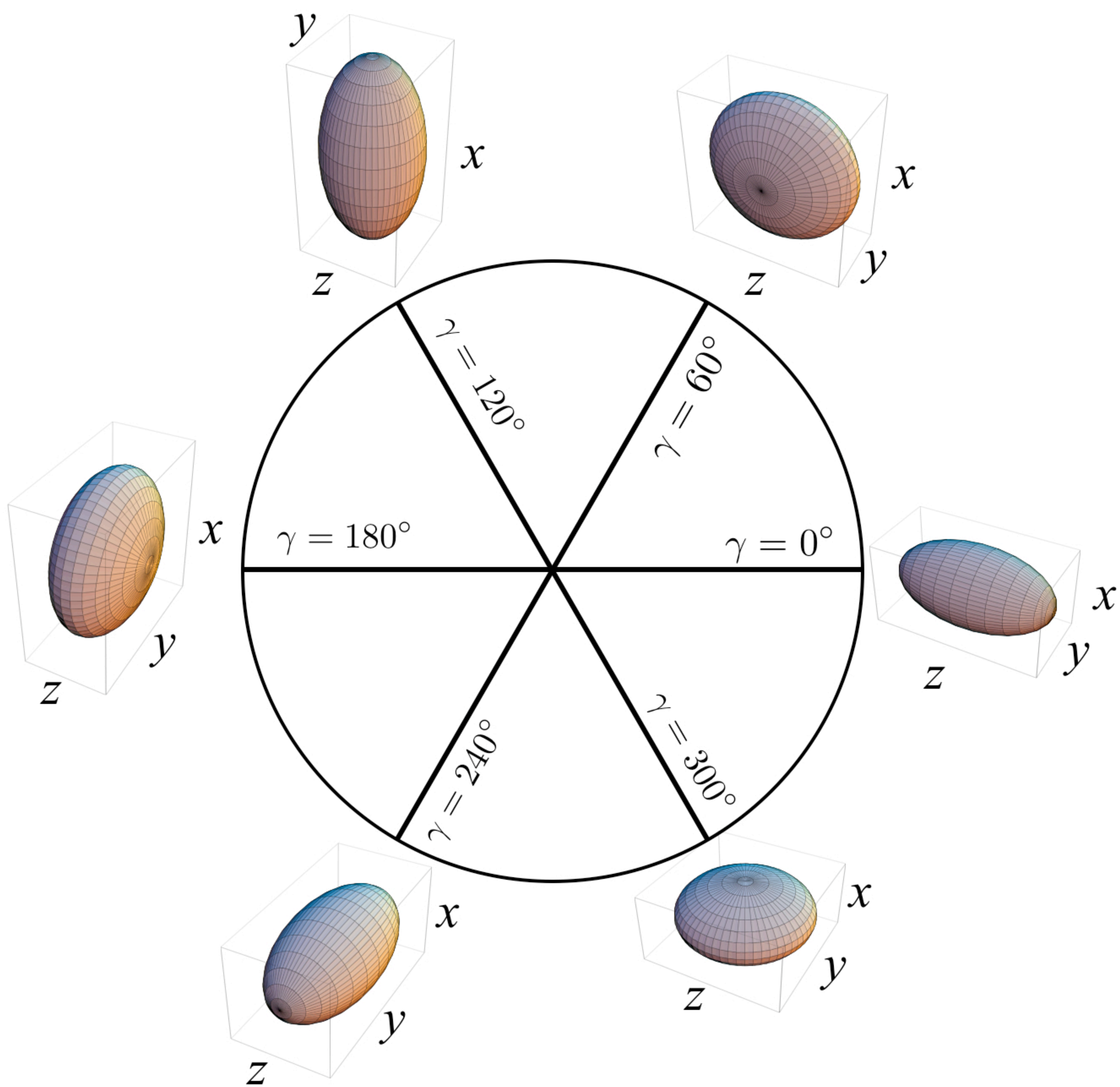
Particle number
and
Triaxial Angular Momentum Projection

The nucleus ^{24}Mg

^{24}Mg



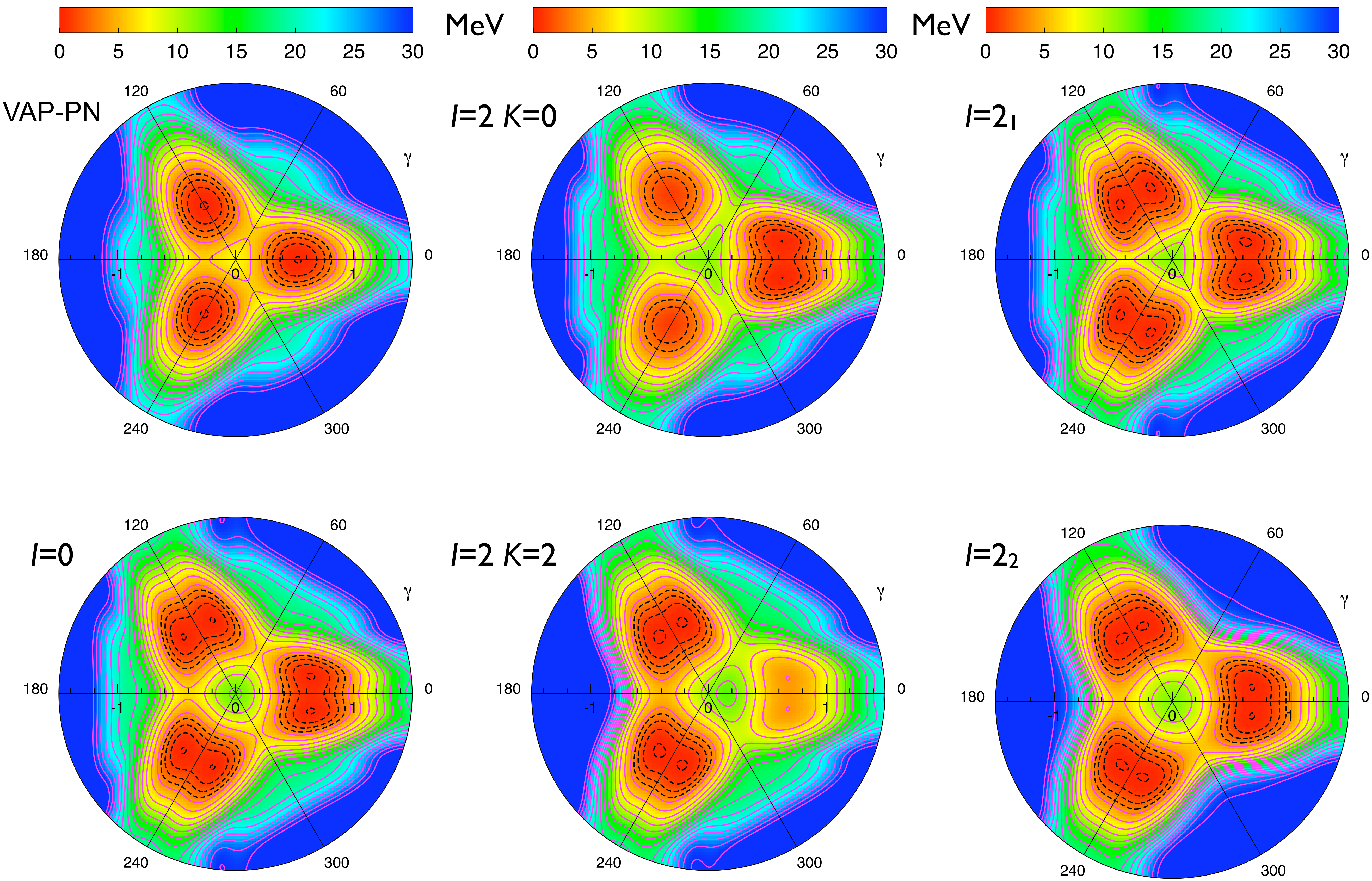
18
16
14
12
10
8
6
4
2
0
E (MeV)
8+
6+
4+
2+
0+
162
150
145
105
1
10
0+
2+
58
8
6
40
0
19
4+
2+
0+
109
44
Axial
6+
4+
2+
0+
155
160
88
5+
4+
3+
2+
140
64
239
5
10
15
8
4+
2+
0+
7
Experiment



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

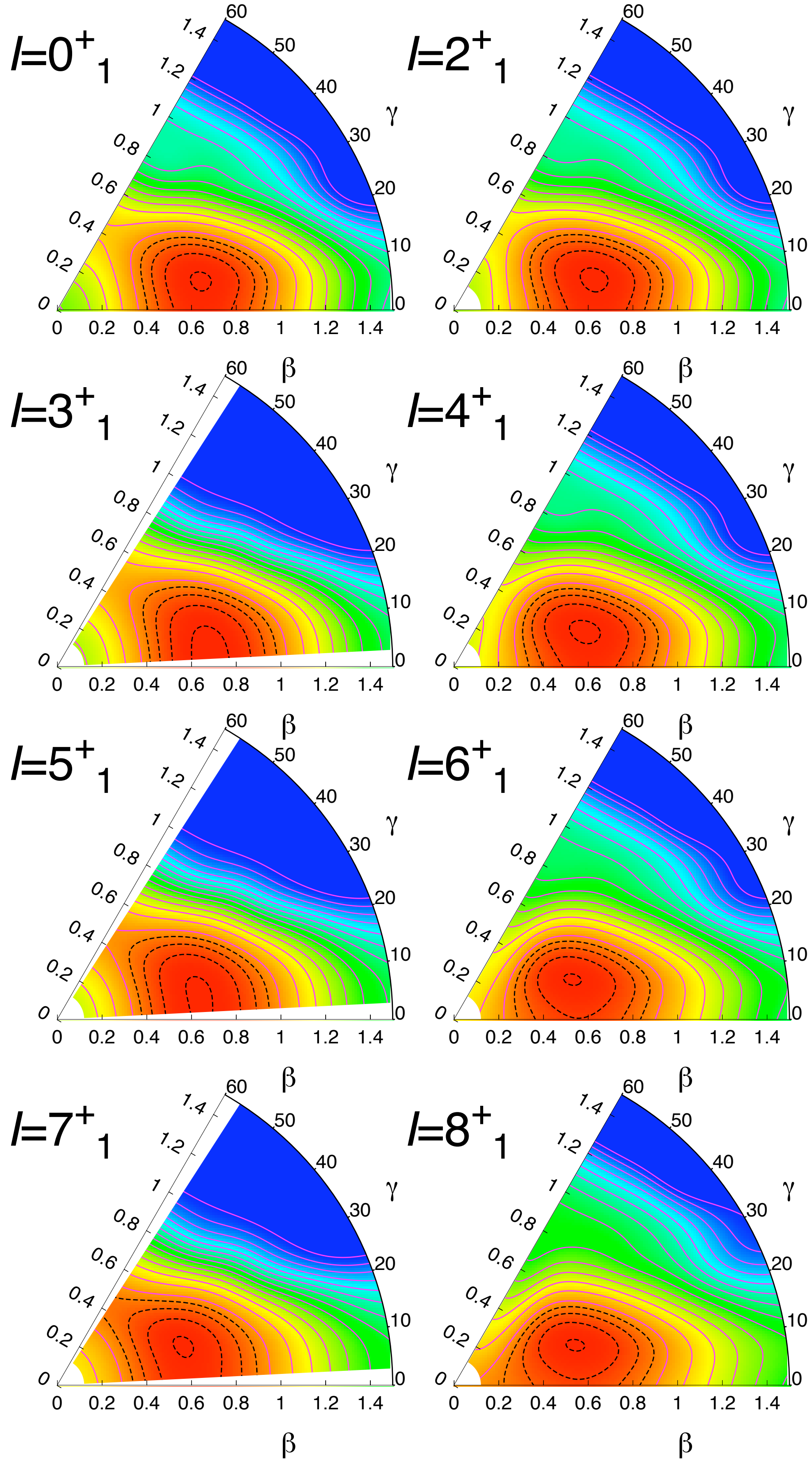
Energy contour plots in the (β,γ) plane

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

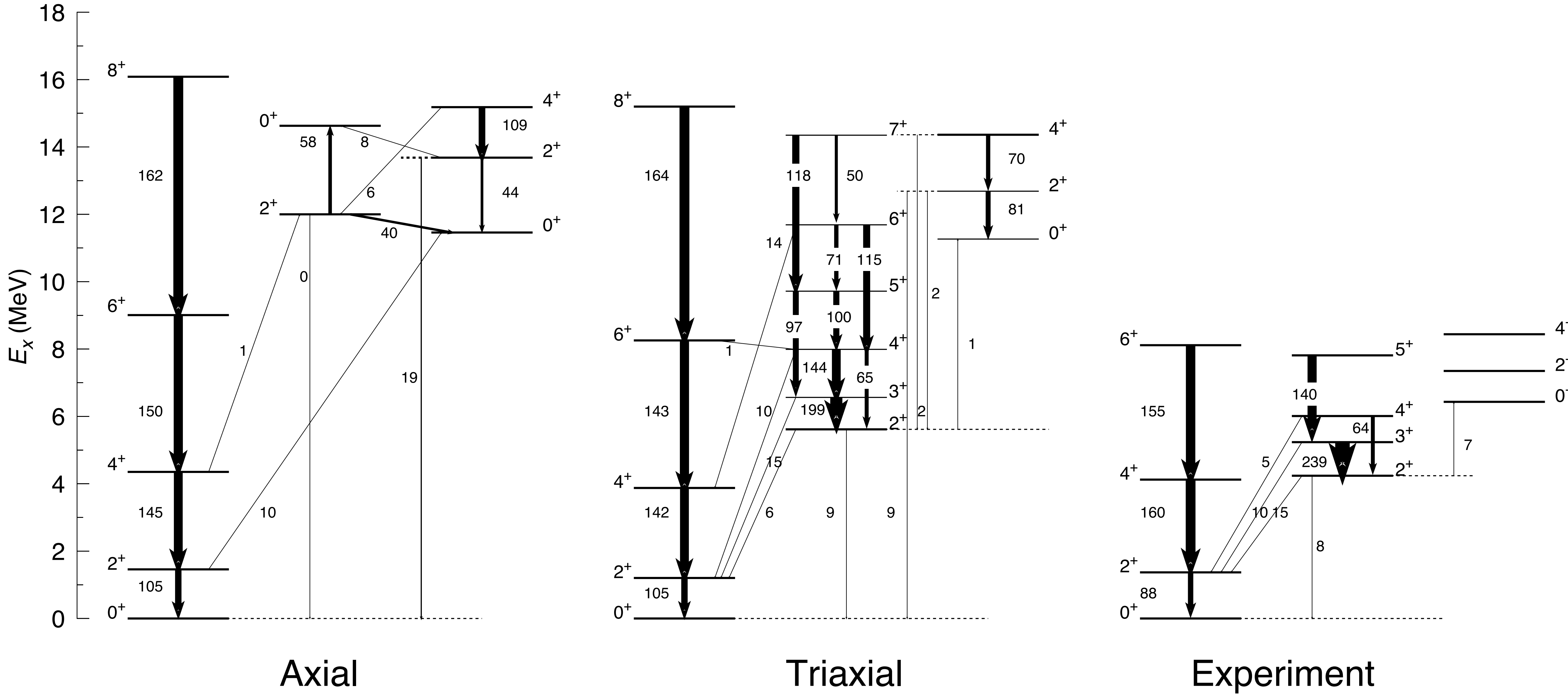


$$|IMK;NZ;\beta\gamma\rangle = P^I_{MK} P^N P^Z |\Phi(\beta,\gamma)\rangle$$

Projected energies in the (β,γ) plane

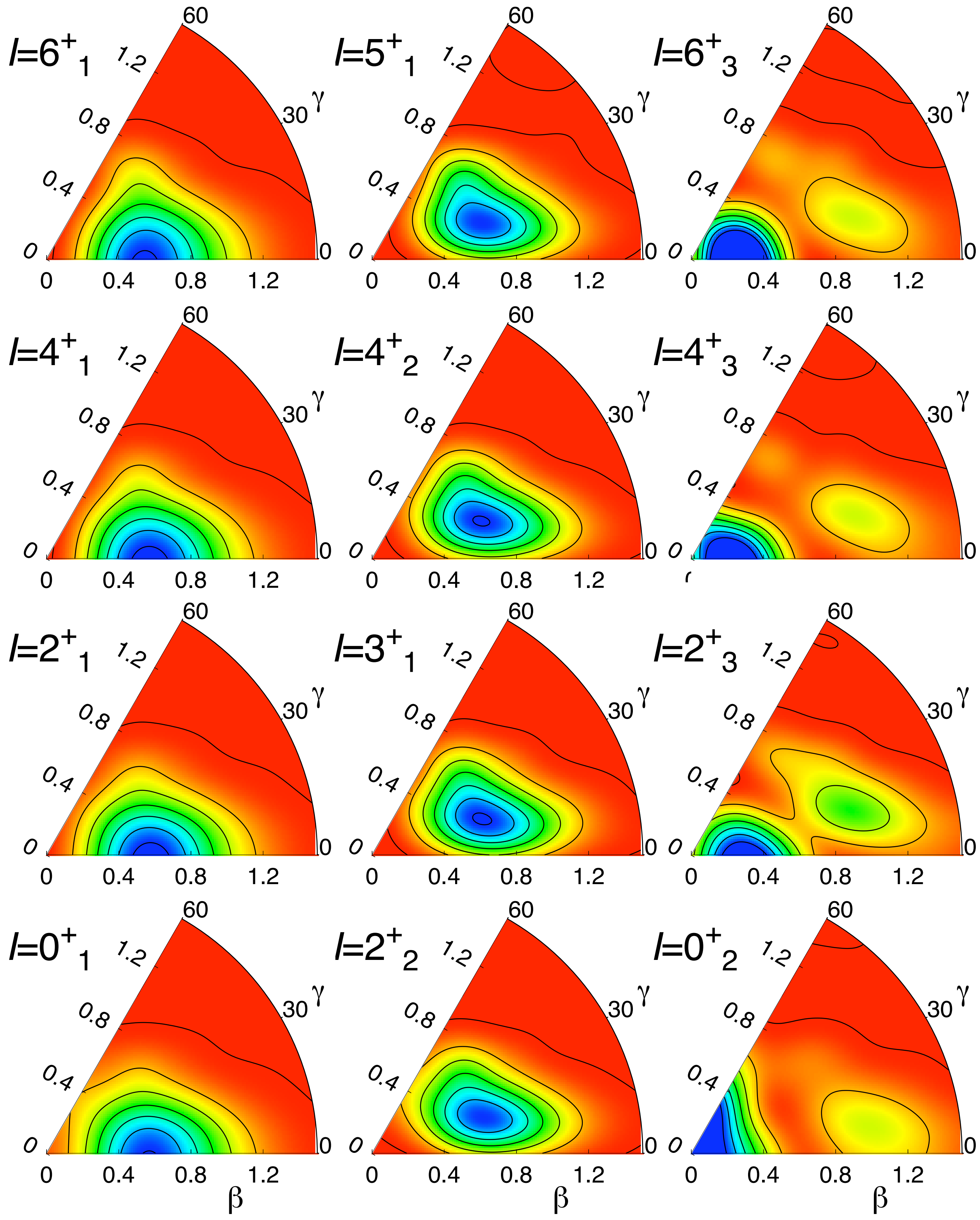


^{24}Mg



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

Collective wave functions in the (β,γ) plane



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

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

and the Lagrange multipliers determined by the conditions:

$$\langle\phi|\hat{Q}|\phi\rangle = q_2, \qquad \langle\phi|(\Delta\hat{N})^2|\phi\rangle^{1/2} = \delta.$$

Variational Equations (II)

In the second step we perform the configuration mixing calculations

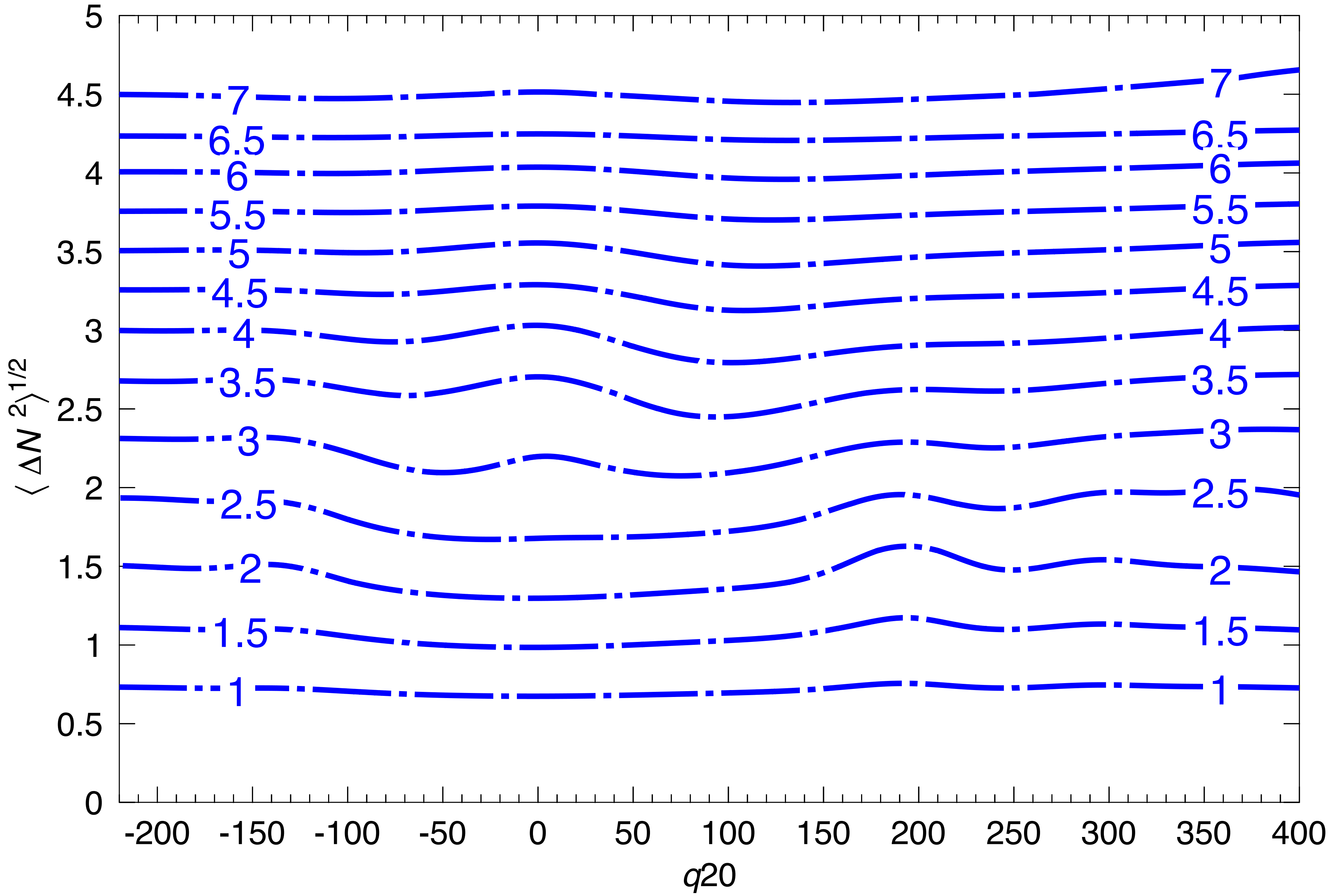
$$|\Psi^{N,I,\sigma}\rangle = \int f^{N,I,\sigma}(q,\delta)\ \hat{P}^I \hat{P}^N \hat{P}^Z\ |\phi(q,\delta)\rangle dq d\delta.$$

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 $\langle(\Delta N)^2\rangle^{1/2} \propto \Delta \propto (-E_{PAIRING})^{1/2}$

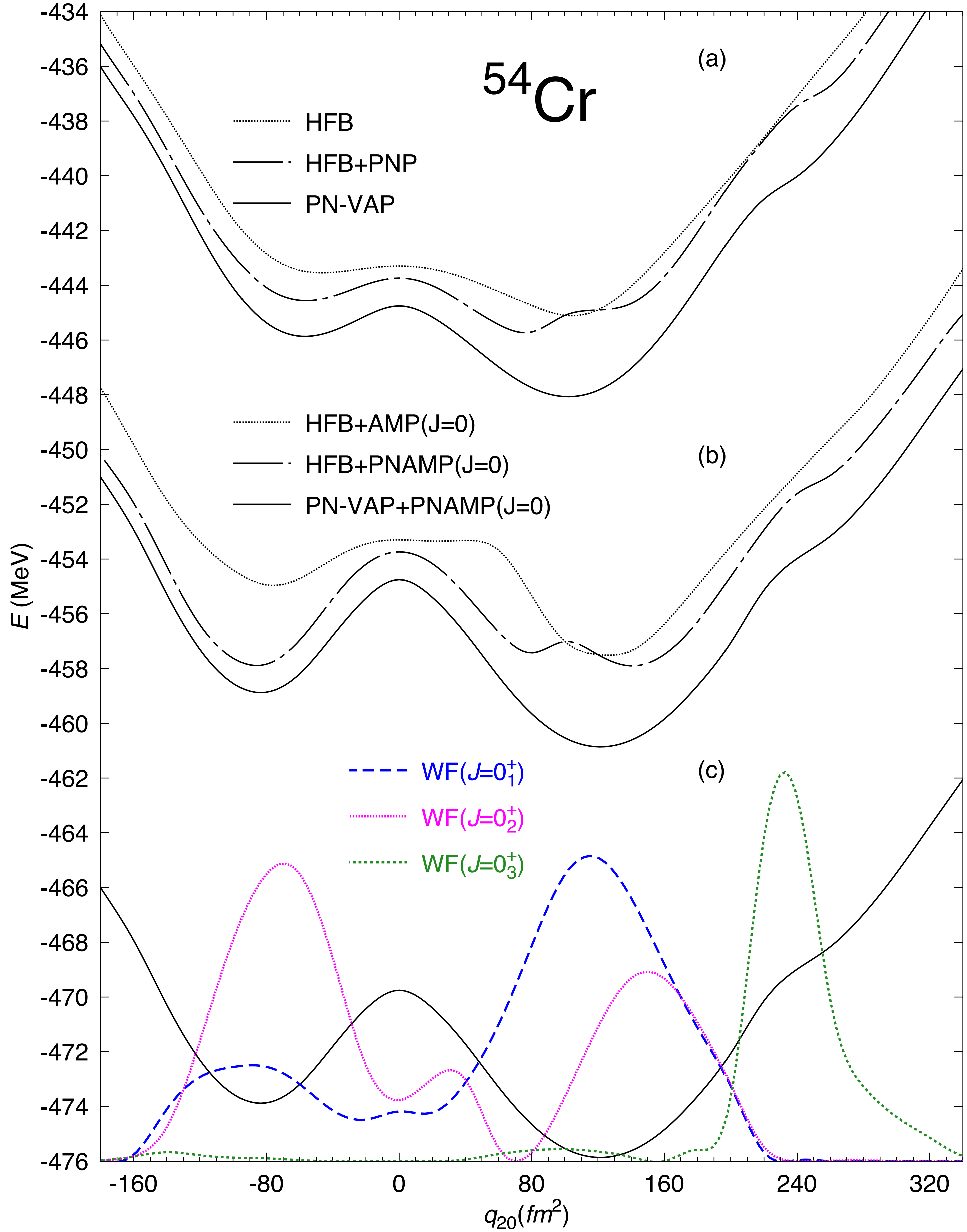


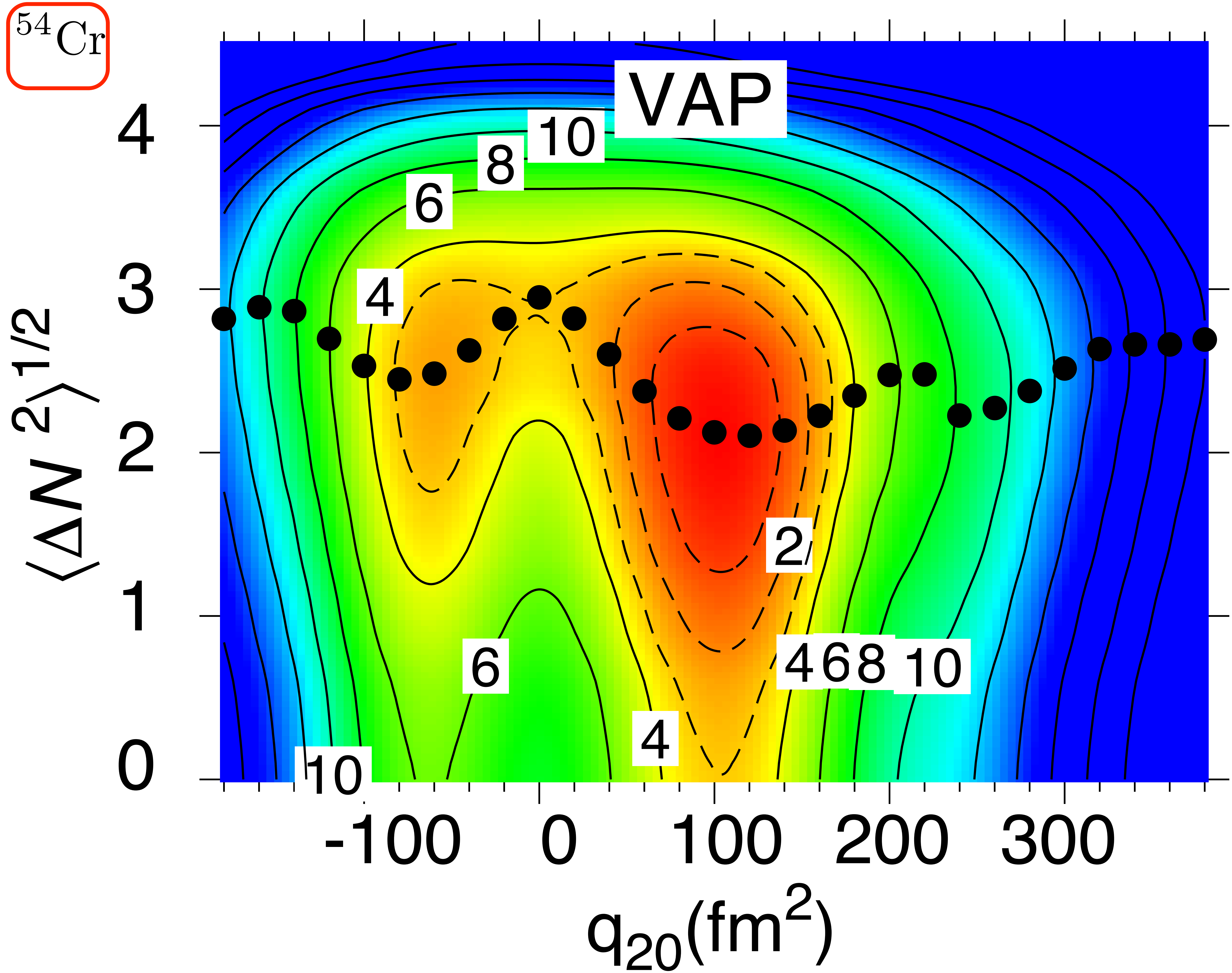
^{54}Cr

Contour curves of the square root of the pairing energies in the plane

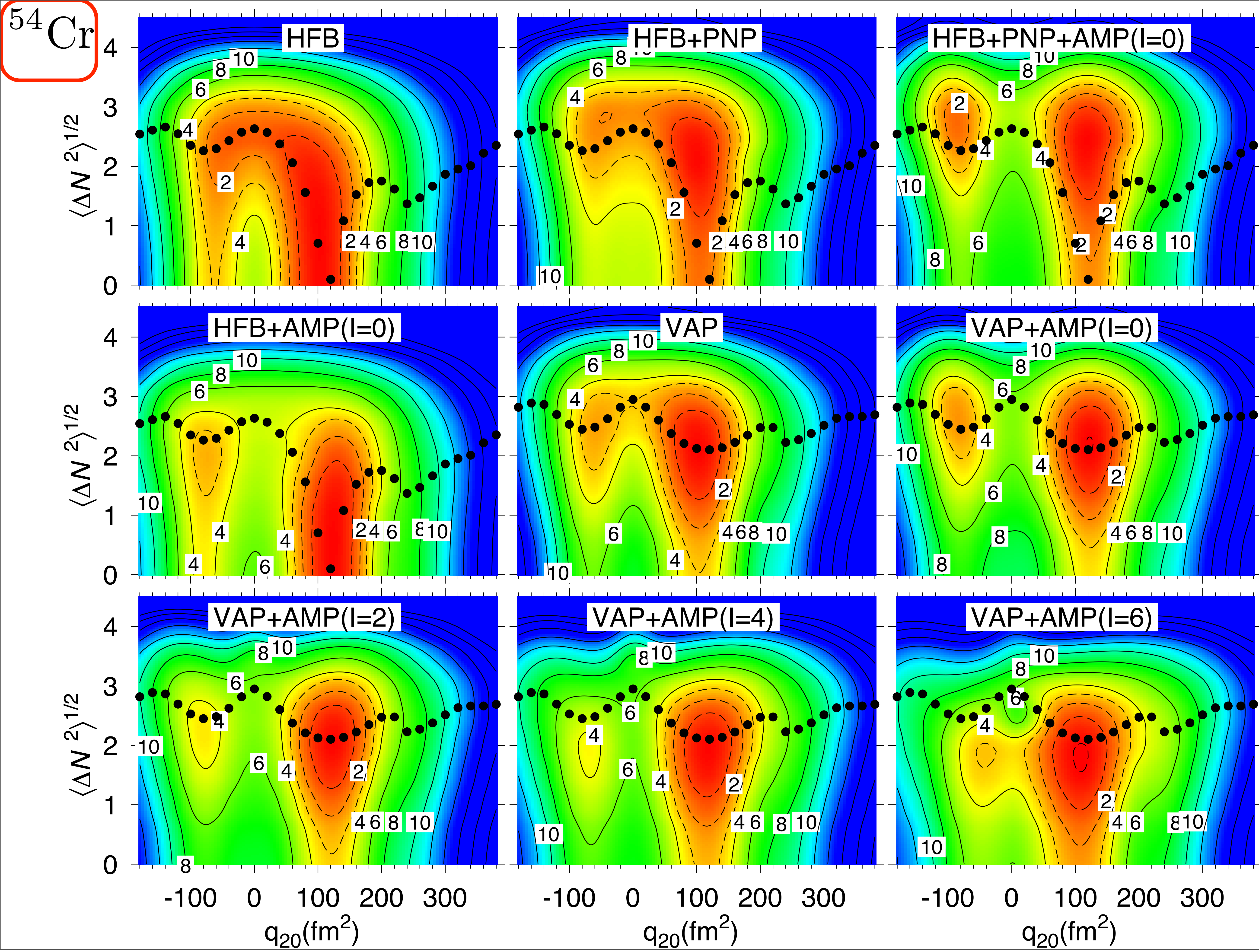
$(q_{20}, \langle(\Delta N)^2\rangle^{1/2})$ with wave functions $P^{I=0}P^Z P^N|\Phi\rangle_{VAP}$

One dimensional calculations

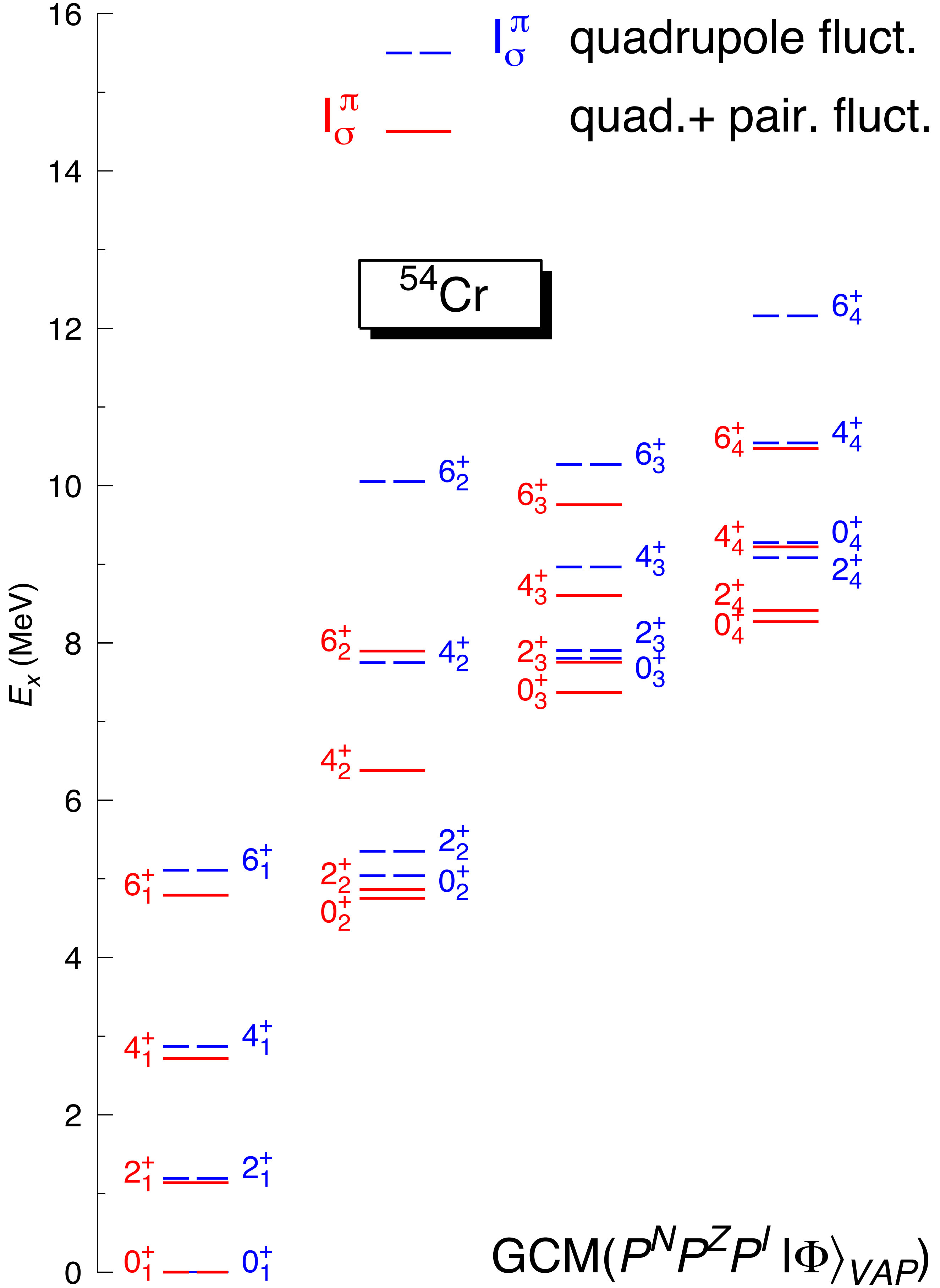




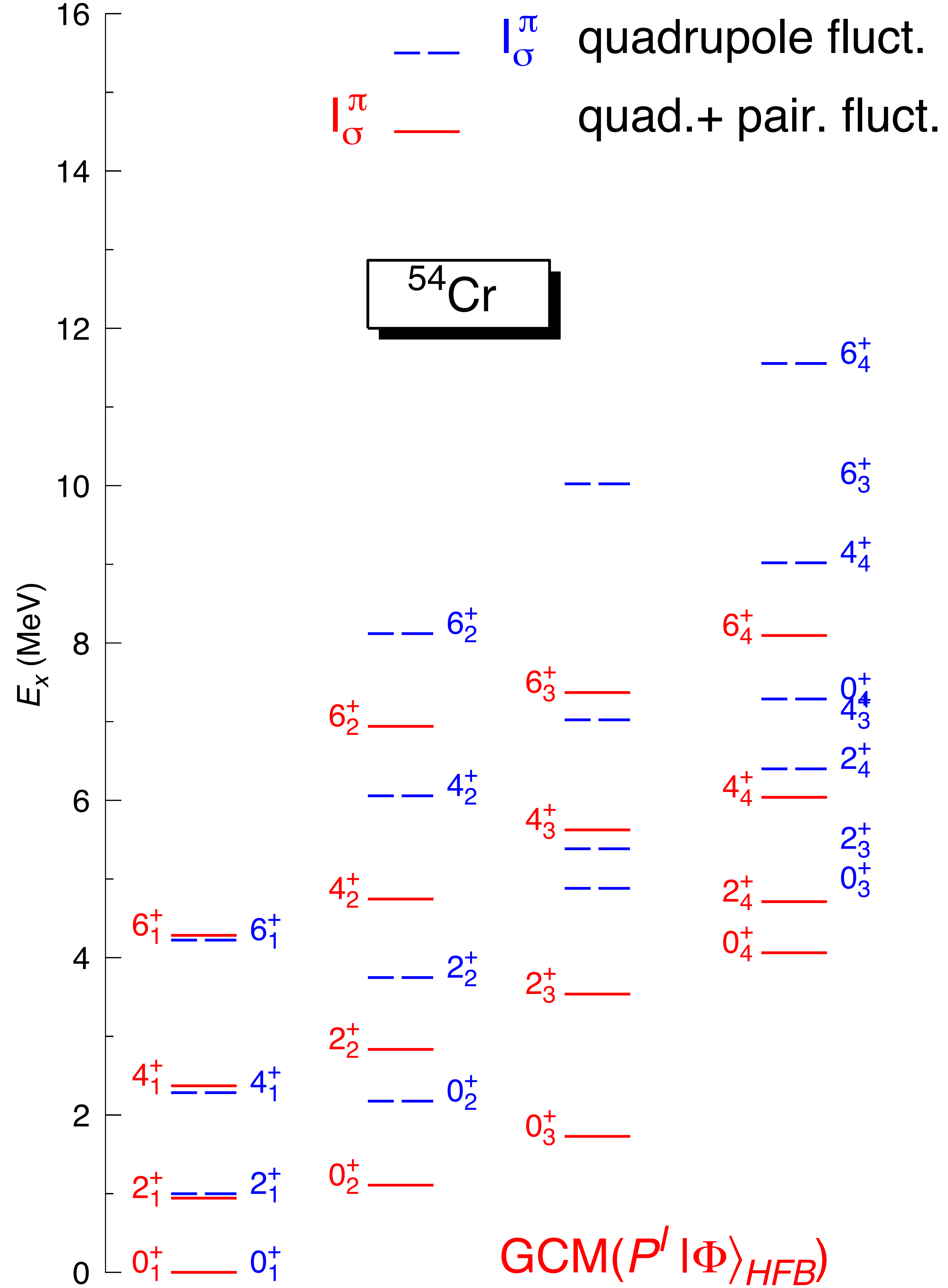
^{54}Cr
VAP
10
8
6
4
2
4 6 8 10
6
4
10
4
3
2
1
0
$\langle \Delta N^2 \rangle^{1/2}$
-100
0
100
200
300
$q_{20}(\mathrm{fm}^2)$

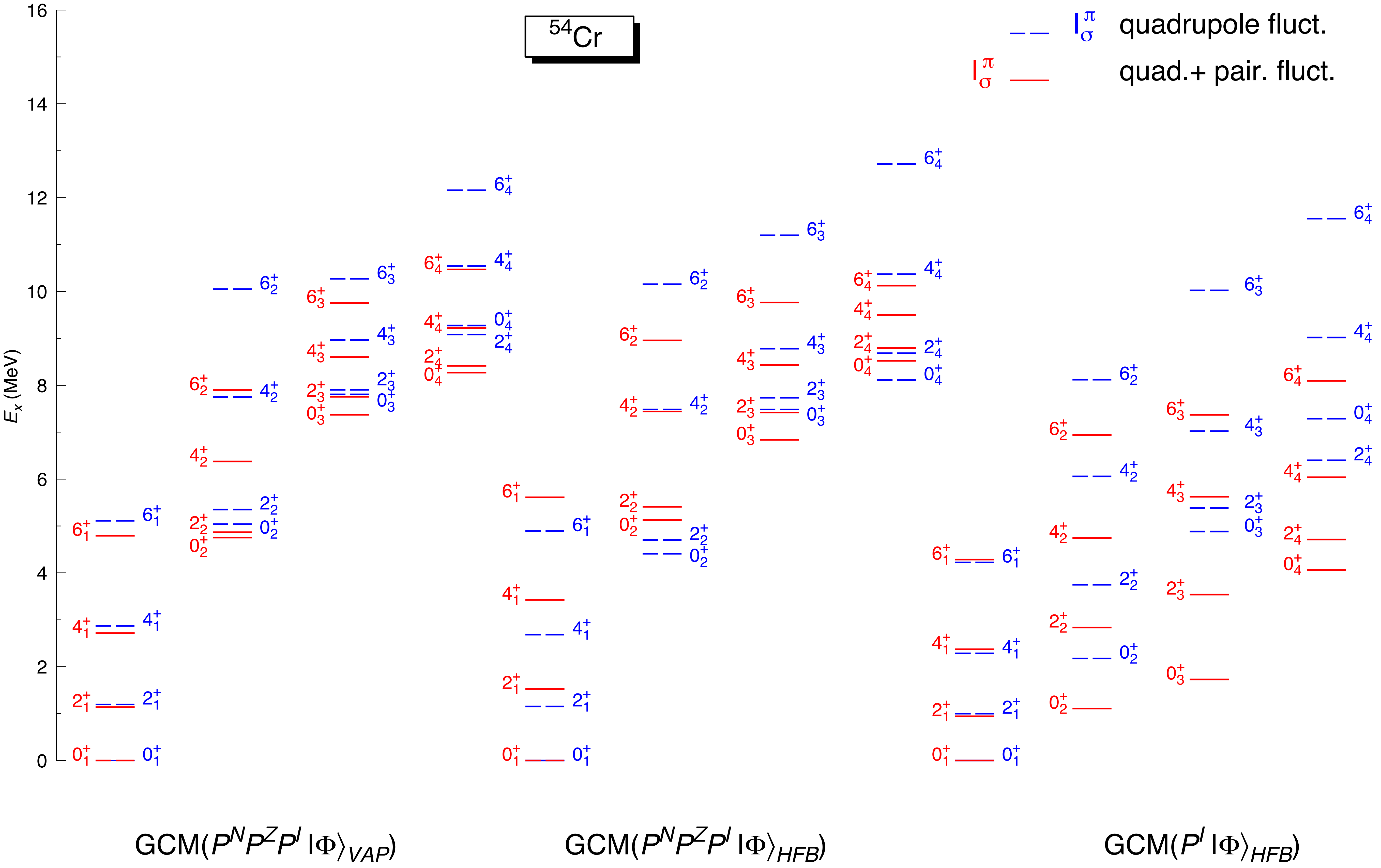


^{54}Cr
HFB
HFB+PNP
HFB+PNP+AMP(I=0)
HFB+AMP(I=0)
VAP
VAP+AMP(I=0)
VAP+AMP(I=2)
VAP+AMP(I=4)
VAP+AMP(I=6)
$\langle \Delta N^2 \rangle^{1/2}$
$q_{20}(fm^2)$



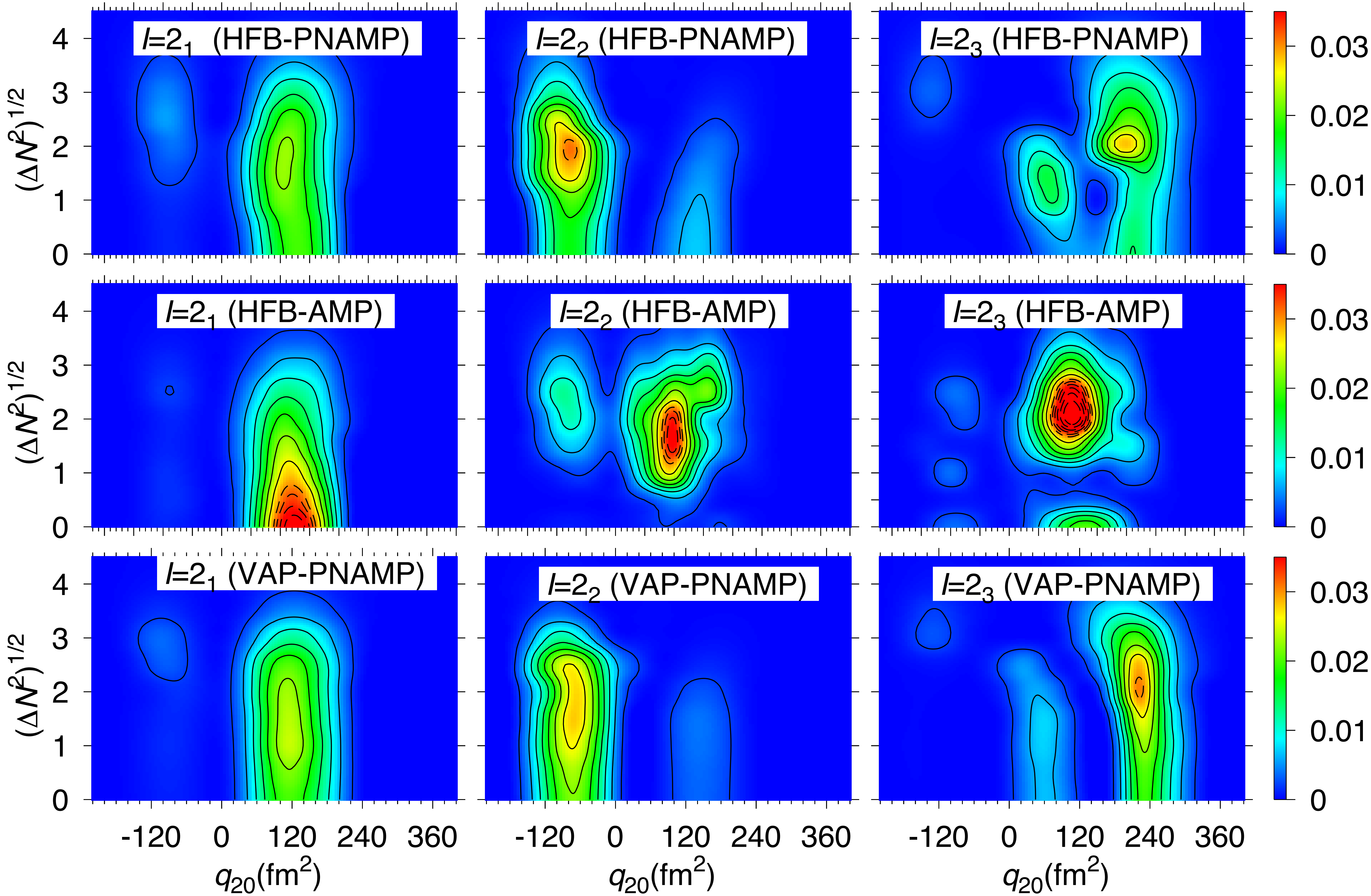
quadrupole fluct.
quad.+ pair. fluct.
54Cr
Ex (MeV)
0
2
4
6
8
10
12
14
16
GCM($P^N P^Z P^I |\Phi\rangle_{VAP}$)


quadrupole fluct.
quad.+ pair. fluct.
54Cr
E_x (MeV)
GCM($P^I |\Phi\rangle_{HFB}$)



^{54}Cr
I^{π}_{σ} quadrupole fluct.
I^{π}_{σ} quad.+ pair. fluct.
E_x (MeV)
0
2
4
6
8
10
12
14
16
GCM($P^N P^Z P^I |\Phi\rangle_{VAP}$)
GCM($P^N P^Z P^I |\Phi\rangle_{HFB}$)
GCM($P^I |\Phi\rangle_{HFB}$)

Wave functions in various approaches

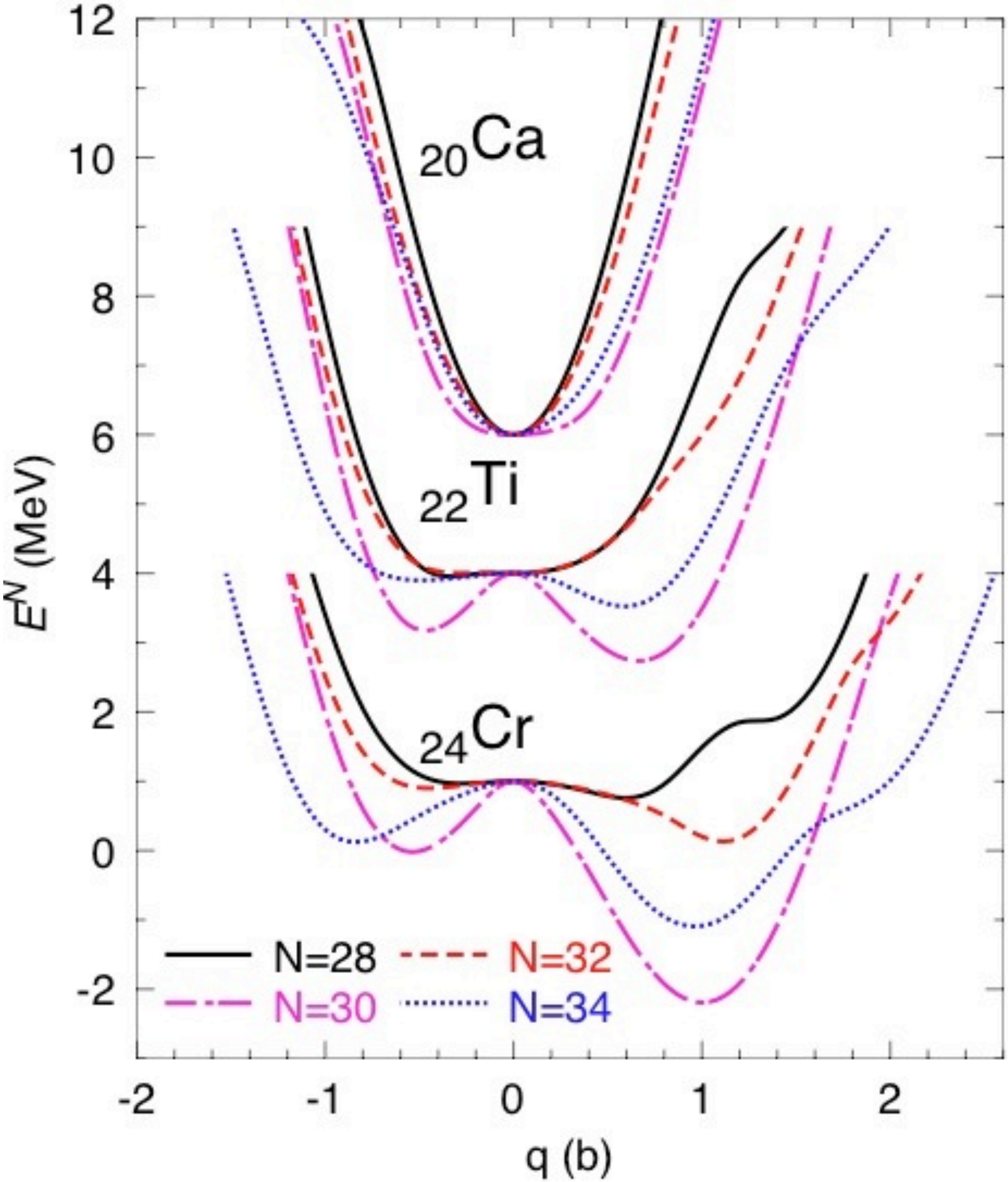


Comparison of the Energy and Quadrupole moments

		2_1^+	2_2^+	2_3^+
HFB+PNAMP	E(2D)	-474.260	-470.457	-468.435
	ΔE(1D-2D)	0.621	0.536	1.166
	Q(2D)	-27.950	13.824	-40.985
	ΔQ(1D-2D)	0.953	0.807	6.21
HFB+AMP	E(2D)	-473.096	-471.417	-470.773
	ΔE(1D-2D)	0.555	1.481	2.551
	Q(2D)	-31.224	-20.381	-26.925
	ΔQ(1D-2D)	1.04	13.615	-0.476
PN-VAP+PNAMP	E(2D)	-475.598	-471.888	-469.372
	ΔE(1D-2D)	0.191	0.637	0.503
	Q(2D)	-29.556	15.299	-42.722
	ΔQ(1D-2D)	-0.114	1.546	-6.841

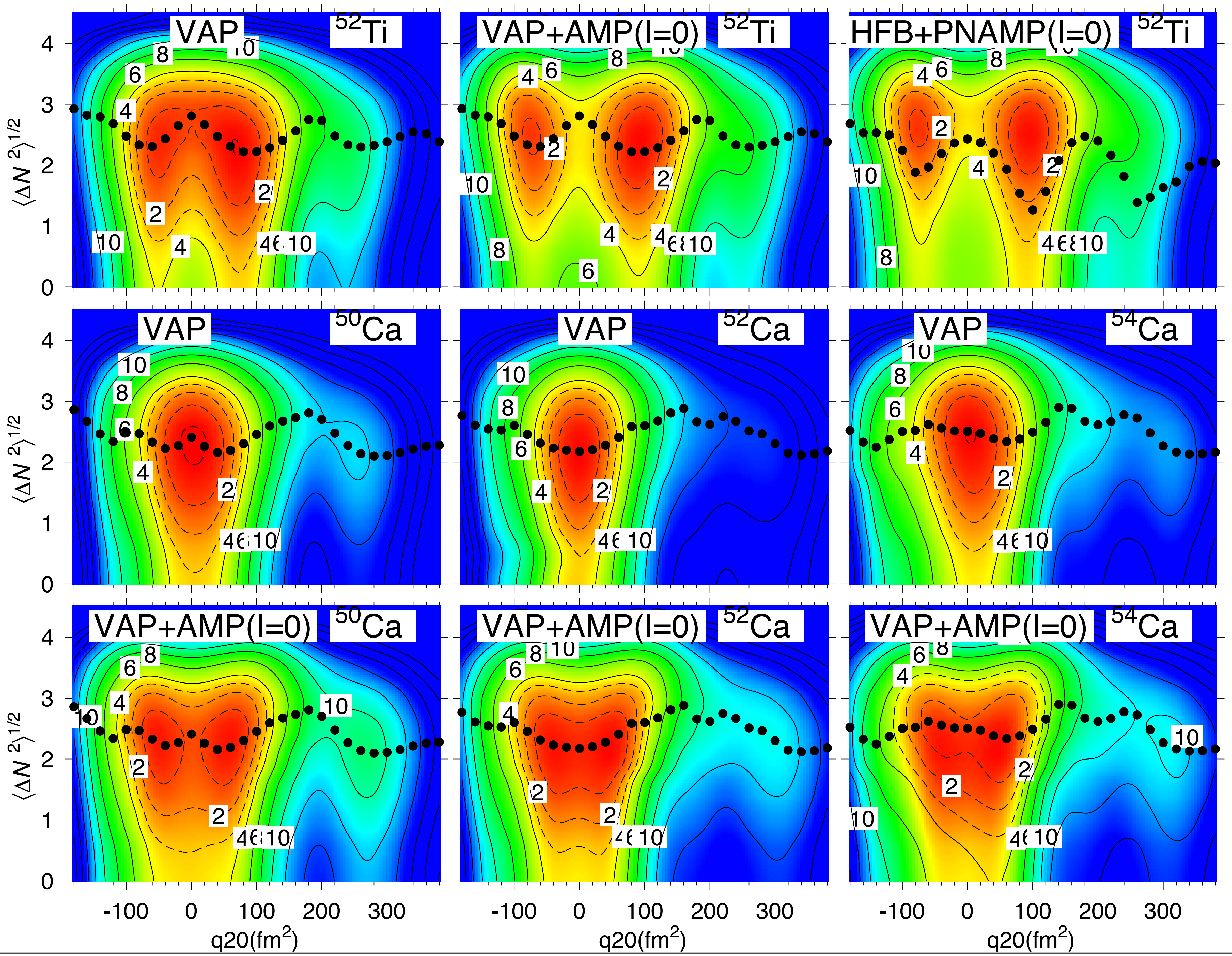
Pairing energies of the lowest 0^+ states

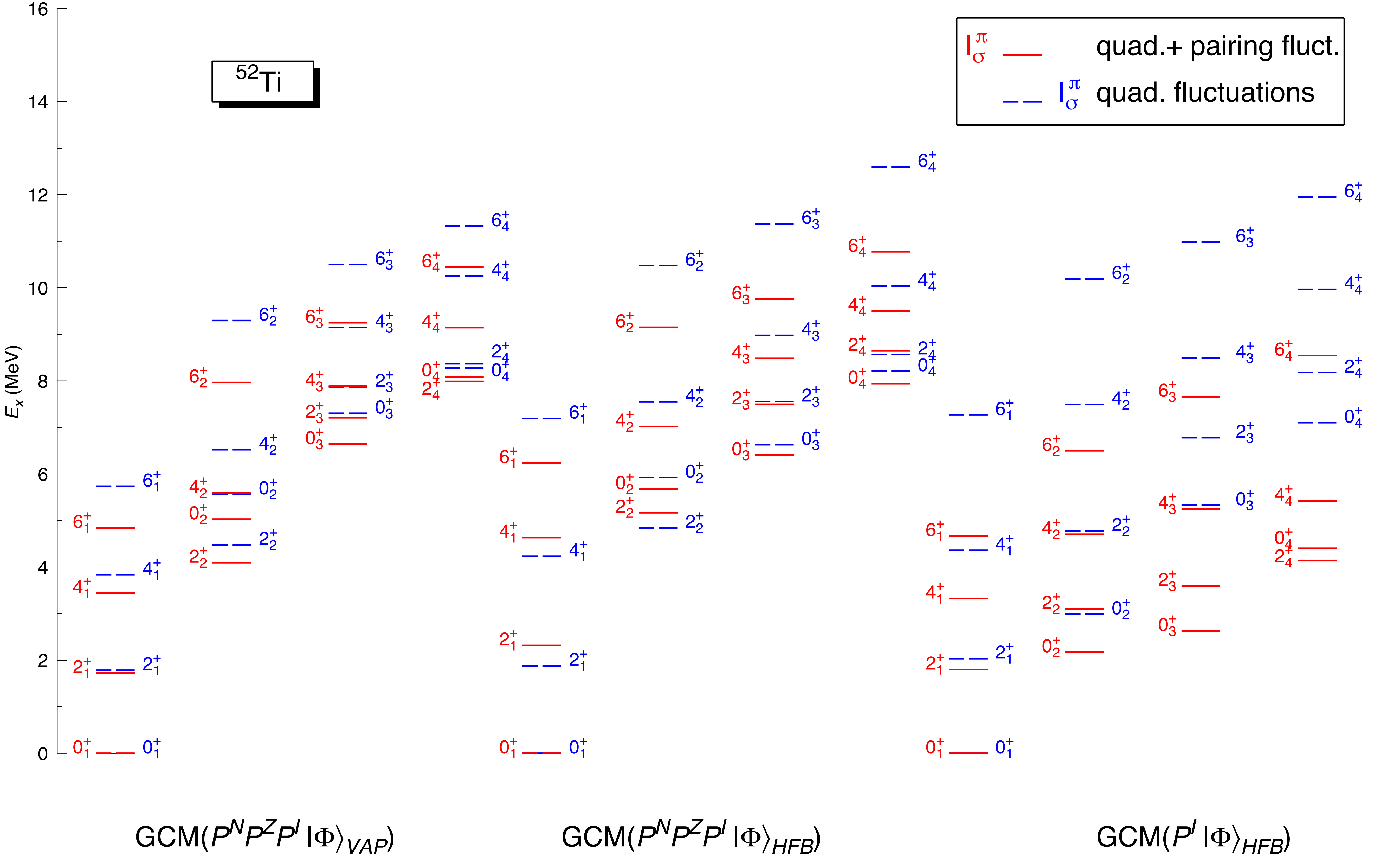
	0_1^+	0_2^+	0_3^+
	$E_P(Z)$, $E_P(N)$	$E_P(Z)$, $E_P(N)$	$E_P(Z)$, $E_P(N)$
HFB+PNAMP (1D)	-2.183, -2.227	-1.994, -2.639	-2.555, -3.339
HFB+PNAMP(2D)	-3.604, -5.009	-2.484, -2.837	-2.884, -5.709
HFB+AMP(1D)	-1.274, -1.977	-1.751, -1.686	-0.151, -3.165
HFB+AMP(2D)	-1.723, -2.989	-3.321, -4.073	-2.881,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



12
10
8
6
4
2
0
-2
E^N (MeV)
$_{20}$Ca
$_{22}$Ti
$_{24}$Cr
N=28
N=32
N=30
N=34
-2
-1
0
1
2
q (b)

Two dimensional energy contour plots in various approaches





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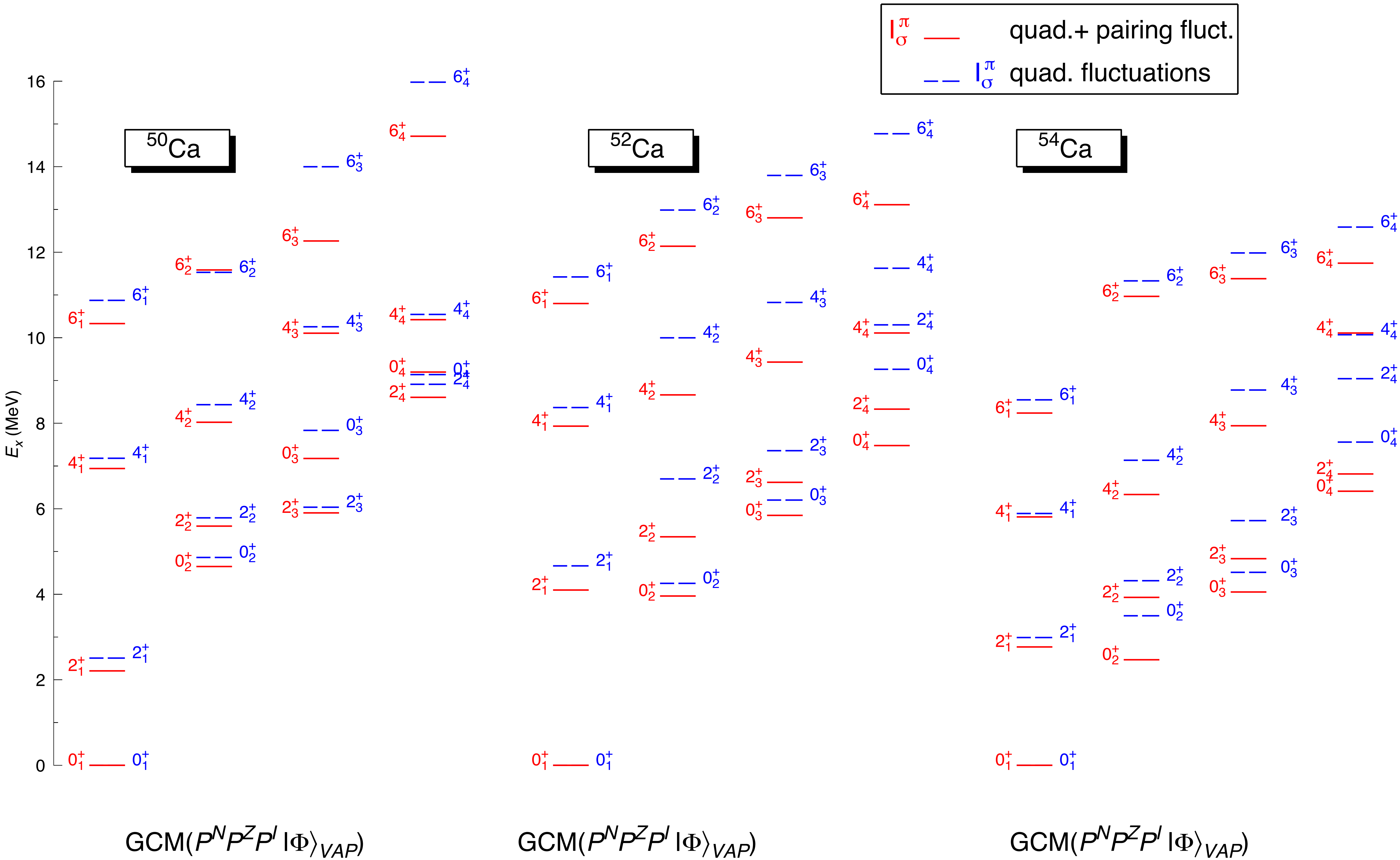

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Energy convergence of the ground state

Approach	^{54}Cr Energy (MeV)	^{52}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

- **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 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).**