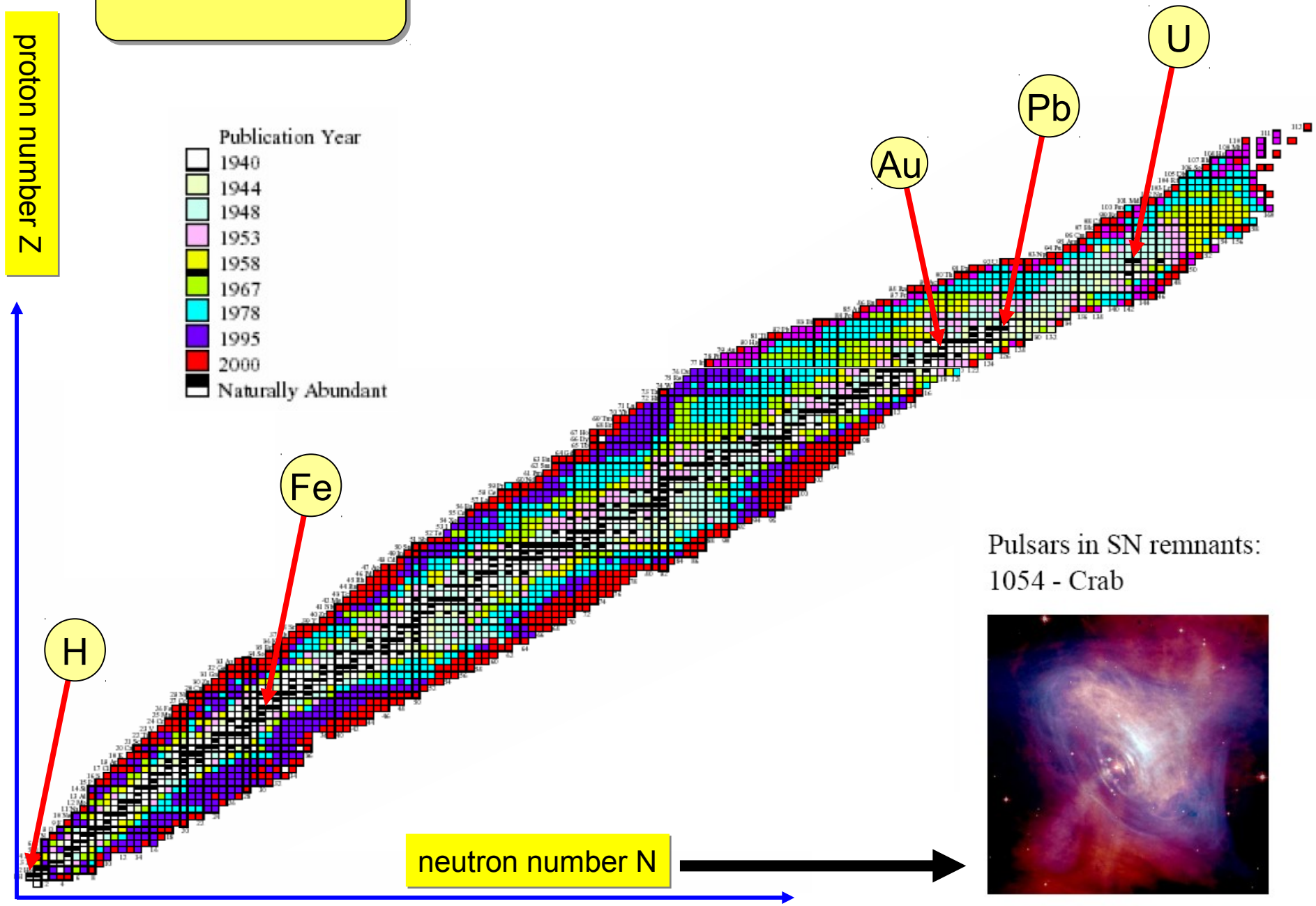
Covariant Density Functional Theory Nuclear Collective Motion

Georgios Lalazissis
Aristotle University of Thessaloniki

Motivation:



Pulsars in SN remnants:
1054 - Crab

Static Kohn-Sham theory:

In order to reproduce shell structure Kohn and Sham introduced a auxiliary single particle potential $v_{\text{eff}}(\mathbf{r})$, defined by the condition, that after the solution of the eigenvalue problem

$$\left\{ -\frac{\hbar^2}{2m}\Delta + v_{\text{eff}}(\mathbf{r}) \right\} \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

the exact density is obtained as $\rho(\mathbf{r}) = \sum_i^A |\varphi_i(\mathbf{r})|^2$.

Obviously to each density $\rho(\mathbf{r})$ there exist such a potential $v_{\text{eff}}(\mathbf{r})$ and one finds

$$v_{\text{eff}}(\mathbf{r}) = f_{\text{ext}}(\mathbf{r}) + v_{\text{H}}(\mathbf{r}) + v_{xc}(\mathbf{r})$$

with $v_{\text{H}}(\mathbf{r}) = \int V(\mathbf{r},\mathbf{r}')\rho(r')d^3r$ and $v_{\text{xc}}(\mathbf{r}) = \frac{\delta E_{\text{xc}}}{\delta \rho(\mathbf{r})}$

Covariant DFT is based on the Walecka model

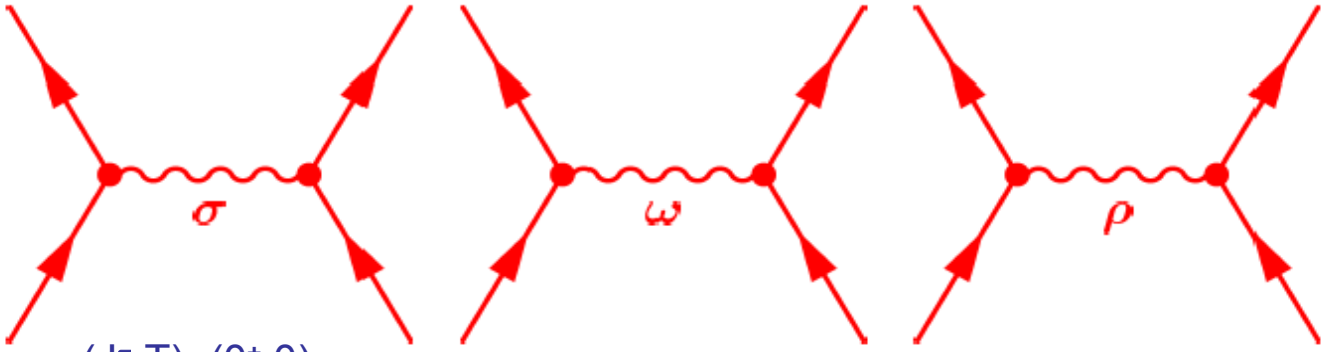
Dürr and Teller, Phys.Rev 101 (1956)

Walecka, Phys.Rev. C83 (1974)

Boguta and Bodmer, Nucl.Phys. A292 (1977)

The nuclear fields are obtained by coupling the nucleons through the exchange of effective mesons through an effective Lagrangian.

$E[\rho]$



$(J^{\pi},T)=(0^{+},0)$ $(J^{\pi},T)=(1^{-},0)$ $(J^{\pi},T)=(1^{-},1)$

$$S(r)=g_{\sigma}\sigma(r) \qquad V(r)=g_{\omega}\omega(r)+g_{\rho}\vec{\tau}\vec{\rho}(r)+eA(r)$$

sigma-meson: attractive scalar field

omega-meson: short-range repulsive

rho-meson: isovector field

How many parameters ?

4 + 3 parameters

symmetric nuclear matter: E/A, ρ_0 → G_σ G_ω

finite nuclei (N=Z): E/A, radii → m_σ

spinorbit for free

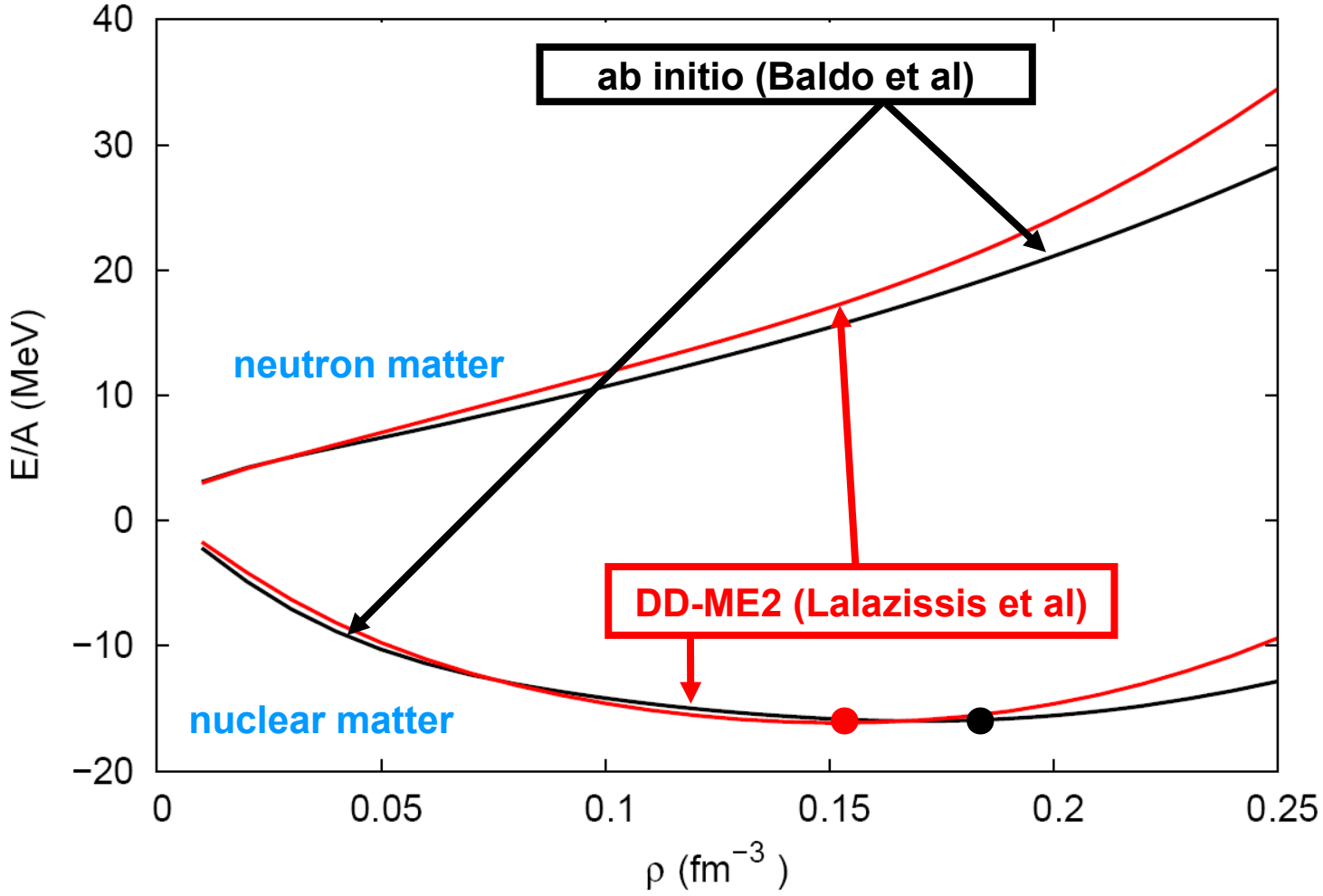
Coulomb (N≠Z):

a_4 → G_ρ

density dependence: T=0 K_∞ → g_2 g_3

T=1 $r_n - r_p$ → a_ρ

Comparison with ab initio calculations:



we find excellent agreement with ab initio calculations of Baldo et al.

Time dependent density functional theory:

Exact solution $|\Psi(t)\rangle$ of a time-dependent Schroedinger equation with initial condition $|\Psi(0)\rangle$

$$i\partial_t|\Psi(t)\rangle = (\hat{H} + f_{\text{ext}}(t))|\Psi(t)\rangle$$

Runge-Gross theorem (1984):

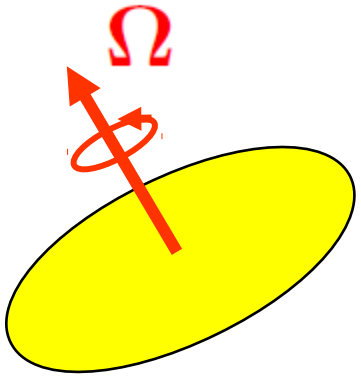
One-to-one correspondence: $\rho(\mathbf{r},t) \iff f_{\text{ext}}(\mathbf{r},t)$ and there exists a fictitious system of non-interacting particles with the wave functions $\varphi_i(\mathbf{r},t)$ satisfying

$$i\partial_t\varphi_i(\mathbf{r},t) = \left[-\nabla^2/2m + v_{\text{eff}}[\rho](\mathbf{r},t)\right]\varphi_i(\mathbf{r},t).$$

for a $v_{\text{eff}}[\rho](\mathbf{r},t)$ and $\rho(\mathbf{r},t) = \sum_i^A |\varphi_i(\mathbf{r},t)|^2$ is the exact density of the interacting many-body system. $v_{\text{eff}}[\rho](\mathbf{r},t)$ is a function of $\mathbf{r}$ and t, but it is in addition a unique functional of the time-dependent density $\rho(\mathbf{r},t)$.

Rotational excitations:

We assume that the time-dependence is given by a rotation with constant velocity $\boldsymbol{\Omega}$



$$\rho(\boldsymbol{r},t) = e^{-i\boldsymbol{\Omega}\boldsymbol{j}t}\rho(\boldsymbol{r})e^{i\boldsymbol{\Omega}\boldsymbol{j}t}$$

This leads to quasi-static Kohn-Sham equations in the rotations frame

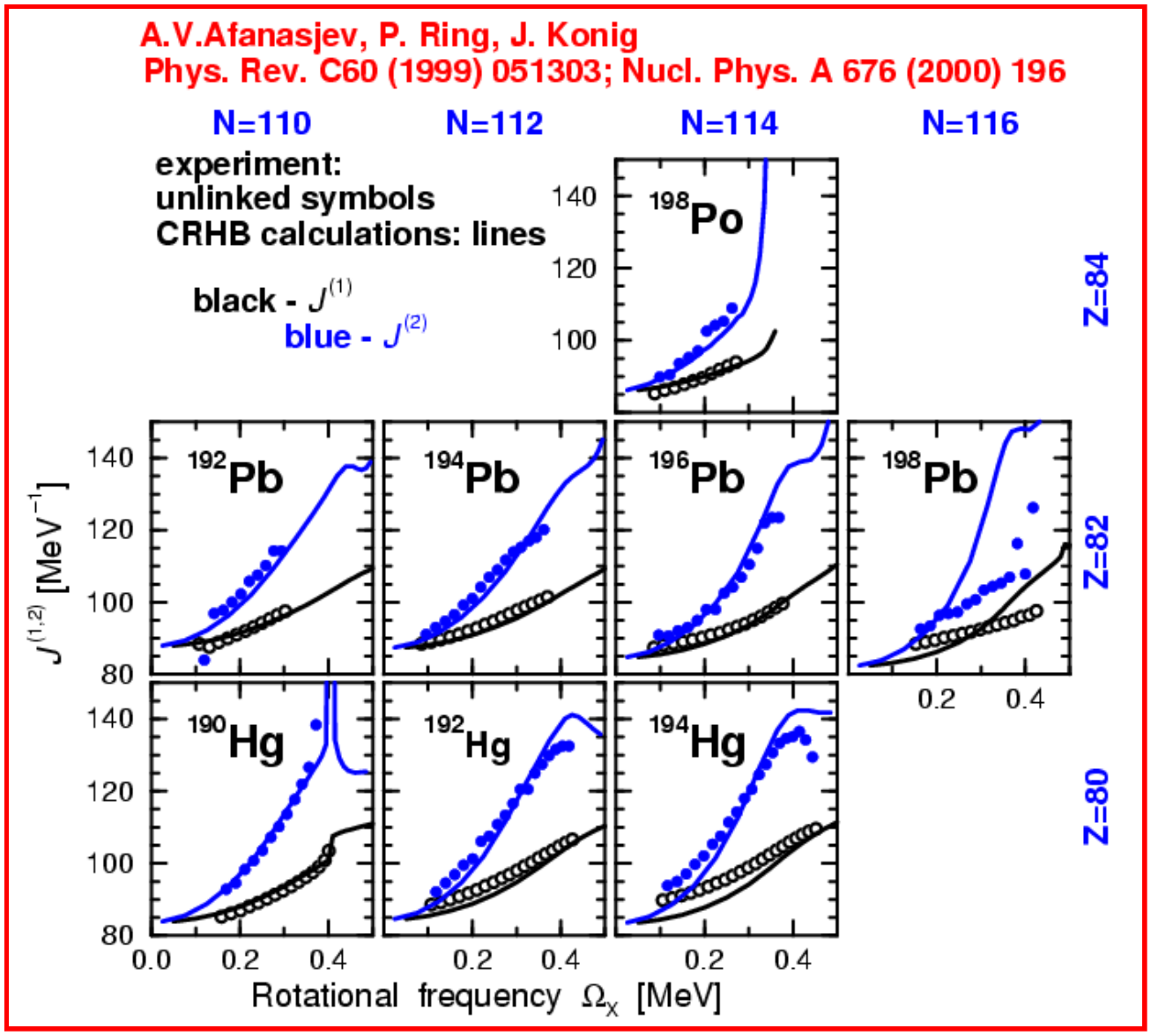
Cranking model: Inglis (1956):

$$\left[-\boldsymbol{\nabla}^2/2m + \upsilon[\rho](\boldsymbol{r}) - \boldsymbol{\Omega}\boldsymbol{j}\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i(\boldsymbol{\Omega})\varphi_i(\boldsymbol{r})$$

with the exact intrinsic density $\rho(\boldsymbol{r}) = \sum_{i=1}^{A} |\varphi_i(\boldsymbol{r})|^2$

Here we assume, that $\upsilon[\rho](\boldsymbol{r})$ is the static Kohn-Sham potential ("adiabatic approximation")

Superdeformed band in the Hg-Pb region:



Timedependent density functional theory:

Exact solution $|\Psi(t)\rangle$ of a time-dependent Schroedinger equation with initial condition $|\Psi(0)\rangle$

$$i\partial_t|\Psi(t)\rangle = (\hat{H} + f_{\text{ext}}(t))|\Psi(t)\rangle$$

Runge-Gross theorem (1984):

One-to-one correspondence: $\rho(\mathbf{r},t) \iff f_{\text{ext}}(\mathbf{r},t)$ and there exists a fictitious system of non-interacting particles with the wave functions $\varphi_i(\mathbf{r},t)$ satisfying

$$i\partial_t\varphi_i(\mathbf{r},t) = \left[-\nabla^2/2m + v_{\text{eff}}[\rho](\mathbf{r},t)\right]\varphi_i(\mathbf{r},t).$$

for a $v_{\text{eff}}[\rho](\mathbf{r},t)$ and $\rho(\mathbf{r},t) = \sum_i^A |\varphi_i(\mathbf{r},t)|^2$ is the exact density of the interacting many-body system. $v_{\text{eff}}[\rho](\mathbf{r},t)$ is a function of $\mathbf{r}$ and t, but it is in addition a unique functional of the time-dependent density $\rho(\mathbf{r},t)$.

Linear response theory:

If $f_{\text{ext}}(\mathbf{r},t)$ is **weak** we have: $\rho(\mathbf{r},t) = \rho_s(\mathbf{r}) + \delta\rho(\mathbf{r},t)$.

and: $v[\rho](\mathbf{r},t) = v_s(\mathbf{r}) + \int dt' \int d^3r' V(\mathbf{r},\mathbf{r}',t-t')\delta\rho(\mathbf{r},t')$.

V is an effective interaction $V(\mathbf{r},\mathbf{r}',t-t') = \left.\frac{\delta v(\mathbf{r},t)}{\delta\rho(\mathbf{r}',t')}\right|_{\rho=\rho_s}$.

For $\delta\rho(\mathbf{r},t) = \int d^3r' \int dt' R(\mathbf{r},\mathbf{r}',t-t') f_{ext}(\mathbf{r}',t')$

we find

$$R(\omega) = R_0(\omega) + R_0(\omega)V(\omega)R(\omega)$$

All these quantities are functionals of the exact ground state density $\rho_s(\mathbf{r})$.

If f_{ext} is weak, these equations are exact, but we do not know the functional $v[\rho(\mathbf{r},t)]$ nor its functional derivative at $\rho = \rho_s$.

The adiabatic approximation:

Here one neglects the memory and assumes that the density changes only very slowly, such that the potential is given at each time by the static potential v_s corresponding to this density.

$$v[\rho](\mathbf{r},t) \approx v_s[\rho_s](\mathbf{r},t)$$

In this approximation $v[\rho]$ is no longer depending on the function $\rho(\mathbf{r},t)$ of 4 variables, but rather on the function $\rho_s(\mathbf{r}) = \rho(\mathbf{r},t)$ depending only 3 variables. The time is just a parameter. We obtain for the effective interaction in the adiabatic approximation

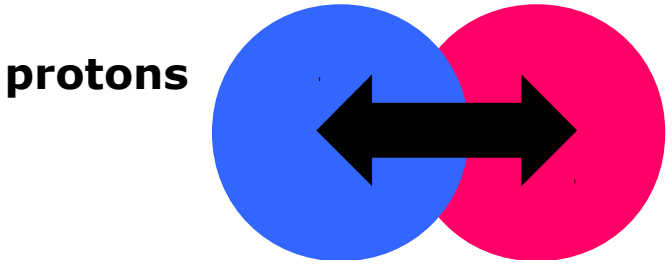
$$V_{ad}(\mathbf{r},\mathbf{r}',t-t') = \frac{\delta E[\rho_s]}{\delta\rho_s(\mathbf{r})\delta\rho_s(\mathbf{r}')}\delta(t-t')$$

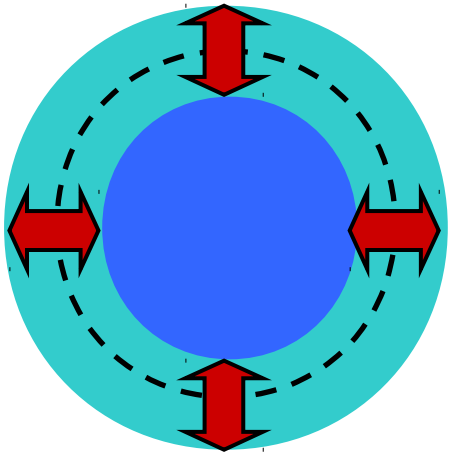
This approximation is well known. It corresponds to the small amplitude limit of the time-dependent mean field equations, i.e. to RPA or in superfluid systems to QRPA and it is extensively used in nuclear physics.

Relativistic (Q)RPA calculations of giant resonances:

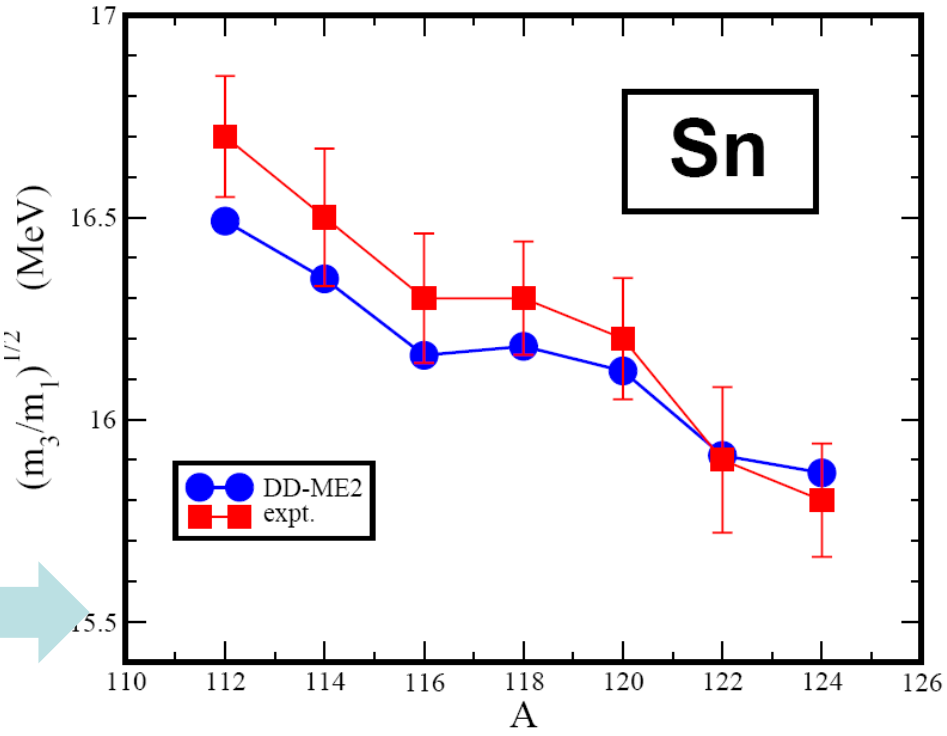
Sn isotopes: DD-ME2 effective interaction + Gogny pairing

Isovector dipole response

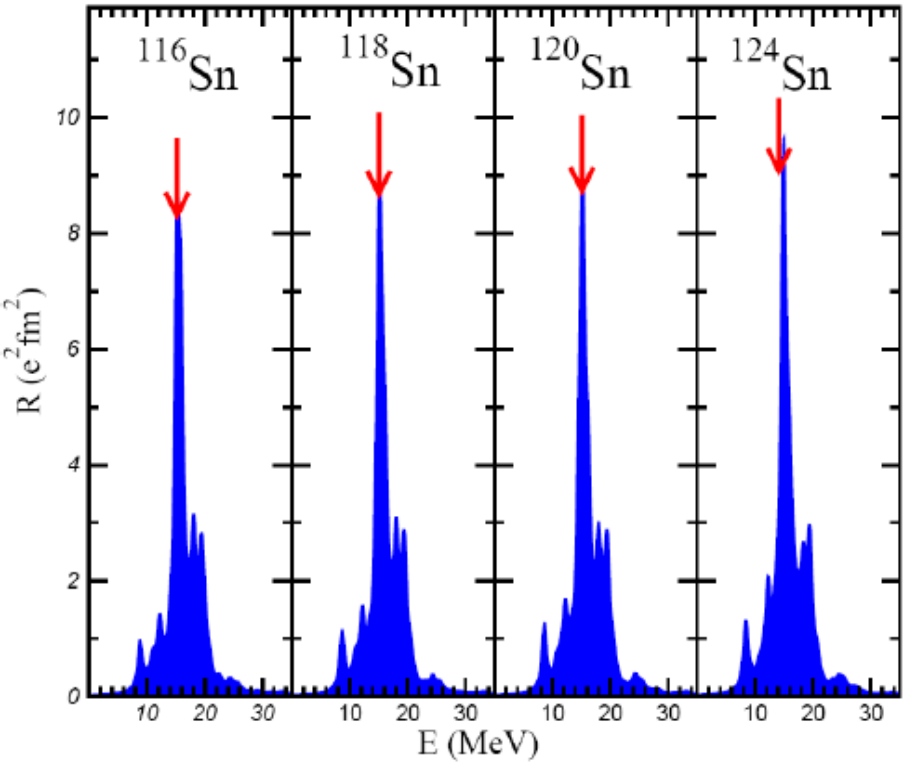




Isoscalar monopole response

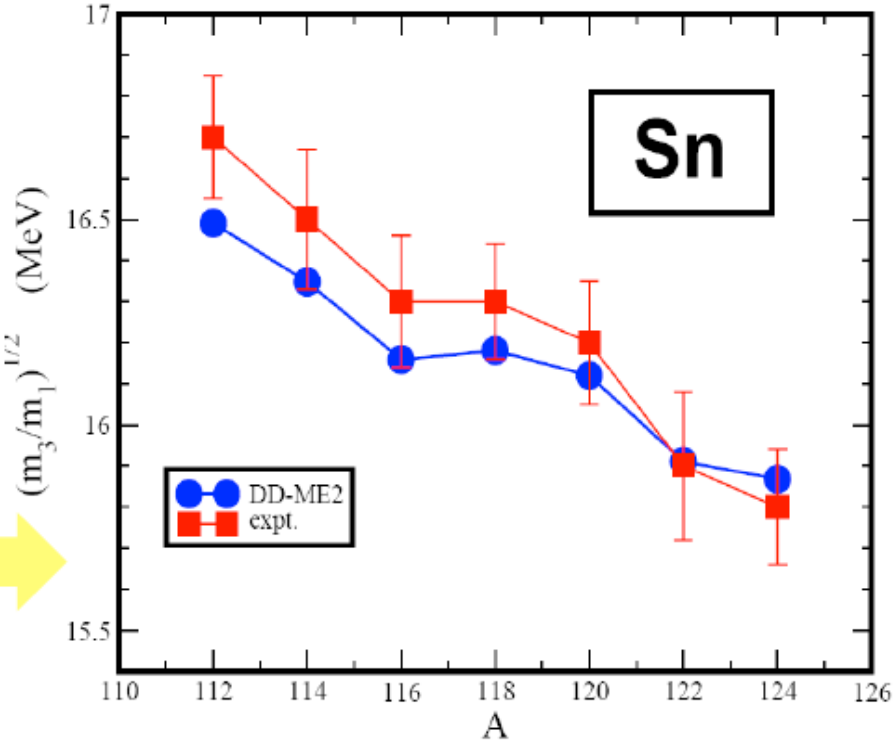


Relativistic (Q)RPA calculations of giant resonances



Isovector dipole response

Isoscalar monopole response

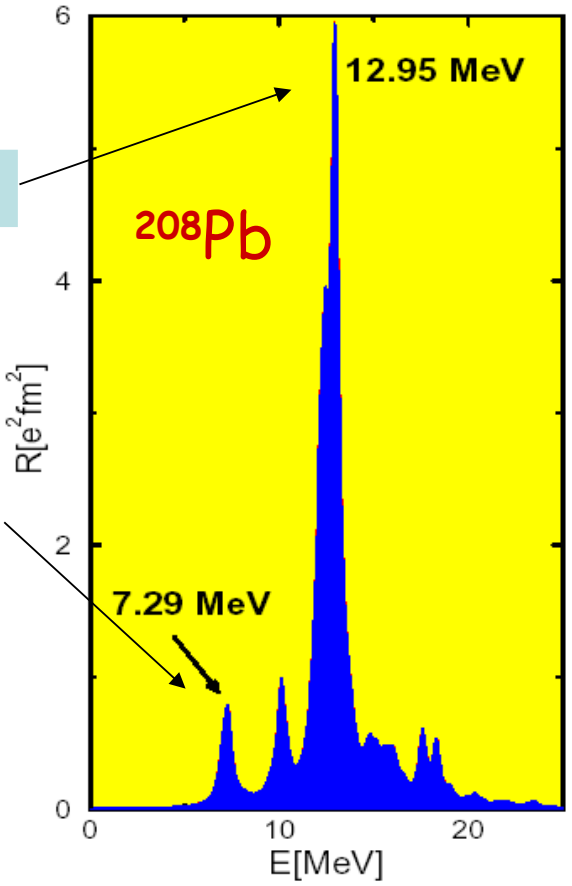


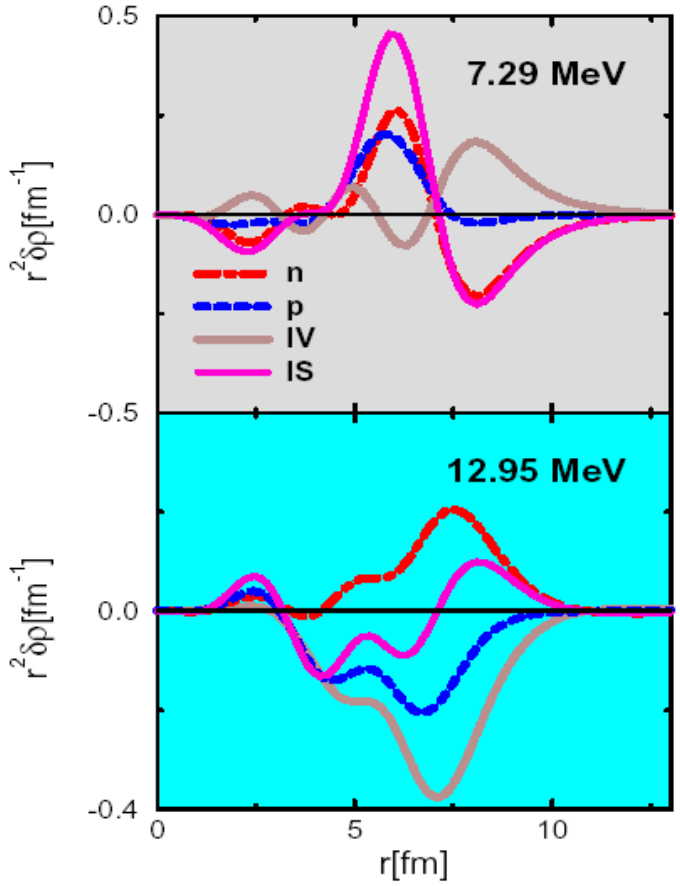
Dipole Strength for ^{208}Pb and transition densities for the peaks at 7.29 MeV
12.95 MeV

Vretenar, Paar, P. R, Lalazissis, Phys. Rev. C63, 047301 (20

Exp GDR at 13.3 MeV

Exp PYGMY centroid at 7.37 MeV

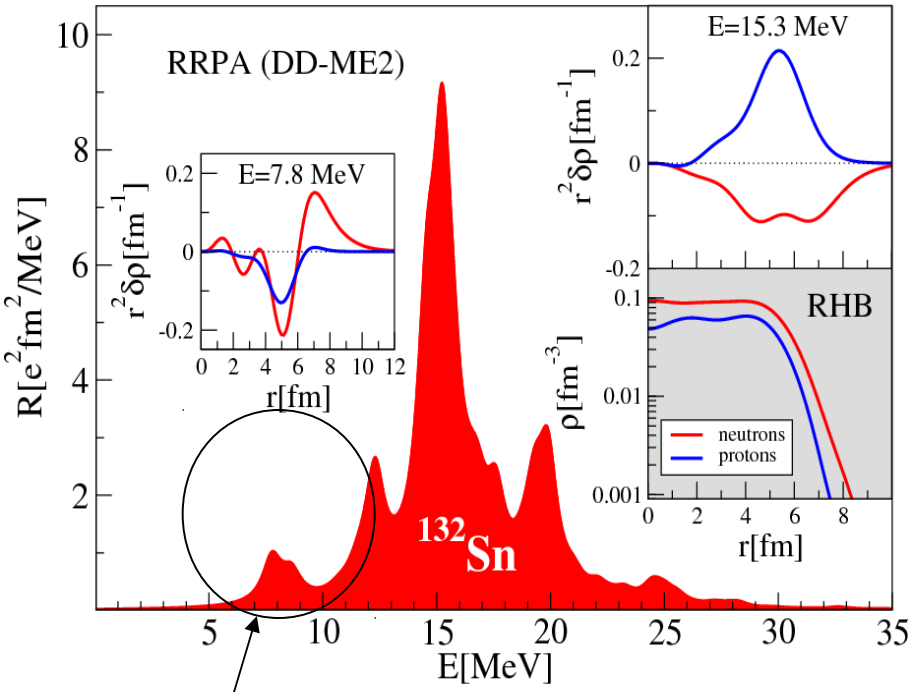




In heavier nuclei low-lying dipole states appear that are characterized by a more distributed structure of the RQRPA amplitude.

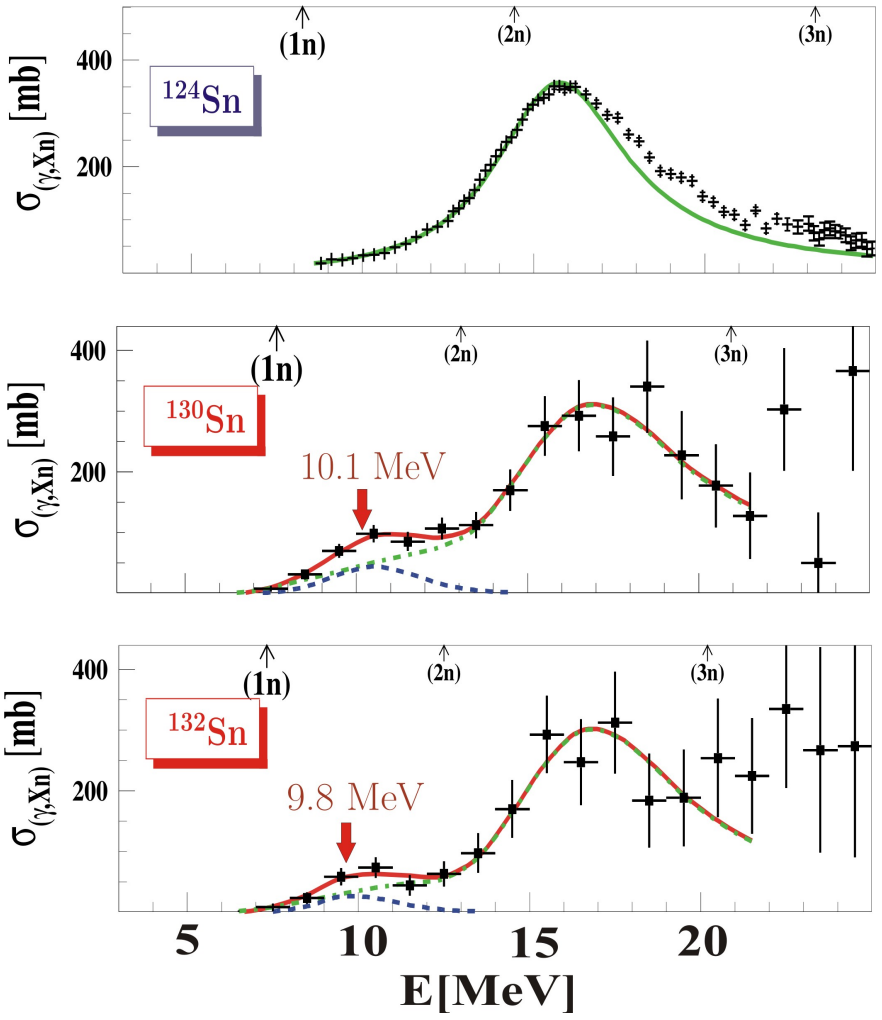
Among several single-particle transitions, a single collective dipole state is found below 10 MeV and its amplitude represents a coherent superposition of many neutron particle-hole configurations.

Pygmy dipole resonance



^{132}Sn at 7.6 MeV	
28.2%	$2d_{3/2} \rightarrow 2f_{5/2}$
21.9%	$2d_{5/2} \rightarrow 2f_{7/2}$
19.7%	$2d_{3/2} \rightarrow 3p_{1/2}$
10.5%	$1h_{11/2} \rightarrow 1i_{13/2}$
3.5%	$2d_{5/2} \rightarrow 3p_{3/2}$
1.9%	$1g_{7/2} \rightarrow 2f_{5/2}$
1.5%	$1g_{7/2} \rightarrow 1h_{9/2}$
0.6%	$1g_{7/2} \rightarrow 2f_{7/2}$
0.6%	$2d_{3/2} \rightarrow 3p_{3/2}$

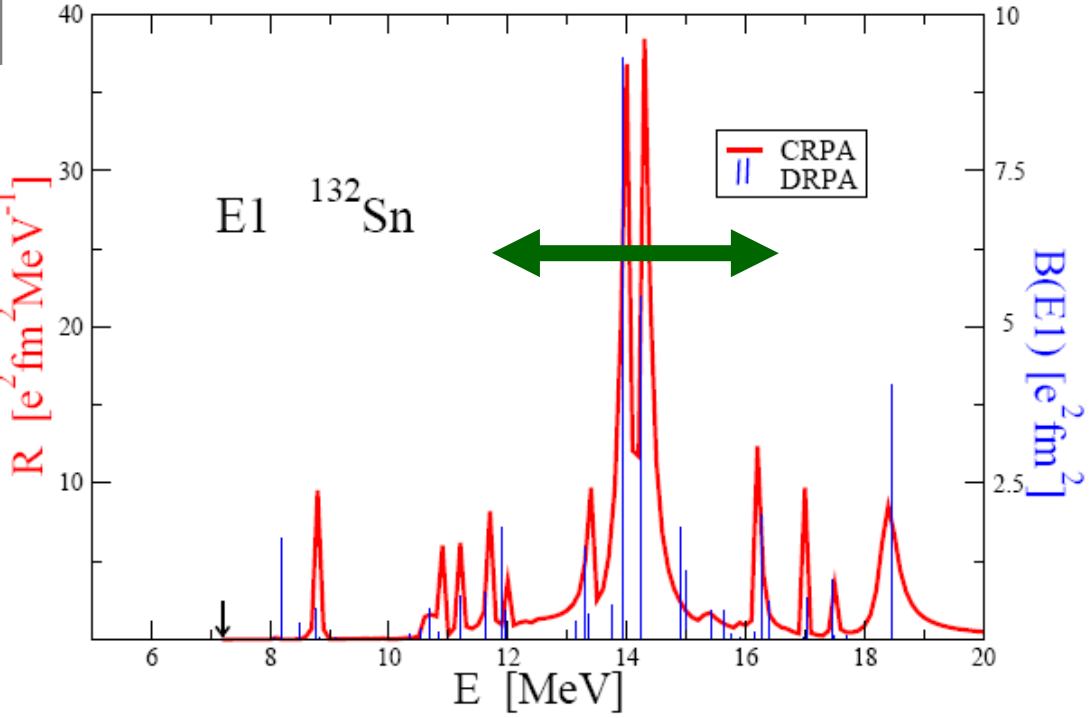
Opening of the closed neutron shell increases collectivity !



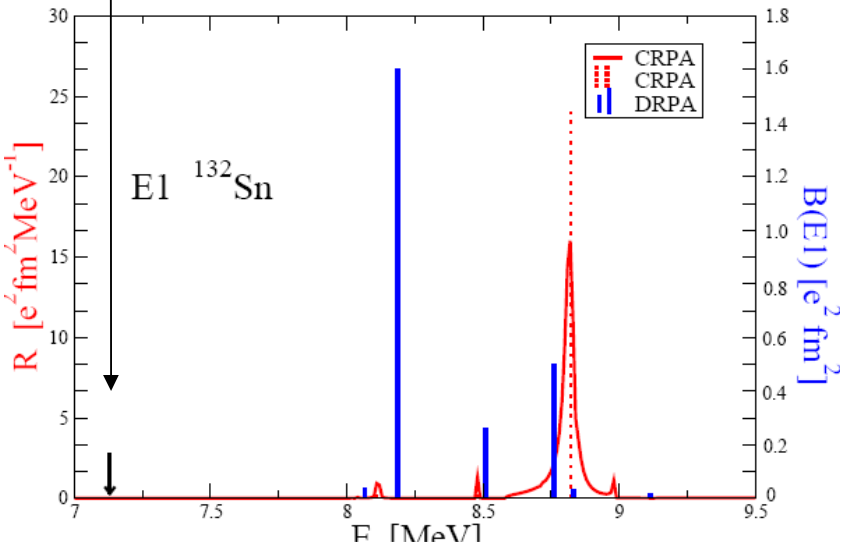
P.Adrich et al., Phys. Rev. Lett. 95, 132501(2005).

E1-continuum RPA

^{132}Sn



neutron threshold:

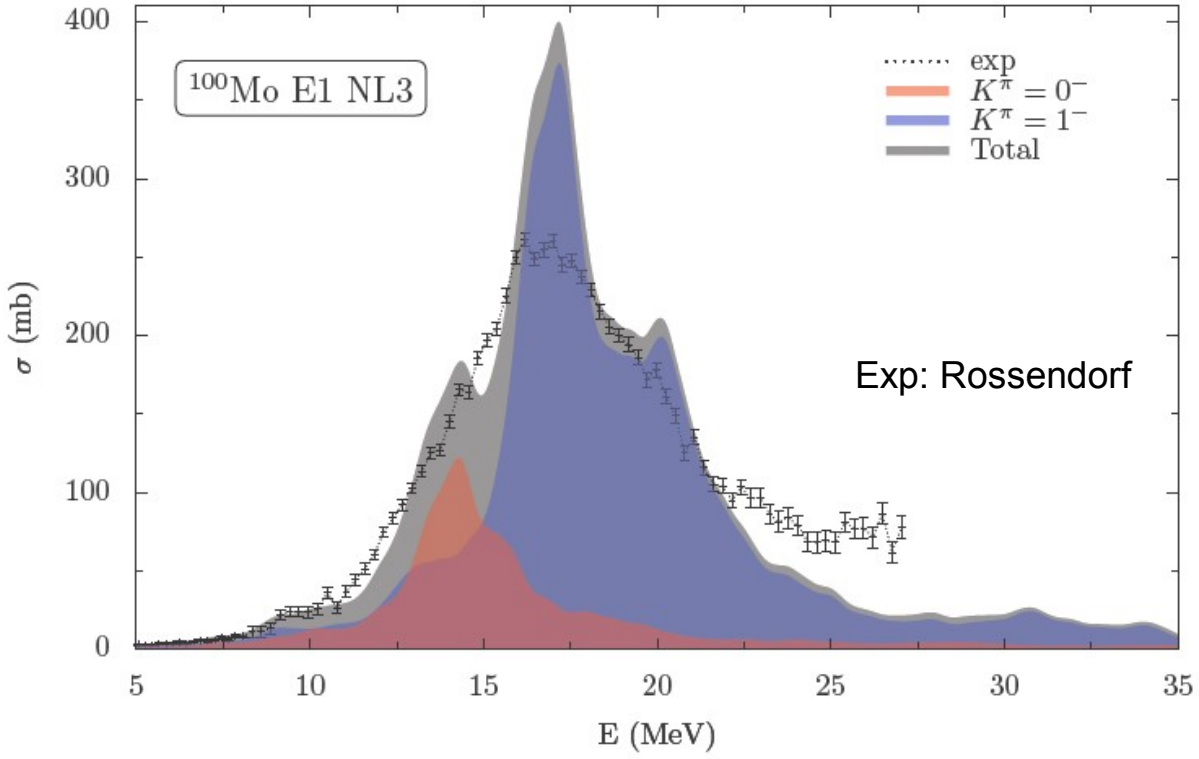


	CRPA		DRPA	
No.	E	B(E1)	E	B(E1)
1	8.11	0.03	8.067	0.037
2	8.48	0.02	8.186	1.601
3	8.82	1.44	8.511	0.260
Σ		1.490		1.898

2.4 % 3.4 % of EWSR

I. Daoutidis, P.R., PRC 80, 024309 (2009)

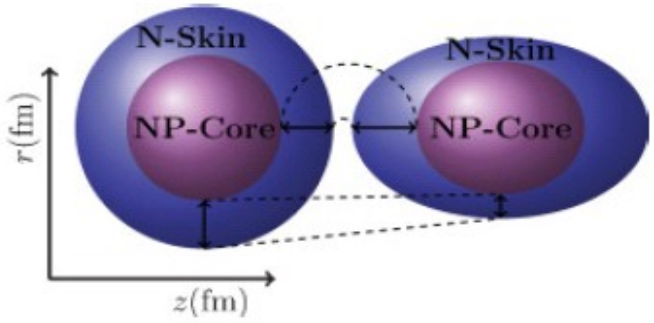
isovector-dipole response in ^{100}Mo



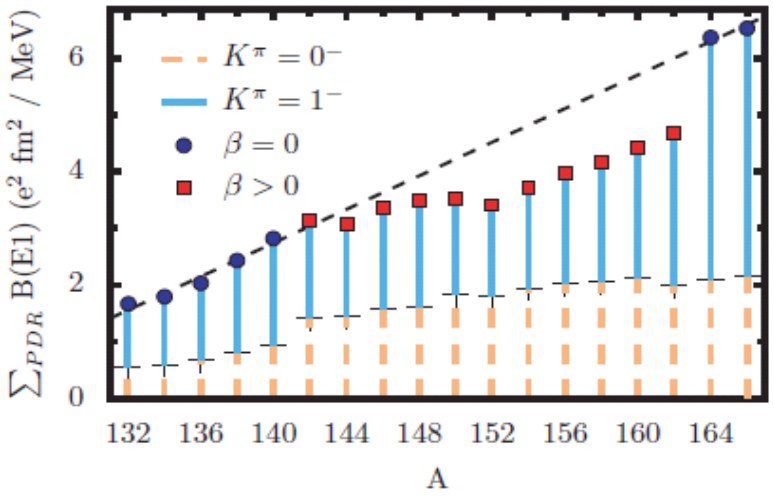
	m_1/m_0	$\sqrt{\frac{m_3}{m_1} - \frac{m_1}{m_0}}$	$\bar{E}_{E1}$	Γ_{E1}
NL3	17.4	1.4	17.2	2.4
DD-ME2	18.3	1.2	18.5	3.3
Exp	18.0	1.4	17.4	3.6

in MeV

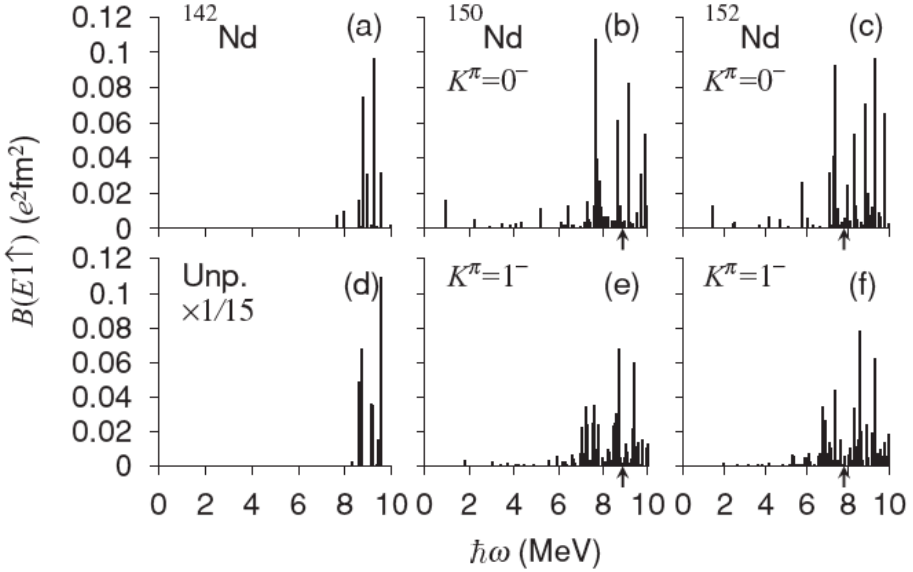
Pygmy in deformed nuclei



The pygmy mode is quenched by the deformation because of the reduction of the n skin



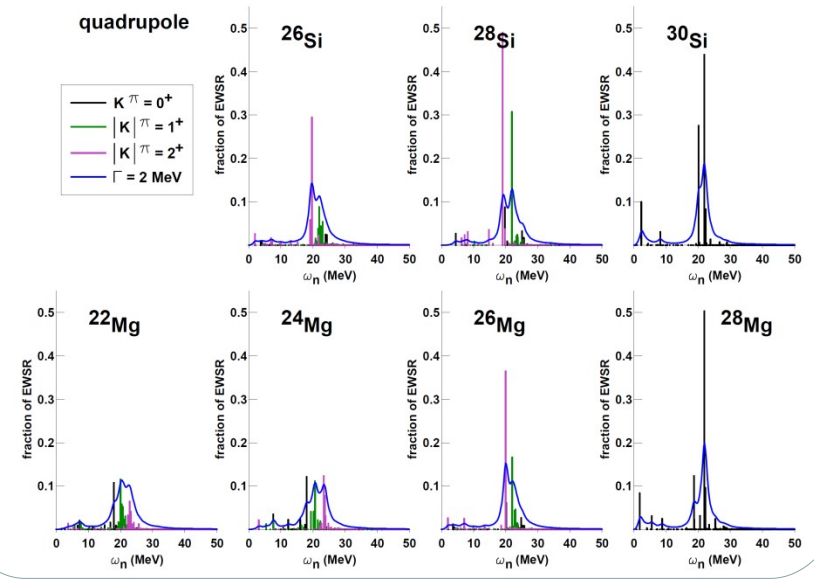
Peña Arteaga, Khan and Ring (2009)



Yoshida and Nakatsukasa (2011)

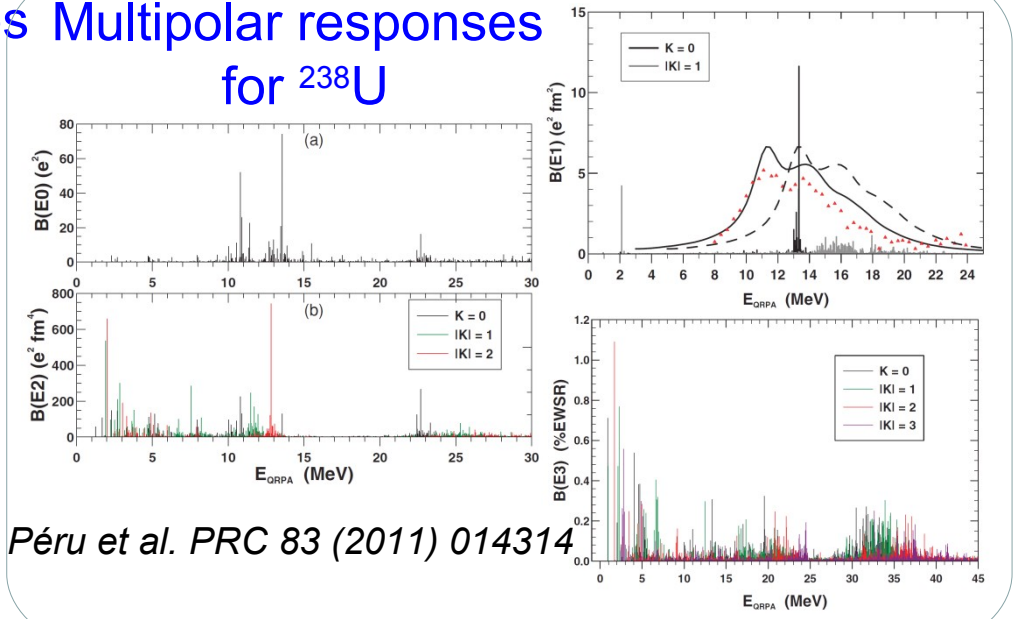
Self-consistent QRPA approach with the Gogny force

ole of deformation on giant resonances



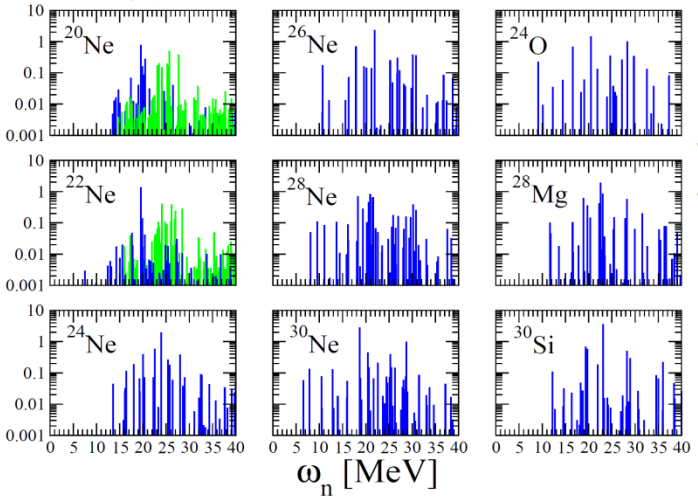
Péru et al. PRC 77 (2008) 044313

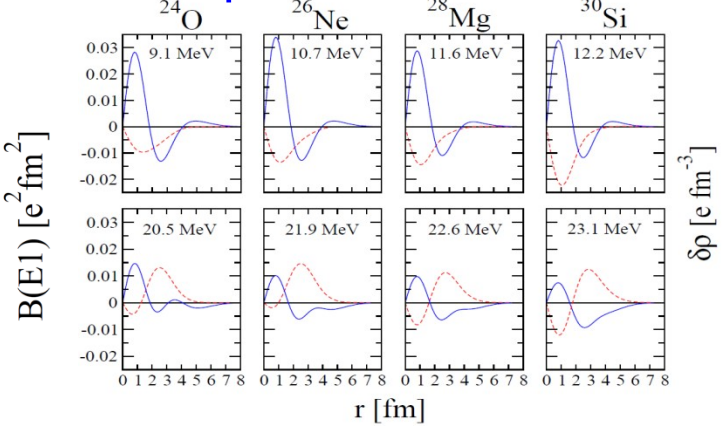
Multipolar responses for ^{238}U



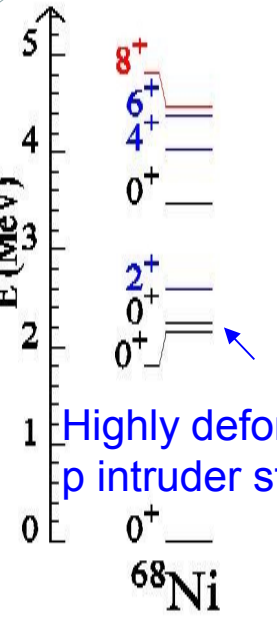
Péru et al. PRC 83 (2011) 014314

w-energy dipole excitations in neon isotopes and N=16 isotones





Martini et al. PRC 83 (2011) 034309



Highly deformed p intruder state

Dijon et al. PRC 85 (2012) 031301

Spin-Isospin Resonances: IAR - GTR

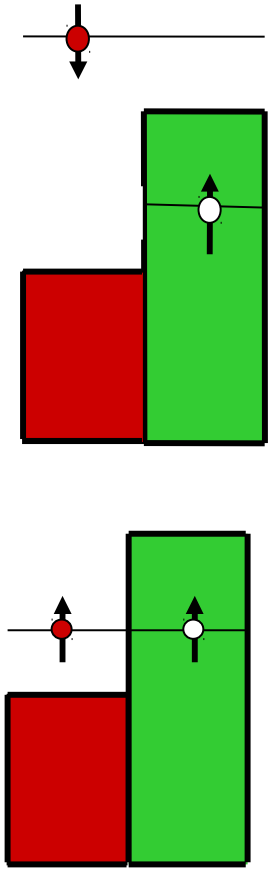
Z,N **Z+1,N-1**

$$|\mathrm{GTR}$$
$$S_- T_+ |Z,N$$

spin flip **σ**

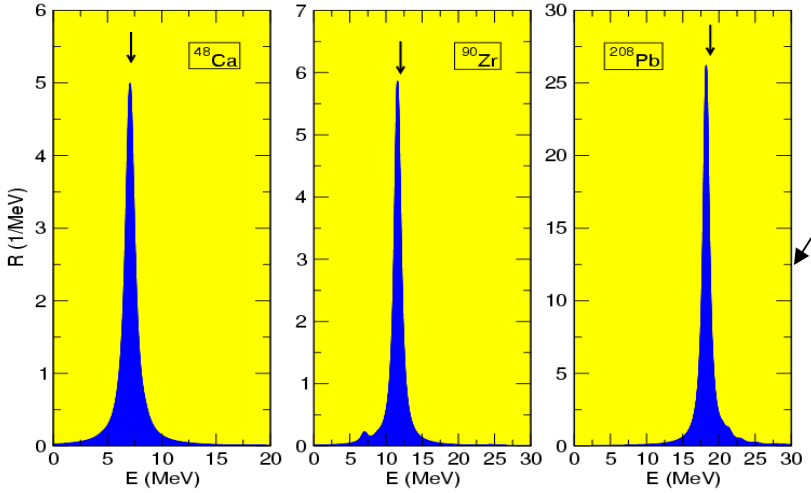
$$|Z,N \longrightarrow |\mathrm{IAR}$$
$$T_+ |Z,N$$

isospin flip **τ**



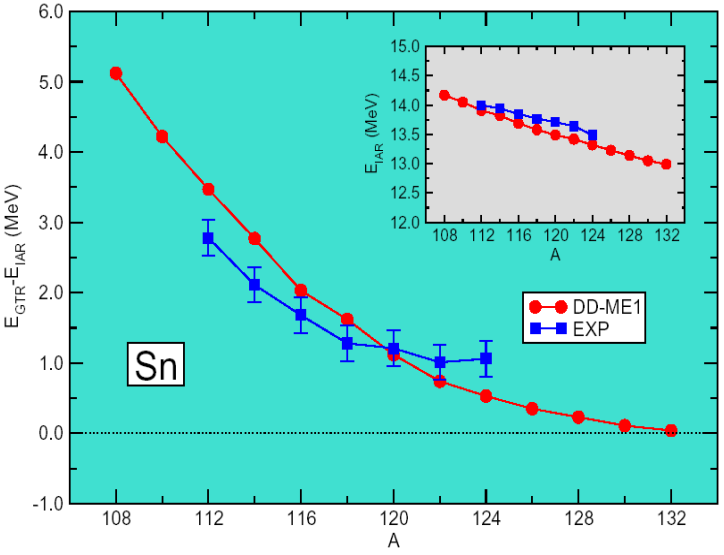
$$E_{\mathrm{GTR}} - E_{\mathrm{IAR}} \sim \Delta(l \cdot s) \sim \frac{\mathrm{dV}}{\mathrm{dr}} \sim \text{neutron skin} = r_n - r_p$$

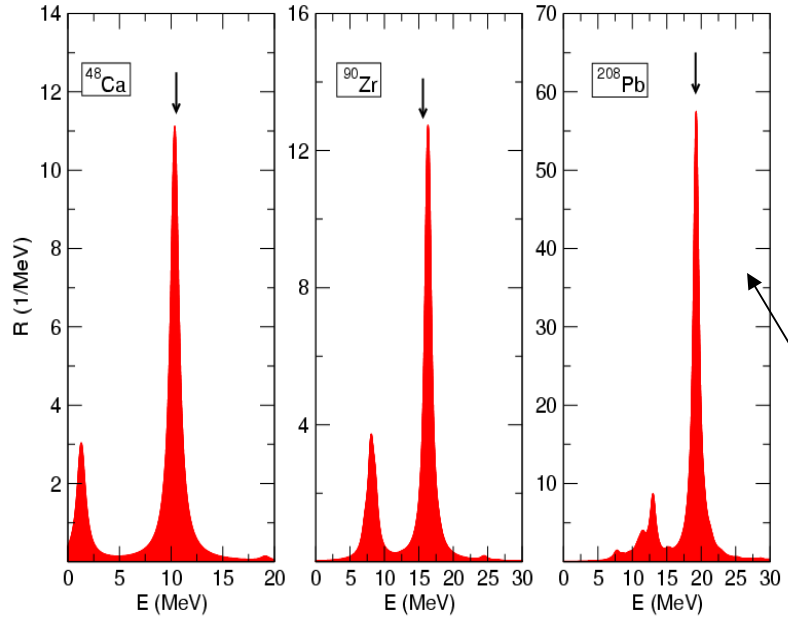
Spin-Isospin Resonances: IAR - GTR



ISOSPIN-FLIP EXCITATIONS

S=0 T=1 $J^{\pi} = 0^{+}$





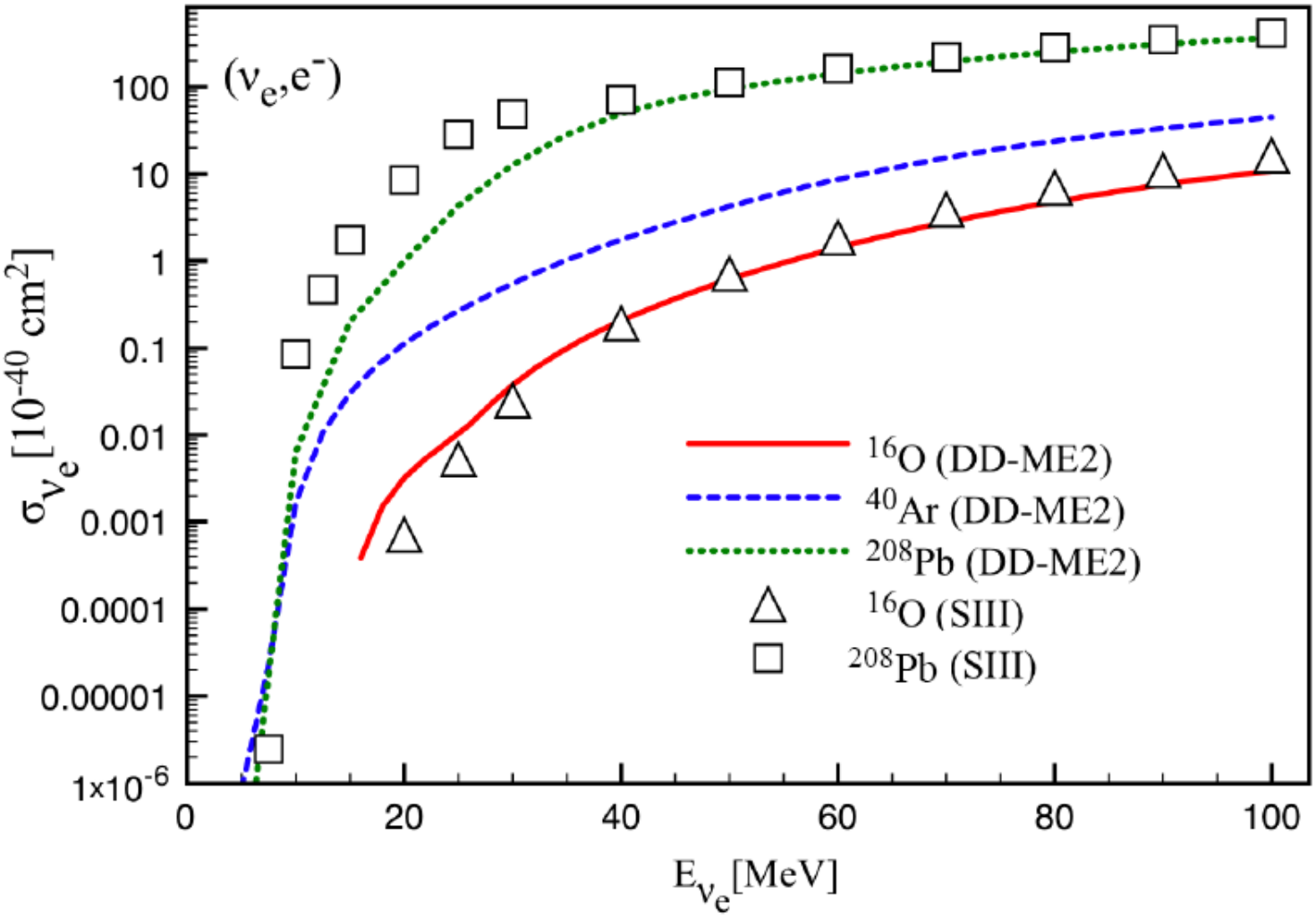
S=1 T=1 $J^{\pi} = 1^{+}$

SPIN-FLIP & ISOSPIN-FLIP EXCITATIONS

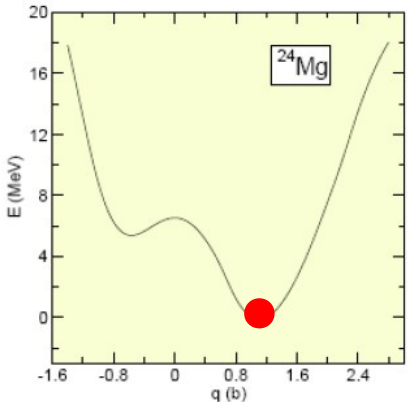
PRC 69, 054303 (2004)

Comparison between RHB+RQRPA and Skyrme-QRPA calculations:

Paar, Vretenar, Marketin, Ring, Phys. Rev. C 77, 024608 (2008)



Problems with the mean field description:



- **Fluctuations** are neglected

  solution: **GCM:** configuration mixing in transitional nuclei

- **Symmetries** are broken

  $$|\Psi\rangle = \int dq\, f(q)\,|q\rangle$$

  no spectroscopy

  solution: **Projection** to good quantum numbers

  derivation of a **Bohr Hamiltonian**

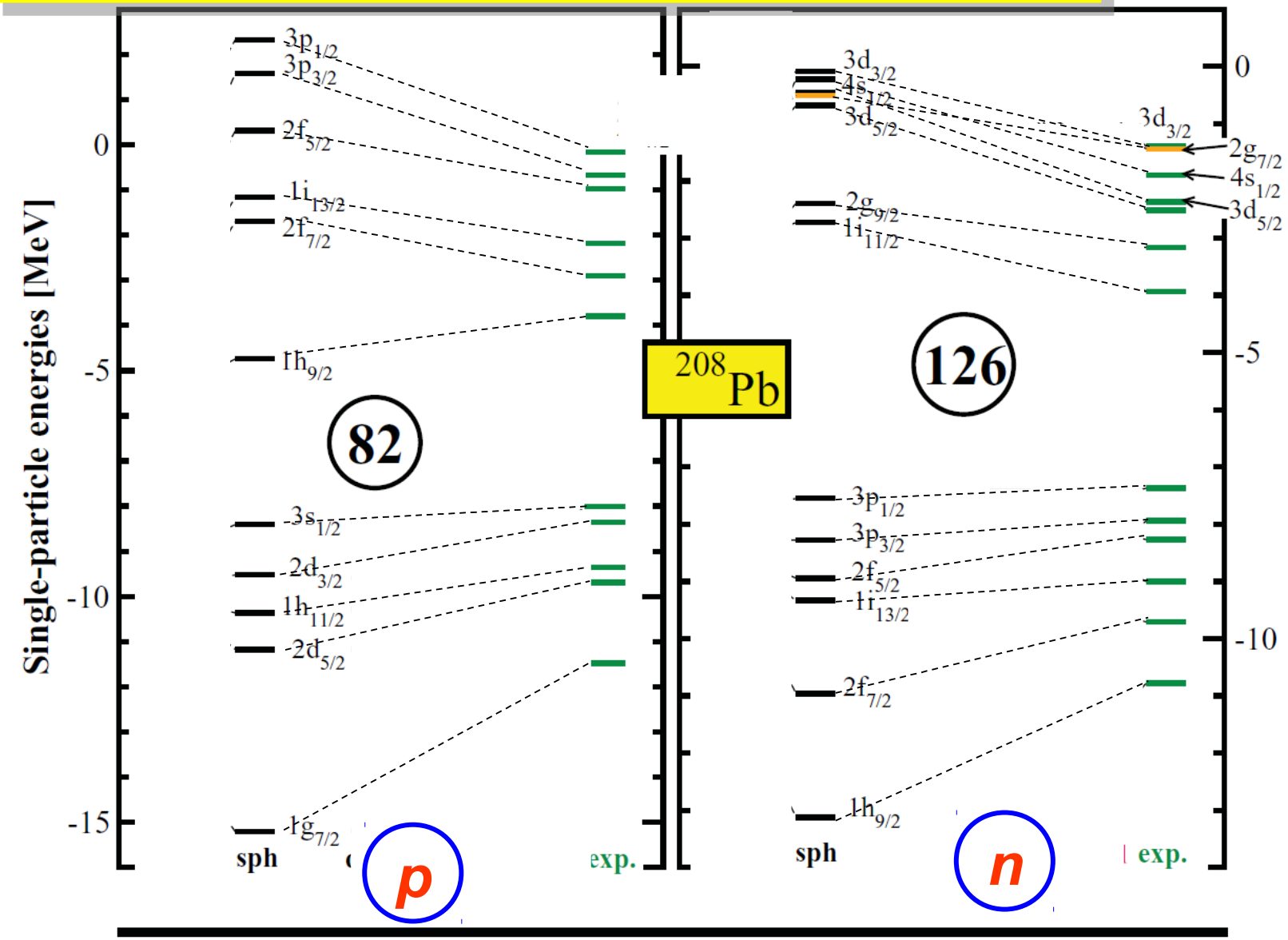
- **Energy dependence** of the self-energy is neglected

  low level density at the Fermi surface (arches in the masses)

  no coupling to many-particle many-hole states in Giant Resonances

  solution: **PVC**: coupling to surface vibrations and complex configurations

Problem: single particle spectra



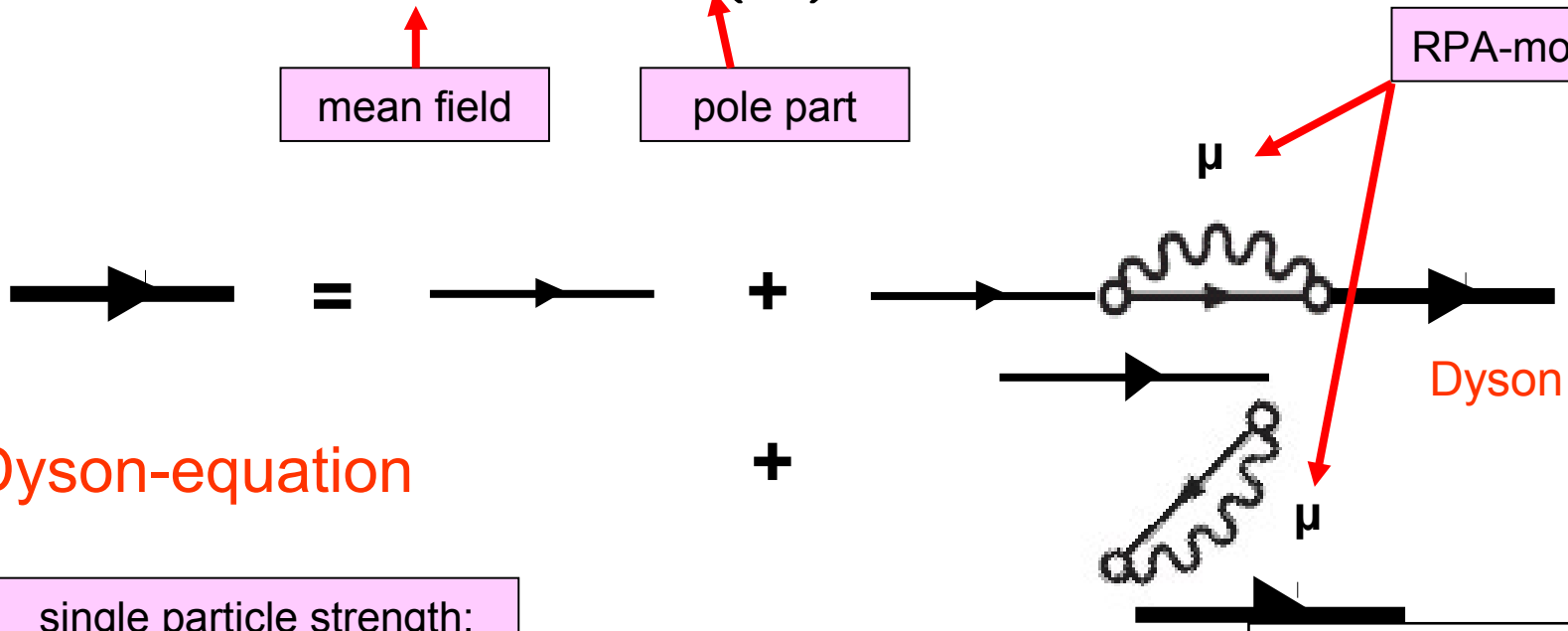
Particle-vibrational coupling (PVC) energy dependent self-energy

eff. Potential v_{eff} → self-energy Σ

$$\Sigma = S + V + \Sigma(\omega)$$

mean field

pole part

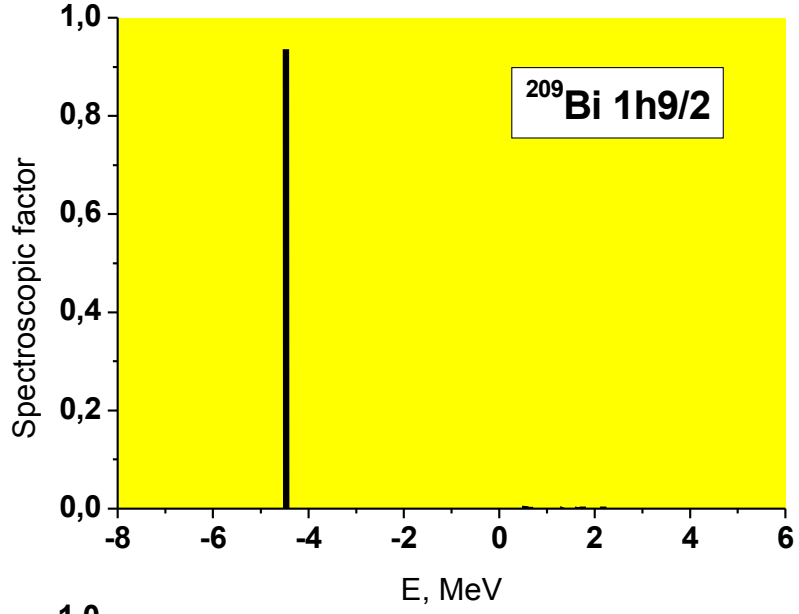


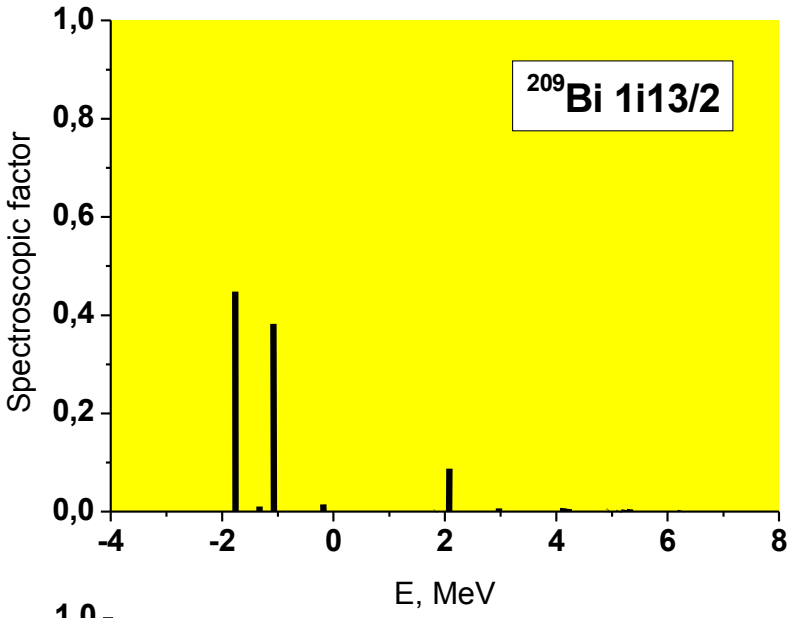
single particle strength:

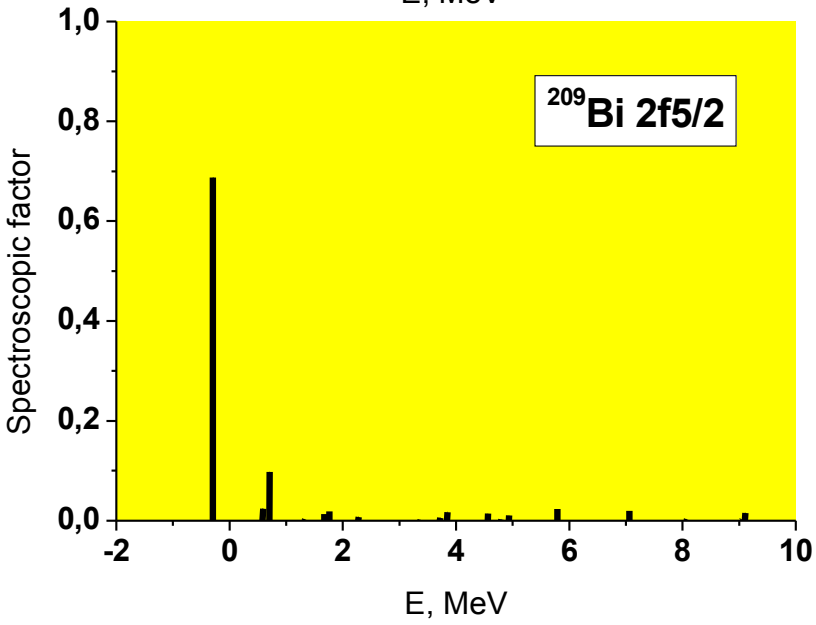
$$S_\nu = \left[1 - \left.\frac{d\Sigma_{\nu\nu}}{d\omega}\right|_{\omega=\epsilon_\nu}\right]^{-1}$$

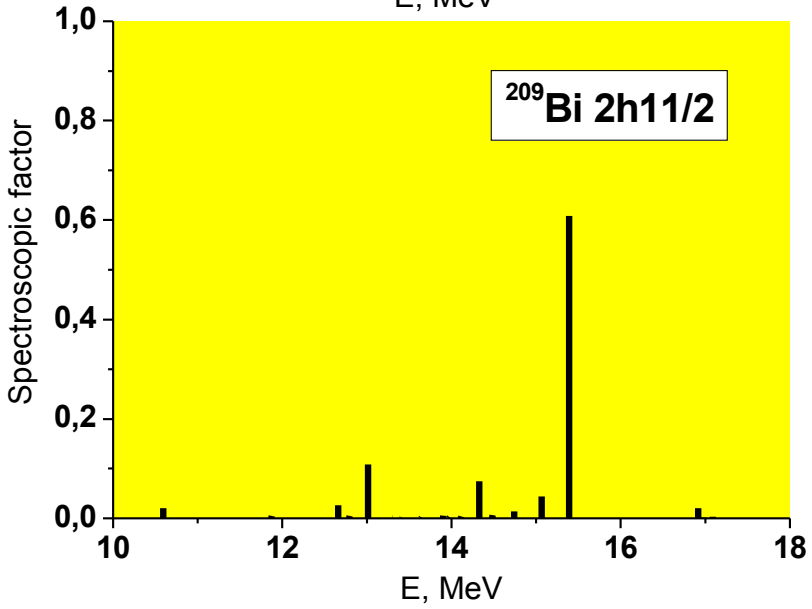
non-relativistic investigations:
Ring, Werner (1973)
Hamamoto, Siemens (1976)
Perazzo, Reich, Sofia (1980)
Bortignon et al (1980)
Bernard, Giai (1980)
Platonov (1981)
Kamerdzhiev, Tselyaev (1986)

Distribution of single-particle strength in ^{209}Bi

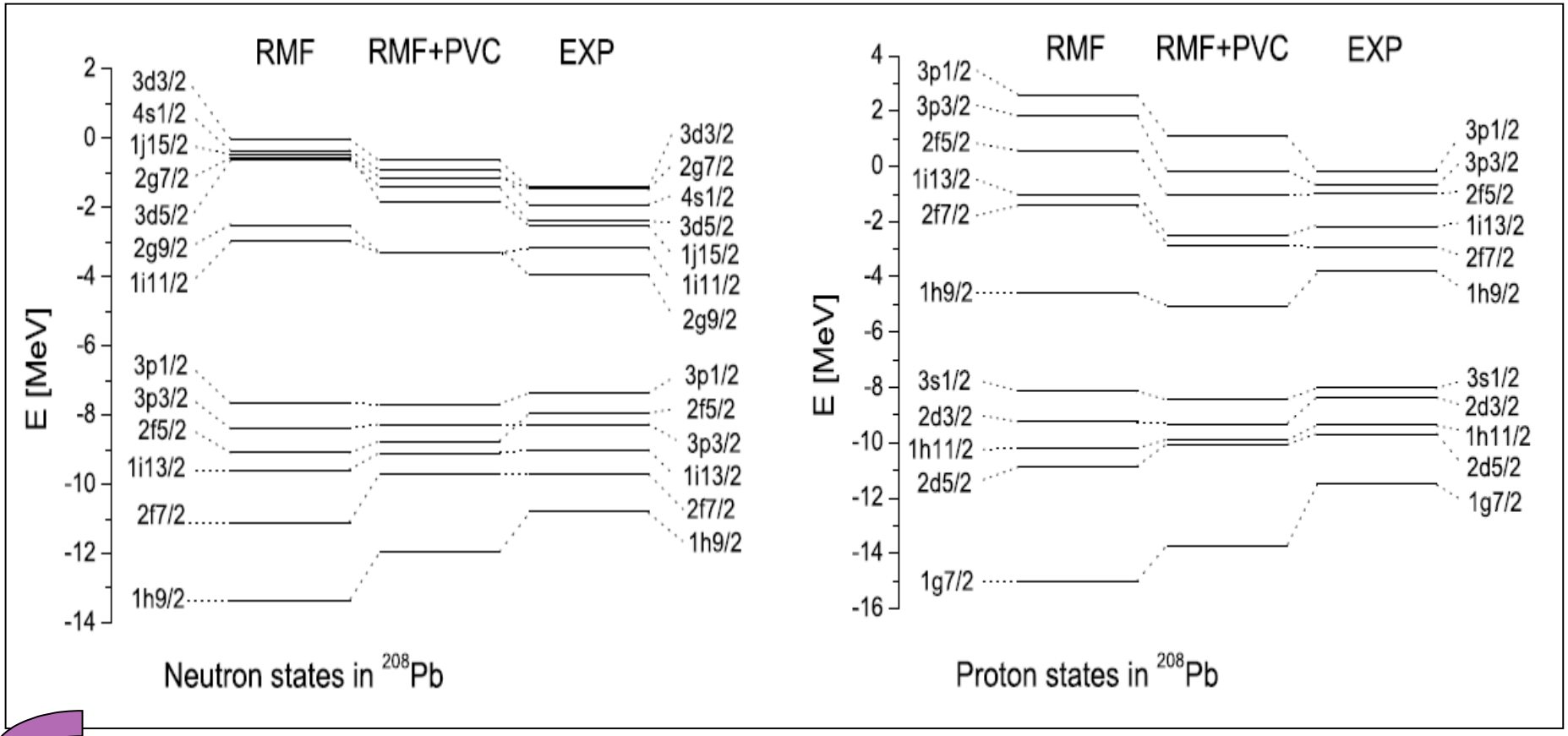








Single particle spectrum in the Pb-region:



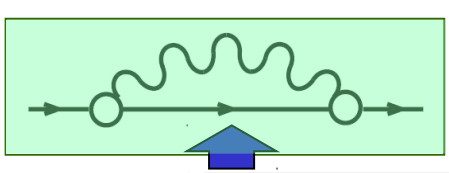
m_{eff} 0.76 0.92 1.0 0.71 0.85 1.0

E. Litvinova and P. R., PRC 73, 44328 (2006)

Width of giant resonances:

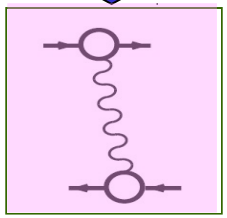
The full response contains energy dependent parts coming from vibrational couplings.

$$V(\omega)=\frac{\delta\Sigma(\omega)}{\delta\rho}$$

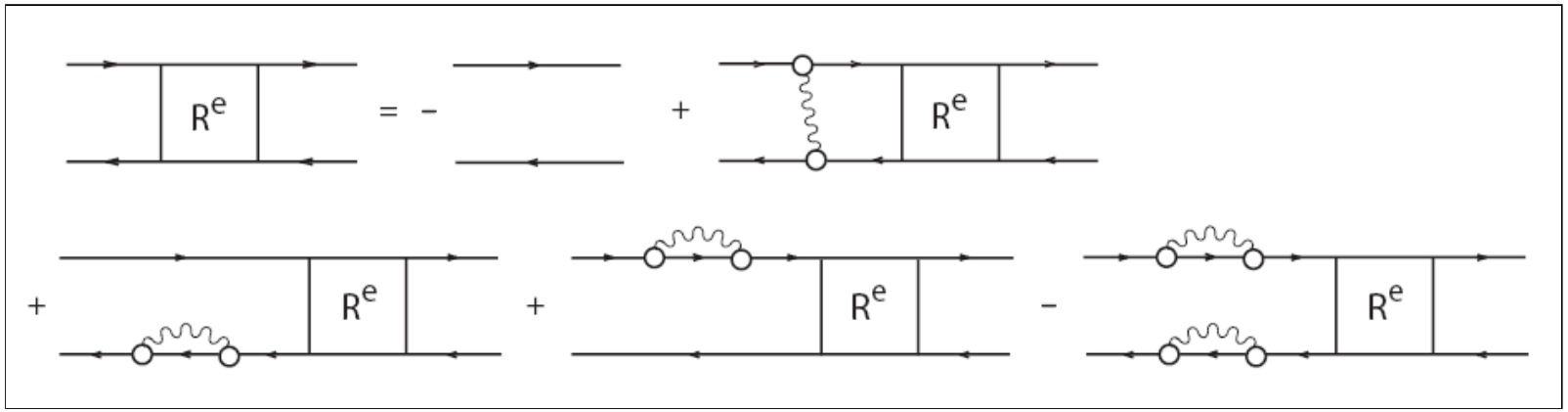


Self energy

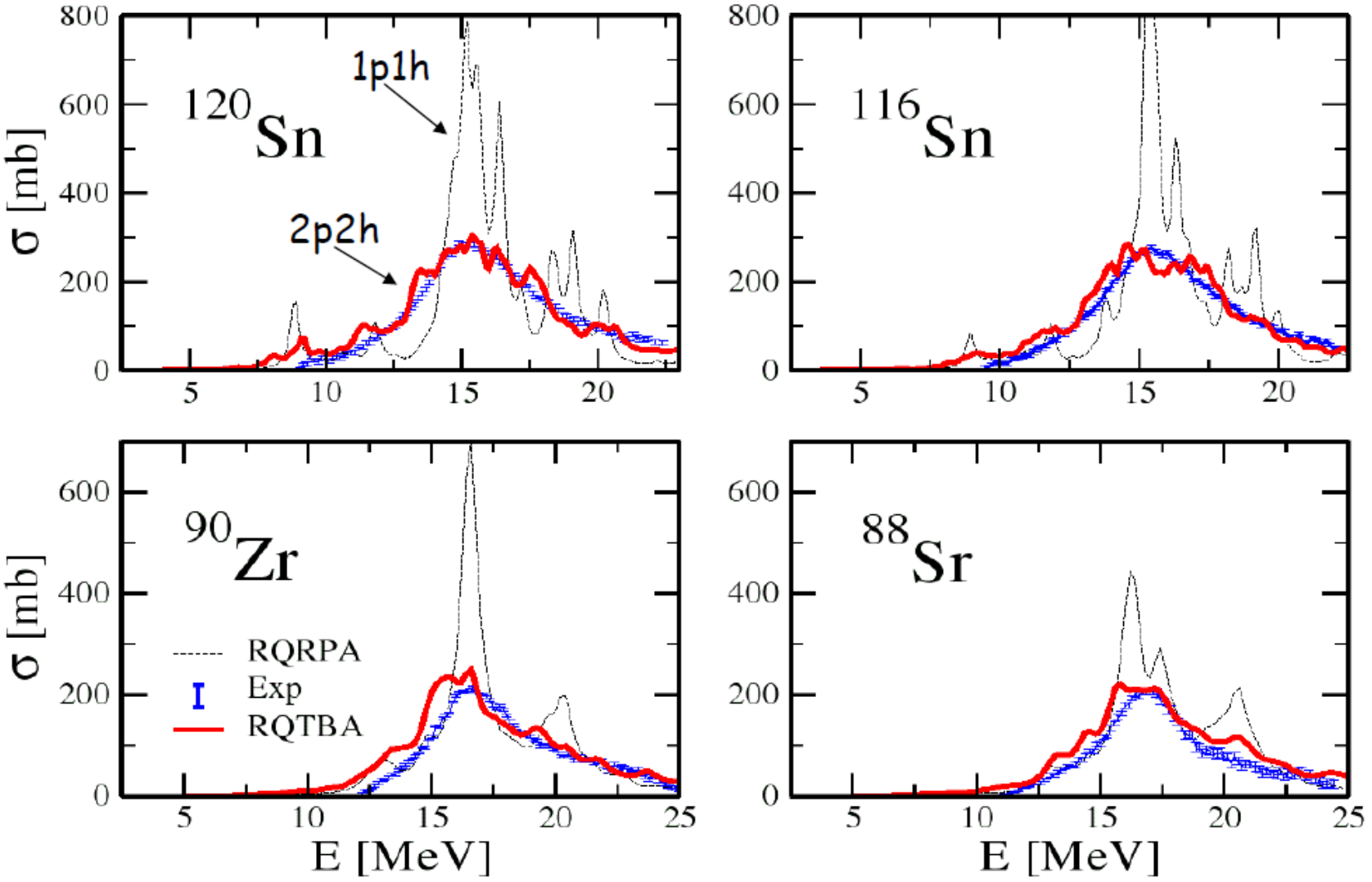
ph-phonon vertices (QRPA)



ph interaction amplitude

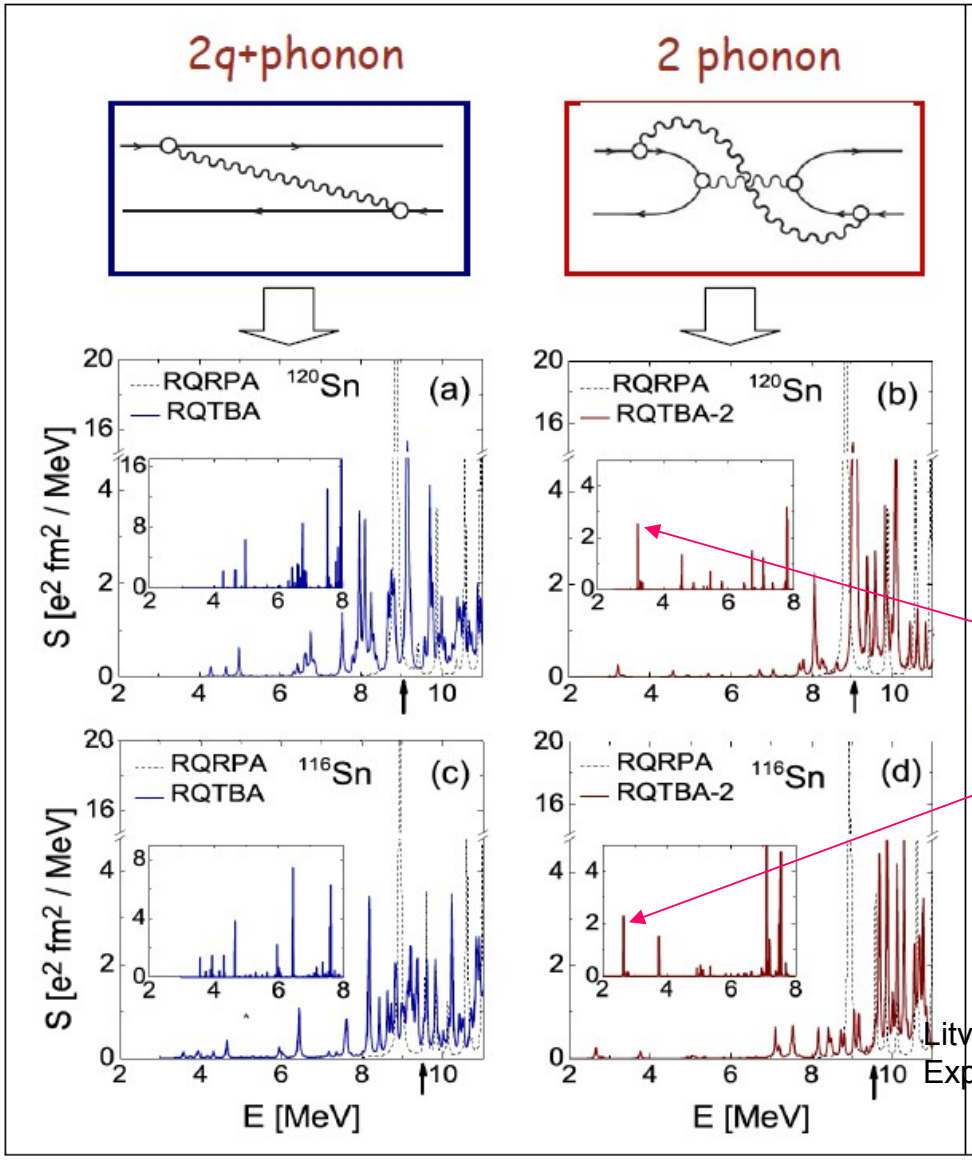


Giant Dipole Resonance within Relativistic Quasiparticle Time Blocking Approximation (RQTBA)



Litvinova, P.R., Tselyaev, PRC 78, 014312 (2008)

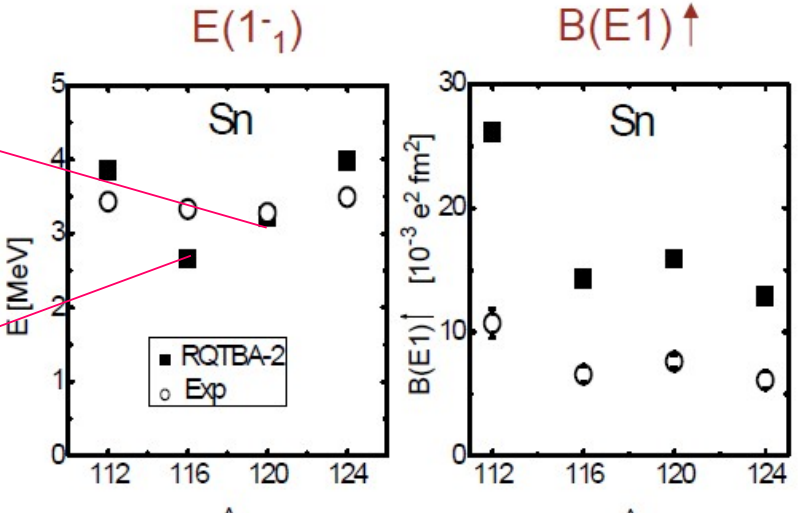
Phonon-phonon coupling:



First two-phonon state 1^-_1

$$3^- \otimes 2^+$$

$$E(1^-_1) \approx E(2^+_1) + E(3^-_1)$$

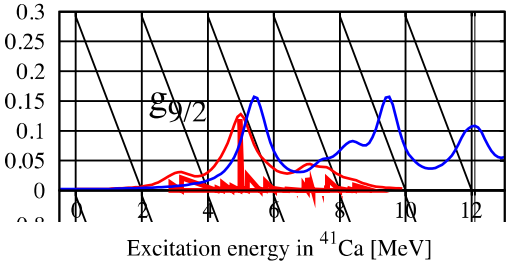


Litvinova, Ring, Tselyaev, PRL 105, 022502 (2010)
Exp: Pysmenetska et al, PRC 73, 017302 (2006)

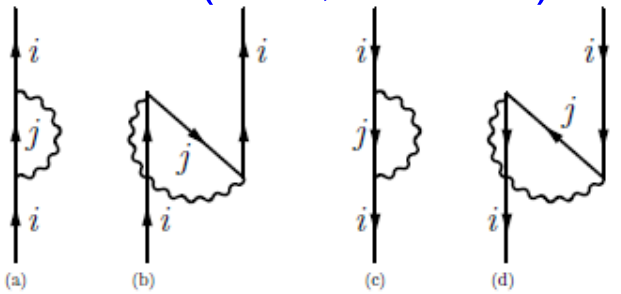
Microscopic **particle-vibration coupling** model applied to single-particle and collective states

- Starting from exact many-body equations the lowest-order approximation to PVC is calculated using consistently an effective interaction (Skyrme)

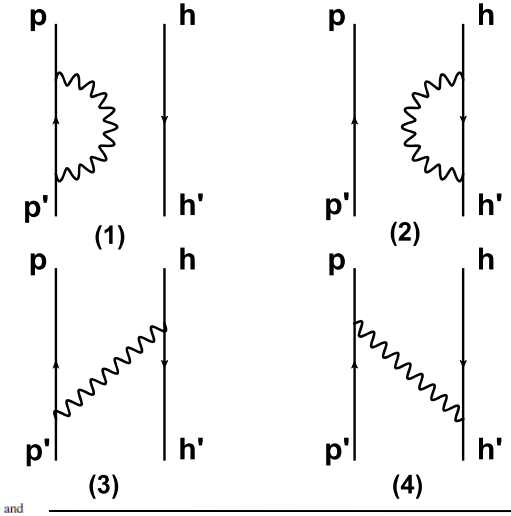
- S.p. states: r.m.s. deviations th. vs. exp. below ≈1 MeV (^{40}Ca, ^{208}Pb …)
- Implementation in the continuum:



$g_{9/2}$ strength
^{41}Ca



- Giant resonances: not only total widths but exclusive data reproduced (γ-decay from ISGQR to 3^-_1 in ^{208}Pb)



M.Brenna, X. Roca-Maza, G. Colò

IVGDR
^{120}Sn

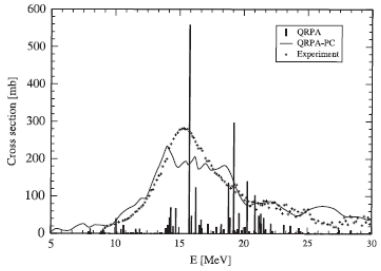


Figure 5. Photoabsorbtion cross section for ^{120}Sn, calculated with the QRPA (vertical bars) and QRPA-PC (solid curve). The theoretical results are shown in comparison with experimental values.

Generator Coordinate Method (GCM)

$$\left\langle \delta\Phi \left| \hat{H} - q\hat{Q} \right| \Phi \right\rangle = 0$$

Constraint Hartree Fock produces
wave functions depending on a generator coordinate q

$$|\Phi(q)\rangle$$

GCM wave function is a
superposition of Slater determinants

$$|\Psi\rangle \int dq\, f(q)\, |q\rangle$$

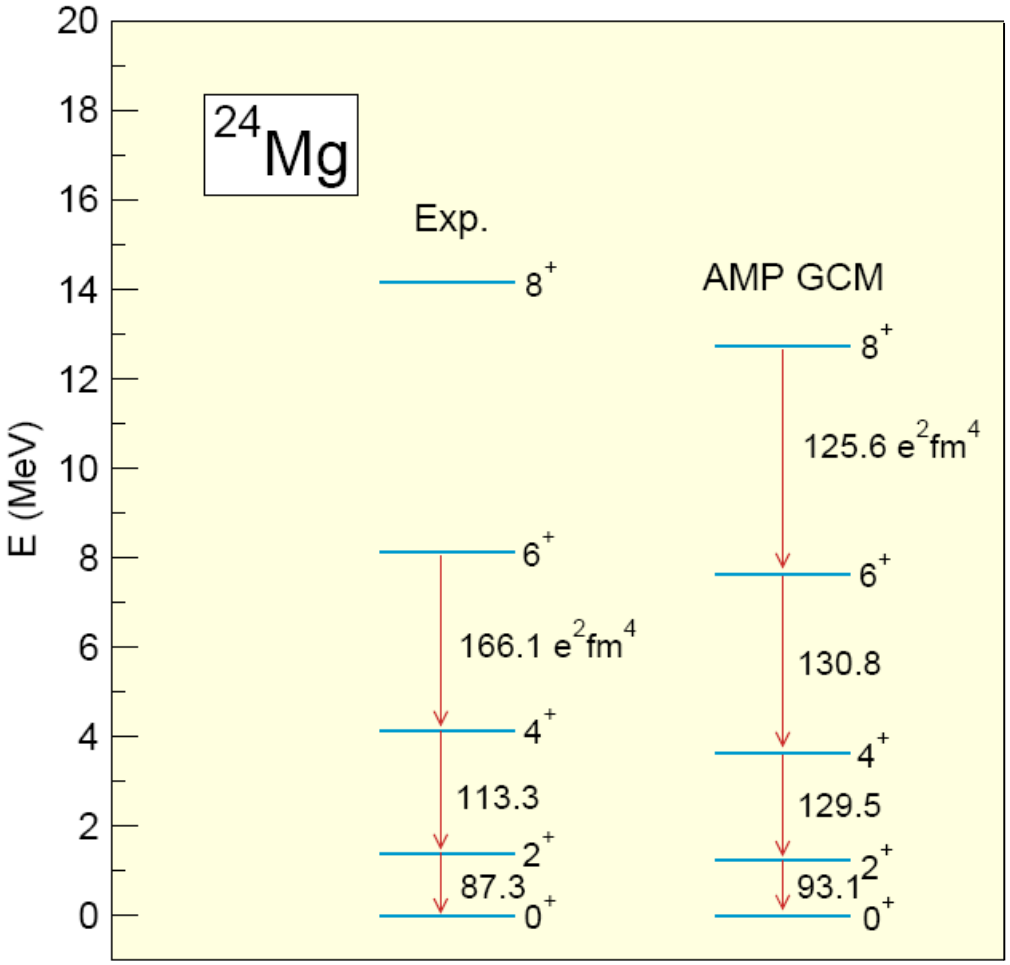
Hill-Wheeler equation:

$$\int dq' \left[\langle q|H|q' \rangle - E \langle q|q' \rangle \right] f(q') = 0$$

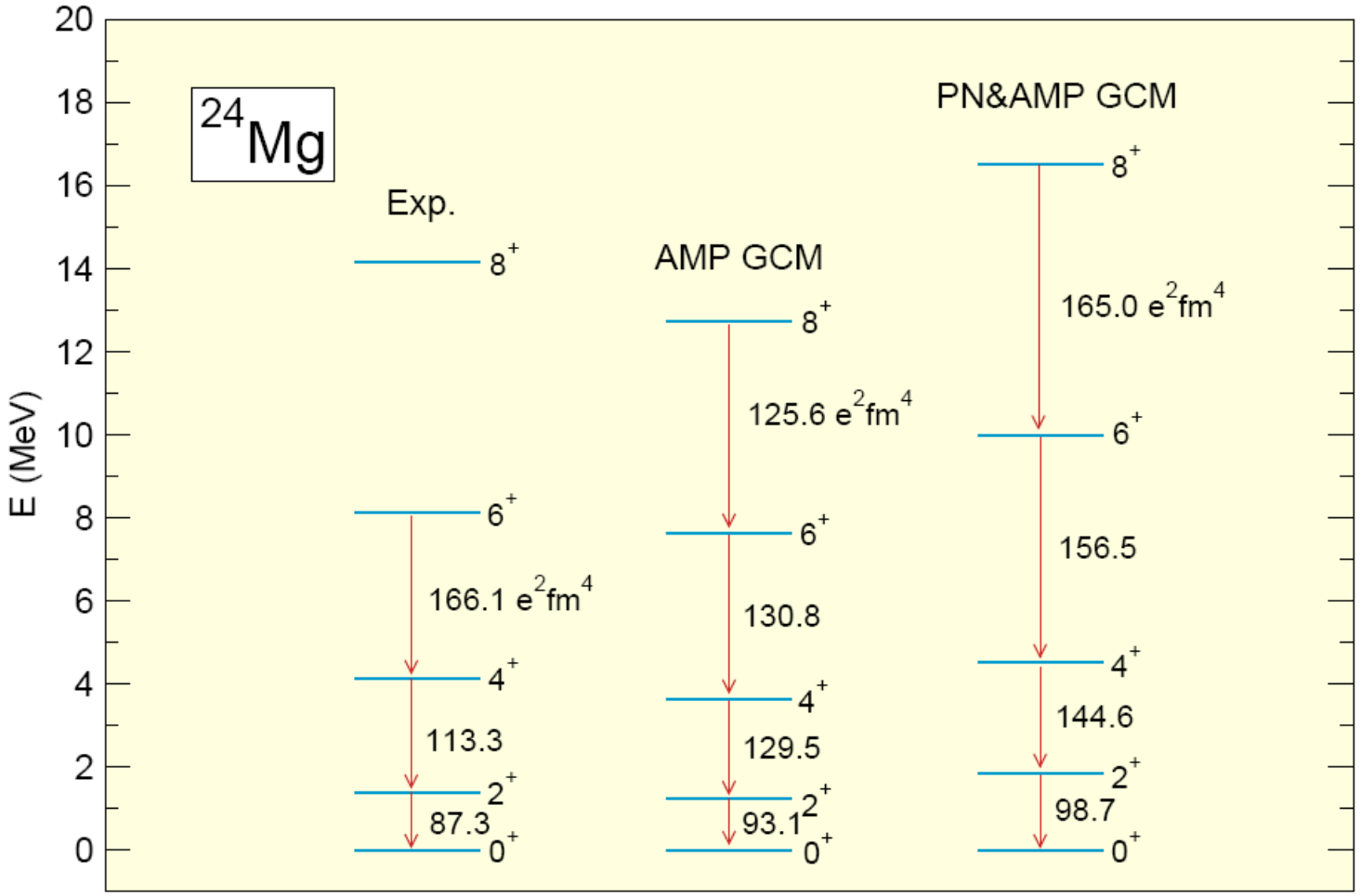
with projection:

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

Spectra in ^{24}Mg



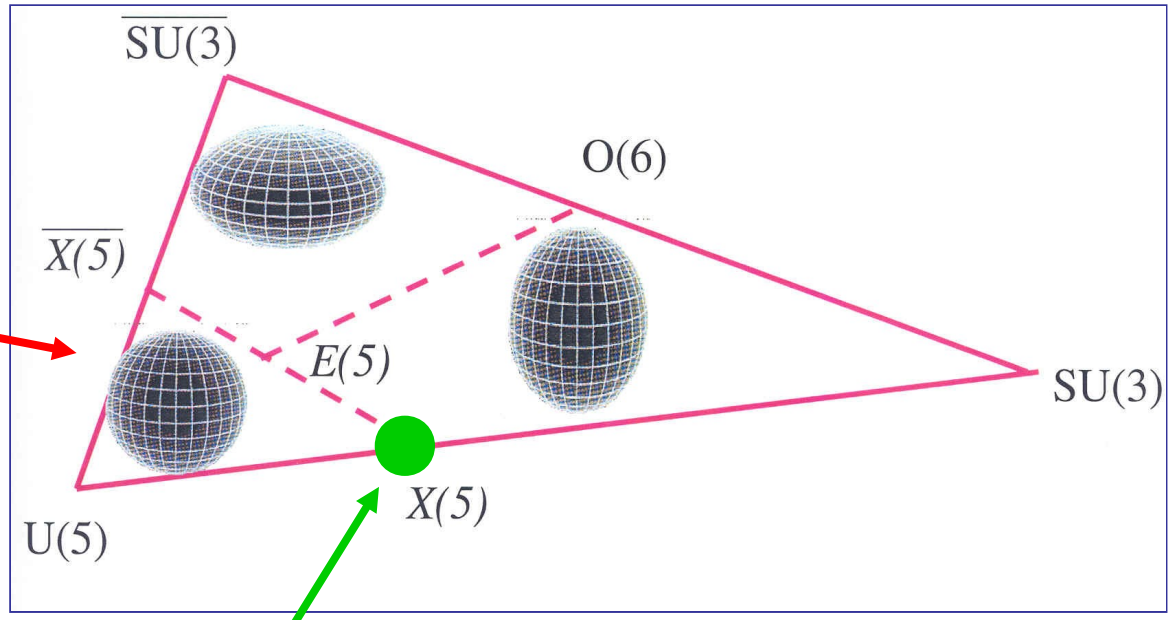
Spectra in ^{24}Mg

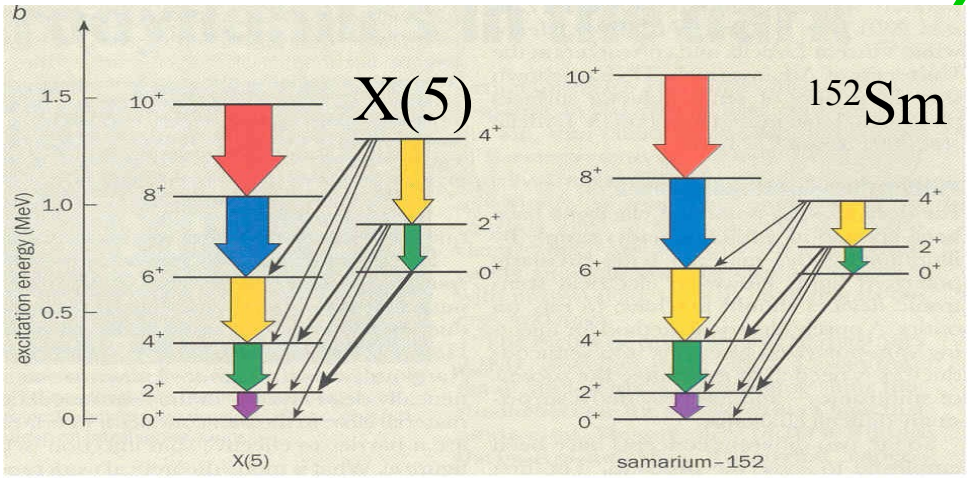


Quantum phase transitions and critical symmetries

Interacting Boson Model

Casten Triangle





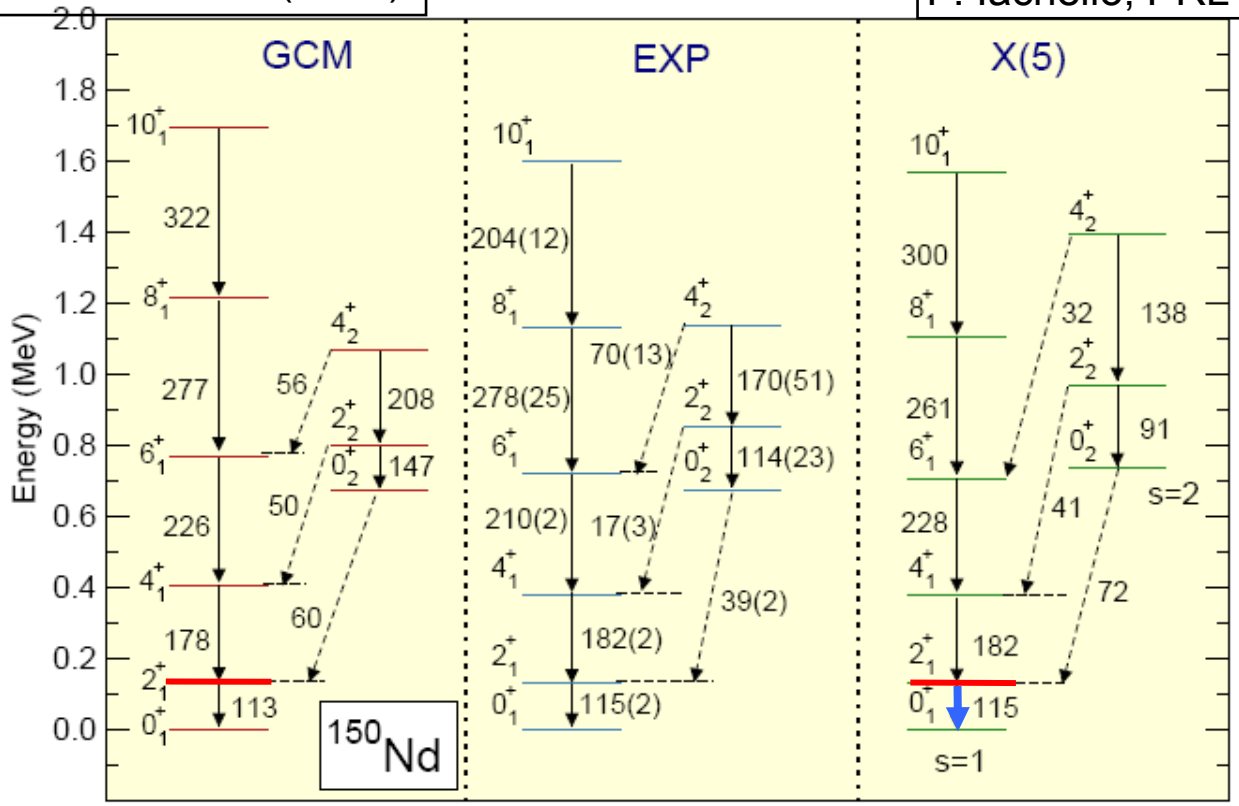
E(5): F. Iachello, PRL 85, 3580 (2000)
X(5): F. Iachello, PRL 87, 52502 (2001)

R.F. Casten, V. Zamfir, PRL 85 3584, (2000)

R. Krücken *et al*, PRL 88, 232501 (2002)

Niksic *et al* PRL 99, 92502 (2007)

F. Iachello, PRL 87, 52502 (2001)

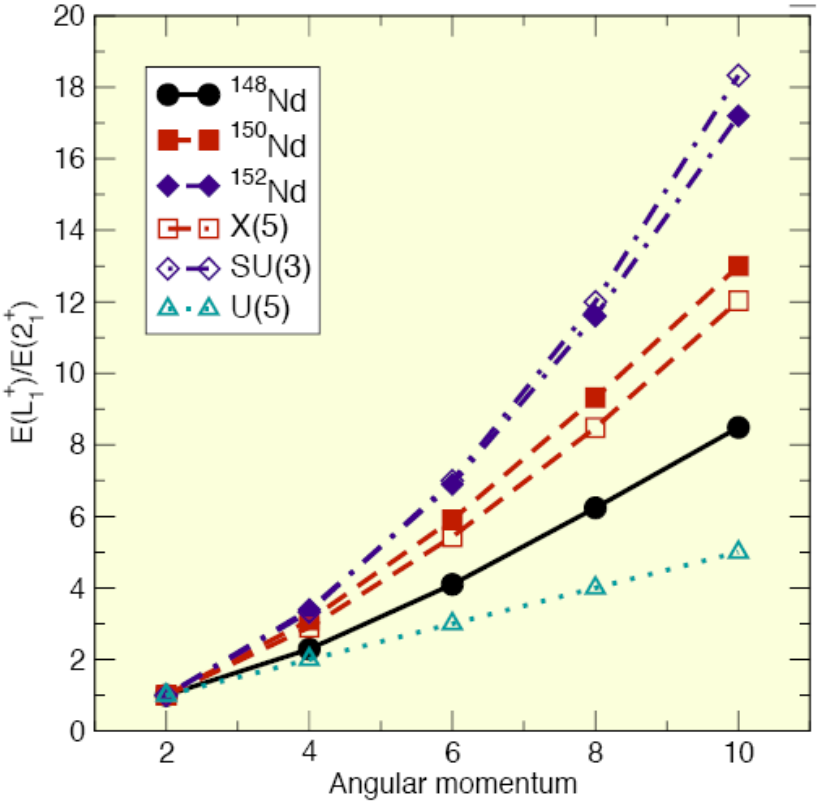


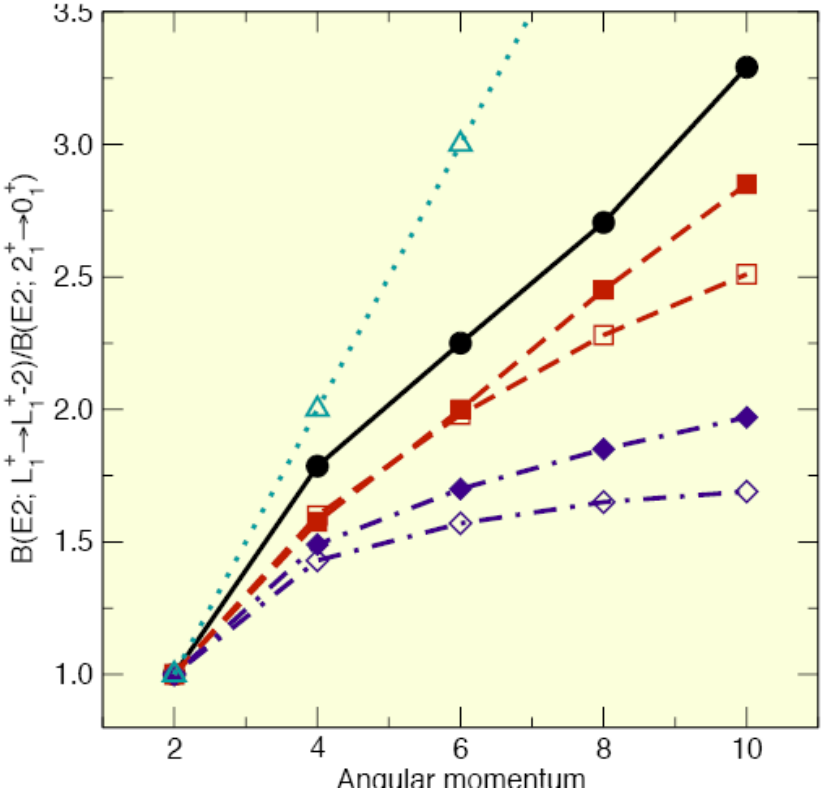
GCM: only one scale parameter: $E(2_1)$

X(5): two scale parameters: $E(2_1)$, $BE2(2_2 \rightarrow 0_1)$

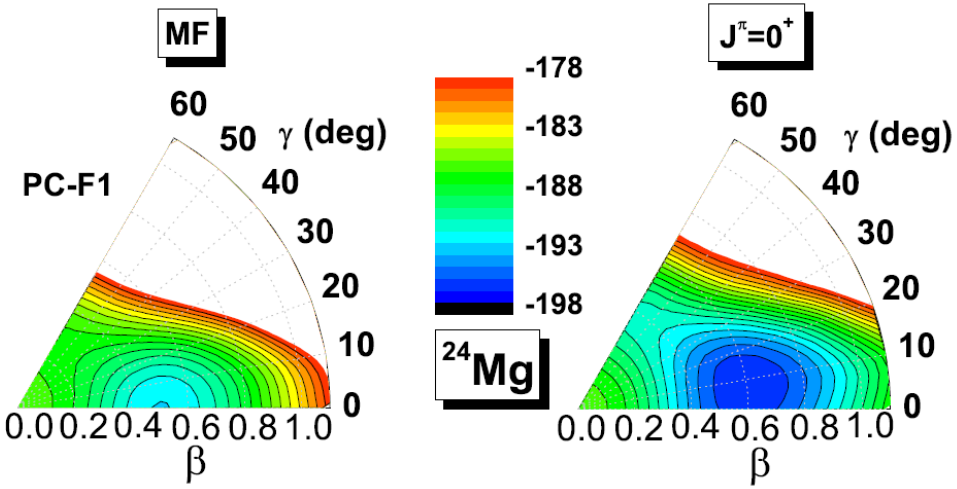
Problem of GCM at this level: restricted to γ=0

B(E2; L → L-2) values and excitation energies for the yrast states: **^{148}Nd**, **^{150}Nd**, and **^{152}Nd**, calculated with the GCM and compared with those predicted by the **X(5)**, **SU(3)** and **U(5)** symmetries.





potential energy suface:



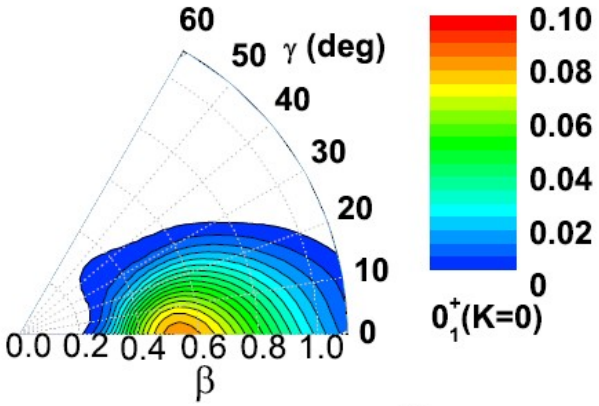
First relativictic full
D GCM calculations

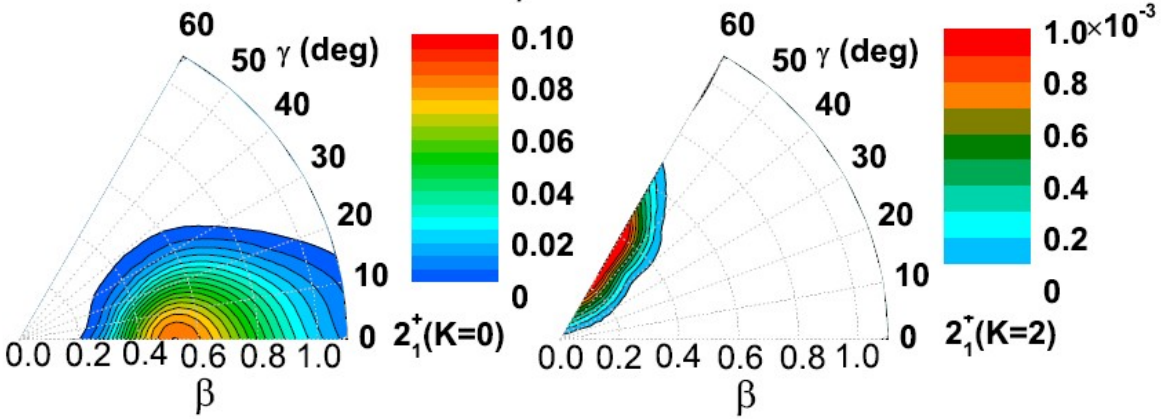
^{24}Mg

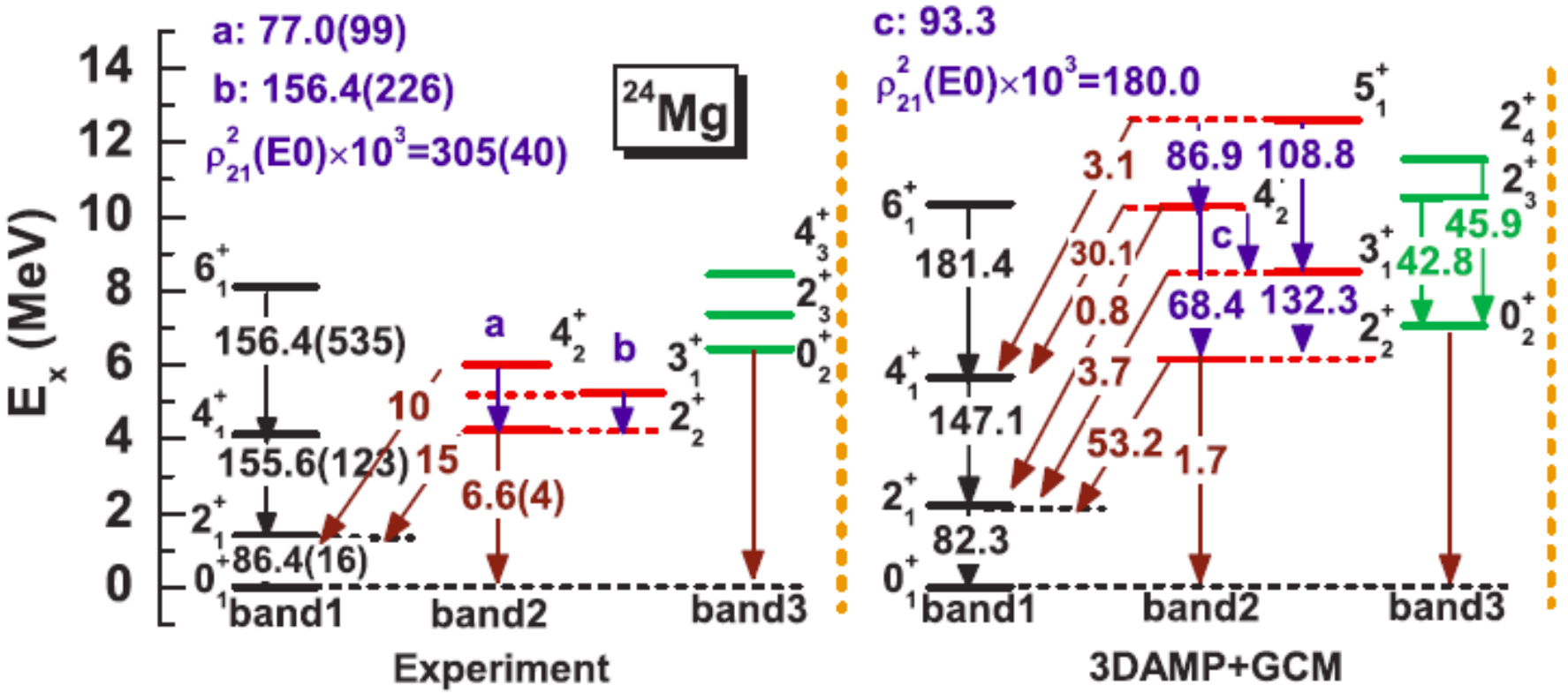
ao et al, PRC 81,044311 (2010)

collective wave functions:

^{24}Mg

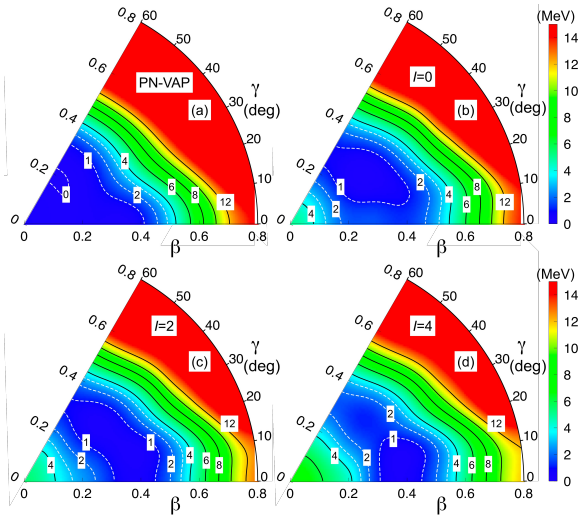


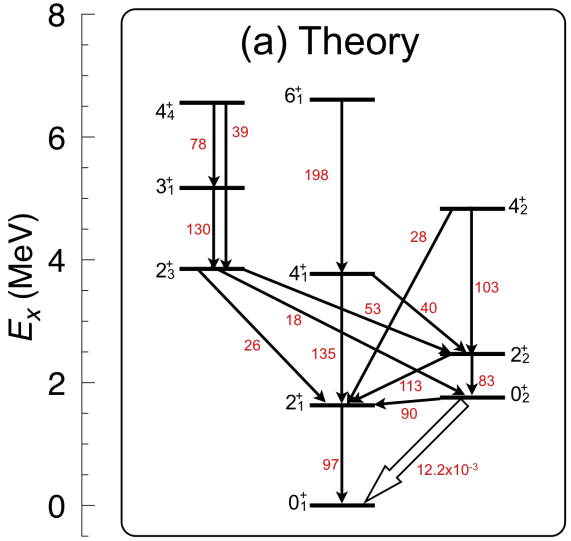


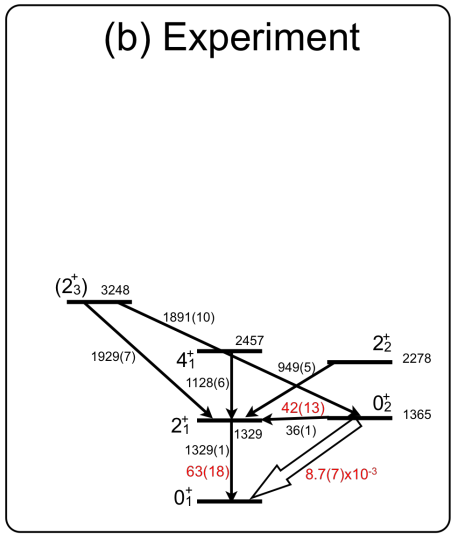


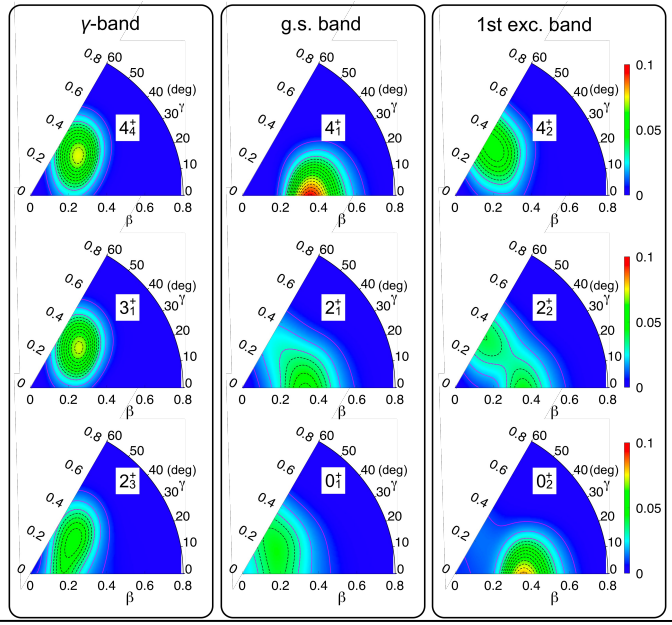
^{24}Mg

1) good agreement in BE2-values (no effective charges)
2) theoretical spectrum is streched
3) β-band has no rotational character









T. Rodriguez, L Egido 2011

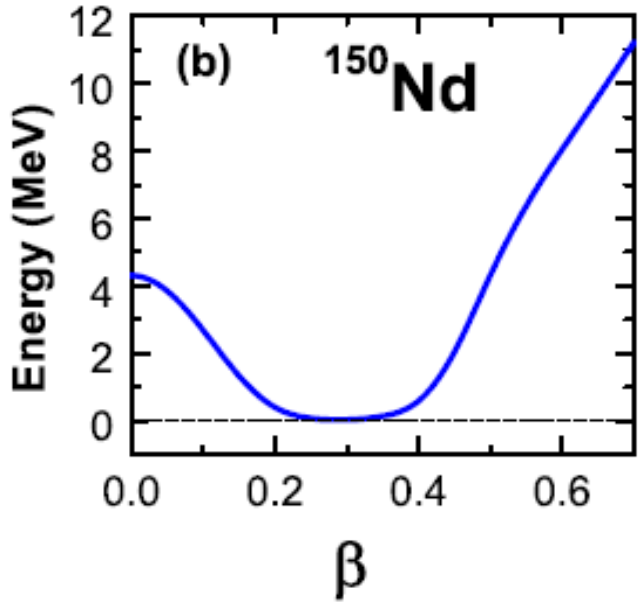
triaxial GCM in q=(β,γ) is approximated by the diagonalization of a 5-dimensional Bohr Hamiltonian:

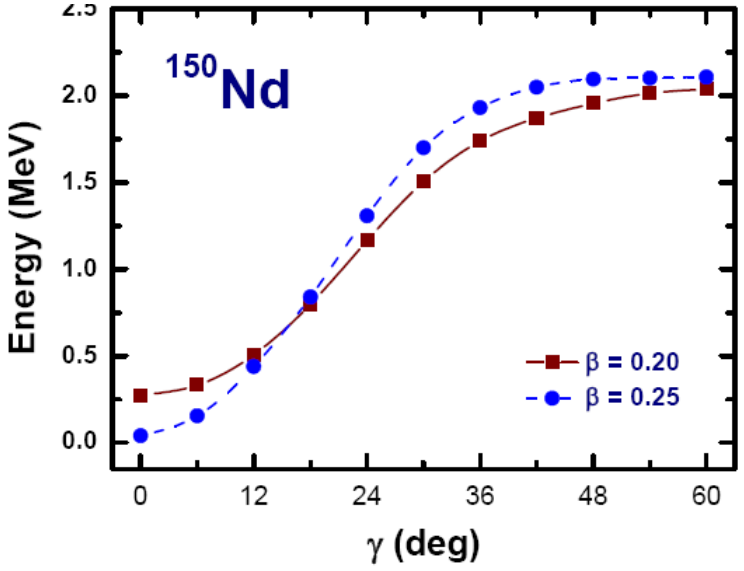
Bohr Hamiltonian: $H = -\frac{\partial}{dq}\frac{1}{2B(q)}\frac{\partial}{dq} + V(q) + V_{corr}(q)$

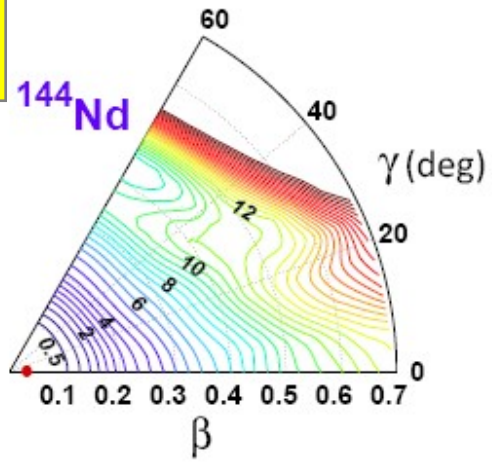
the potential and the inertia functions are calculated microscopically from rel. density functional

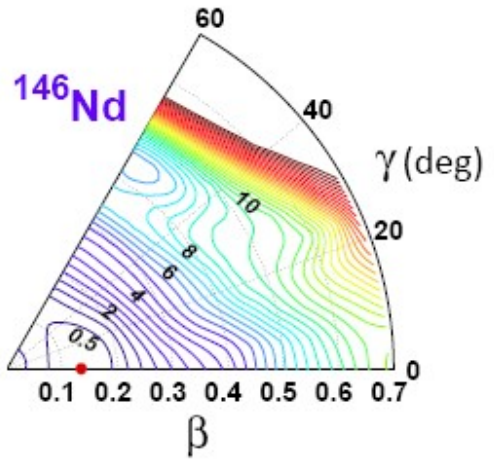
Theory:	Giraud and Grammaticos (1975)	(from GCM)
	Baranger and Veneroni (1978)	(from ATDHF)
Skyrme:	J. Libert,M.Girod, and J.-P. Delaroche (1999)	
RMF:	L. Prochniak and P. R. (2004)	
	Niksic, Li, et al (2009)	

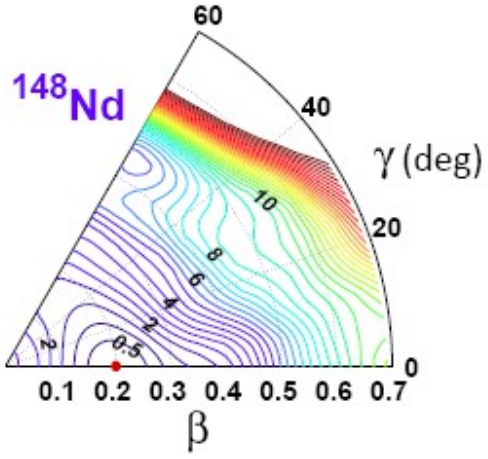
Potential energy surfaces:

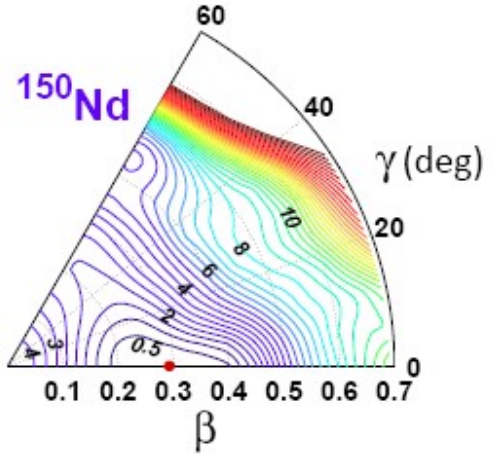


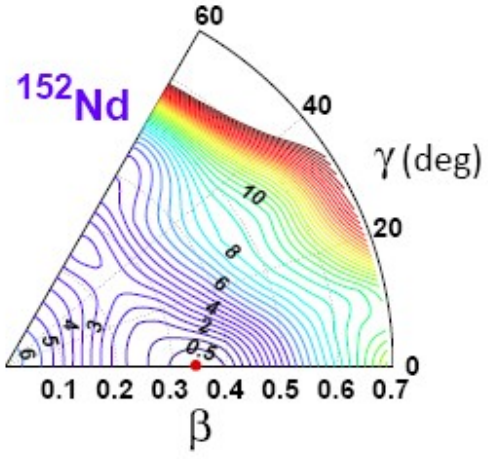


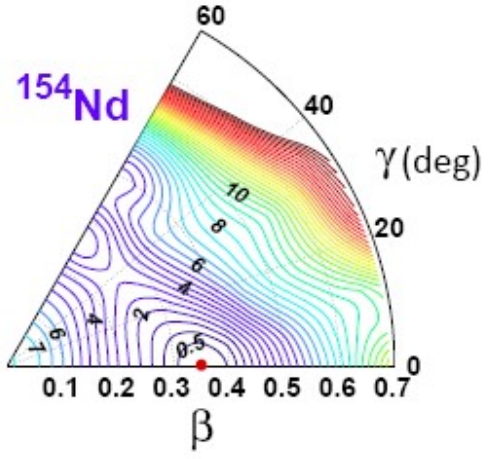






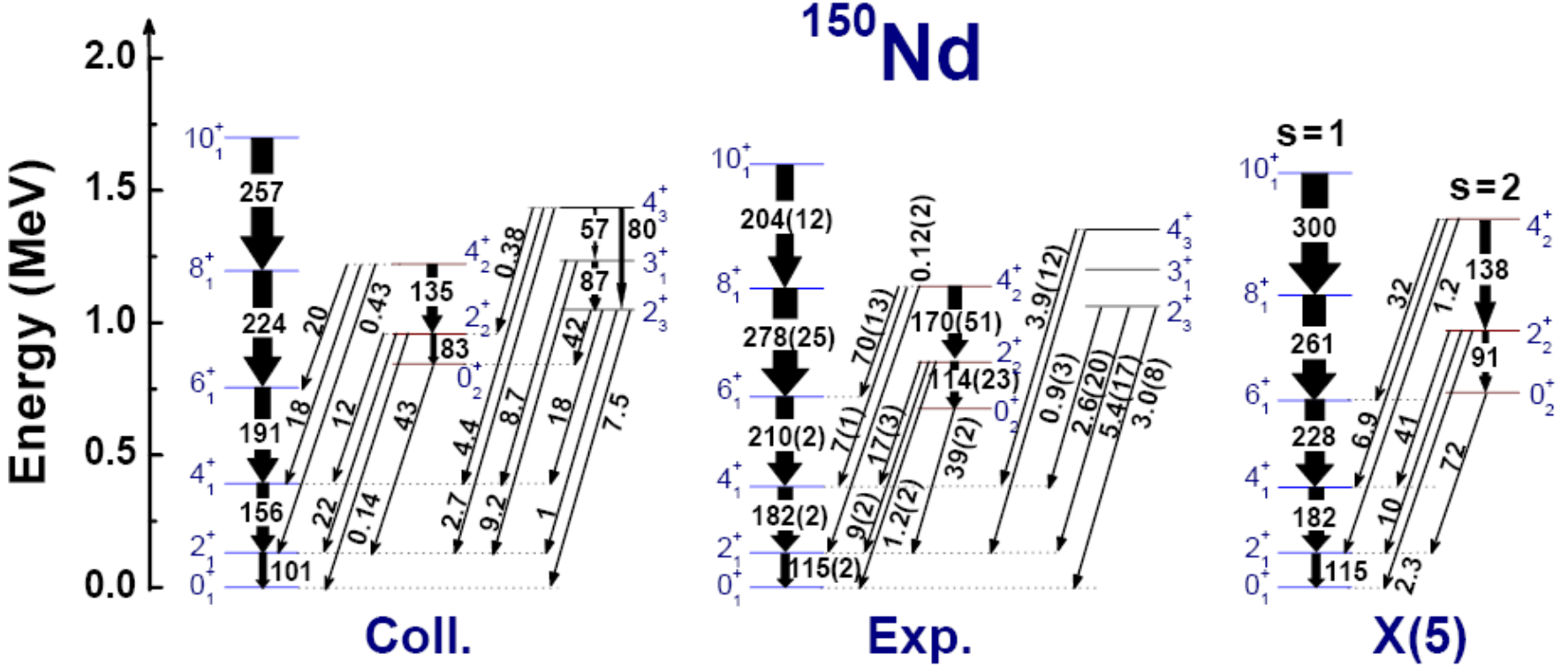






Microscopic analysis of nuclear QPT

- **Spectum**

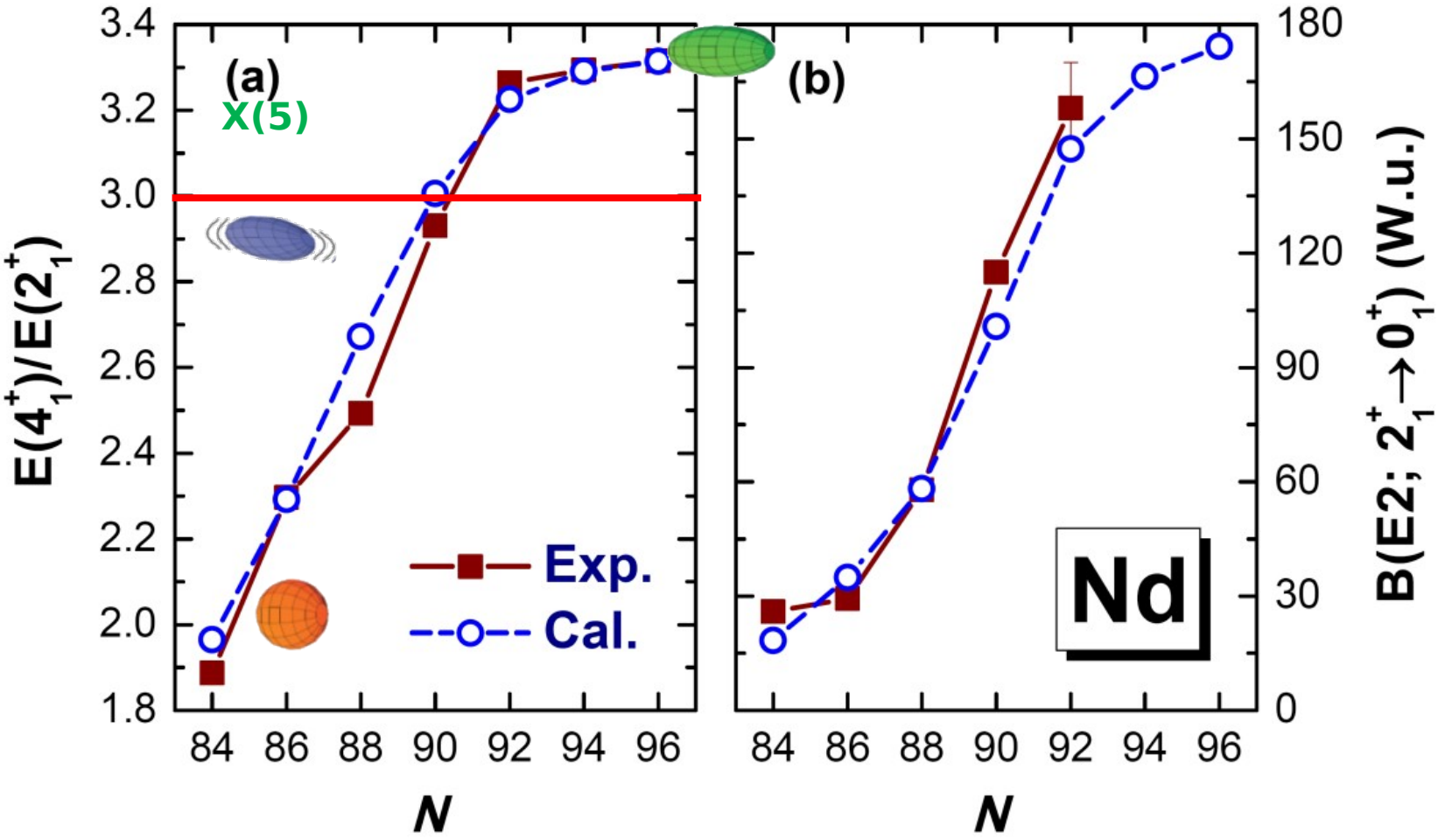


GCM: only one scale parameter: $E(2_1)$

X(5): two scale parameters: $E(2_1)$, $BE2(2_2 \rightarrow 0_1)$

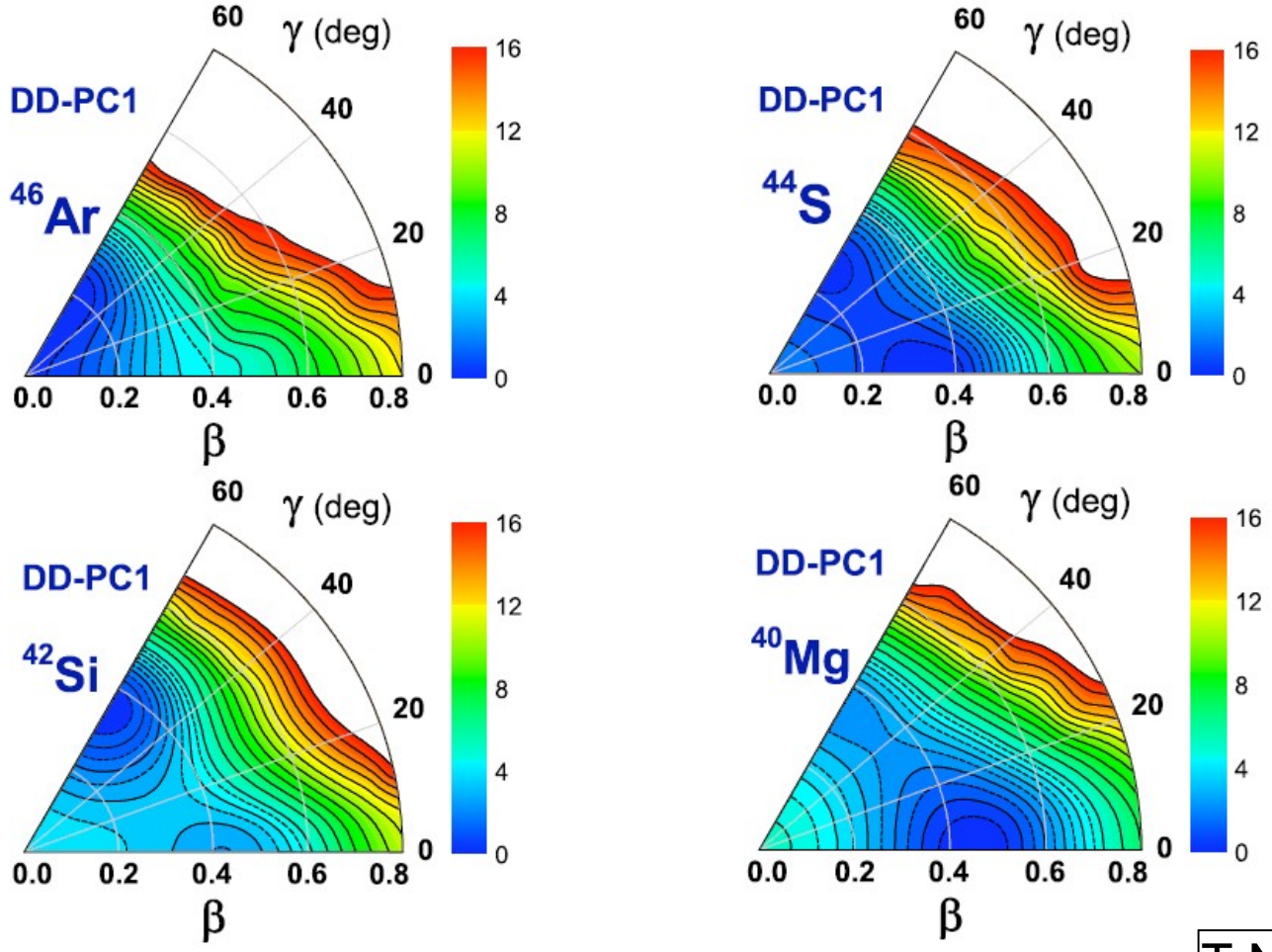
No restriction to axial shapes

Sharp increase of $R_{42}=E(4_1)/E(2_1)$ and $B(E2;2_1\text{-}0_1)$



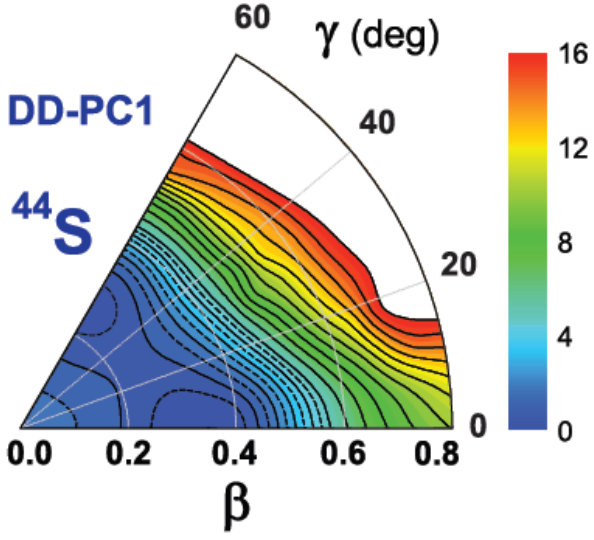
Applications: $N = 28$ isotones

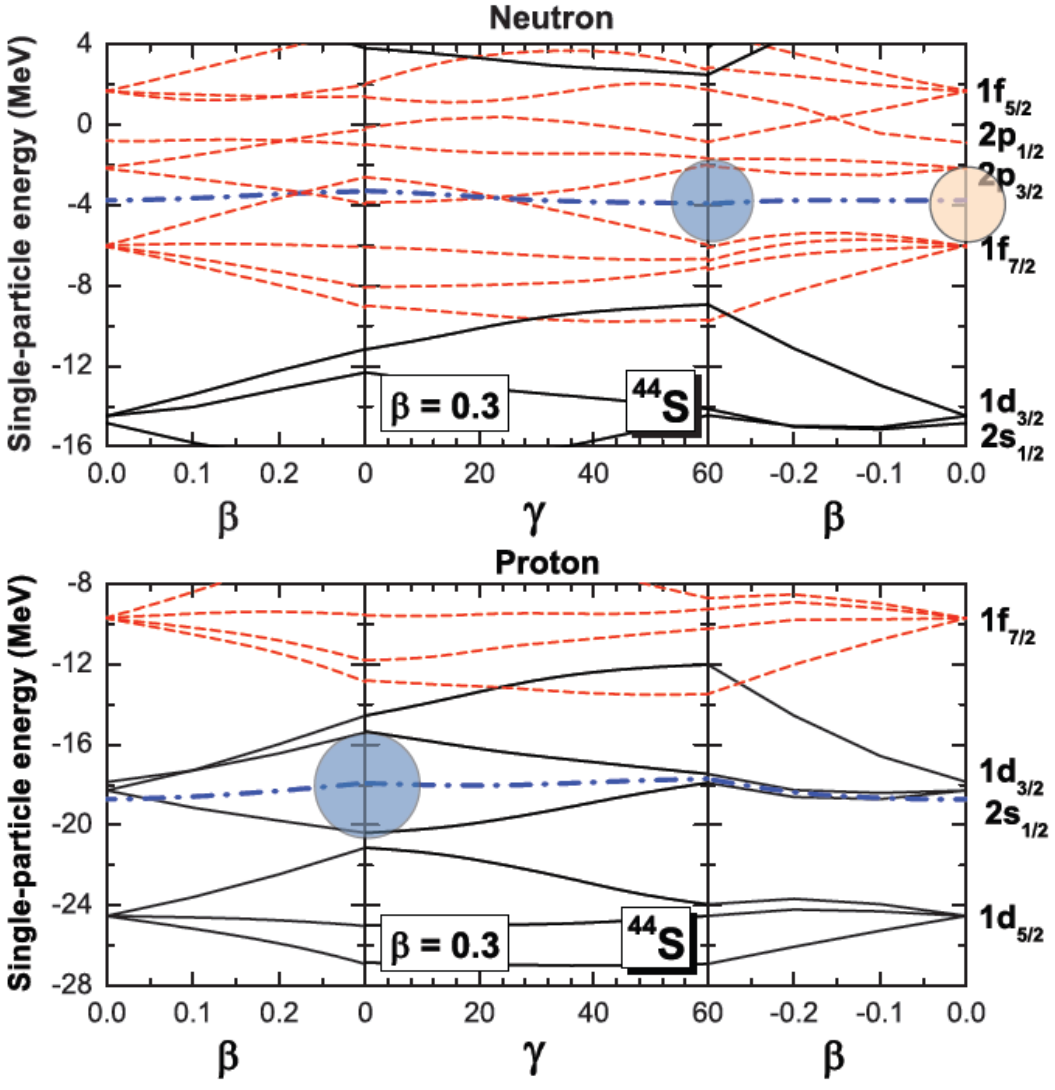
The variation of the mean-field shapes is governed by the evolution of the underlying shell structure of single-nucleon orbitals.



T.Niksic (2011)

^{44}S isotope: single-particle levels

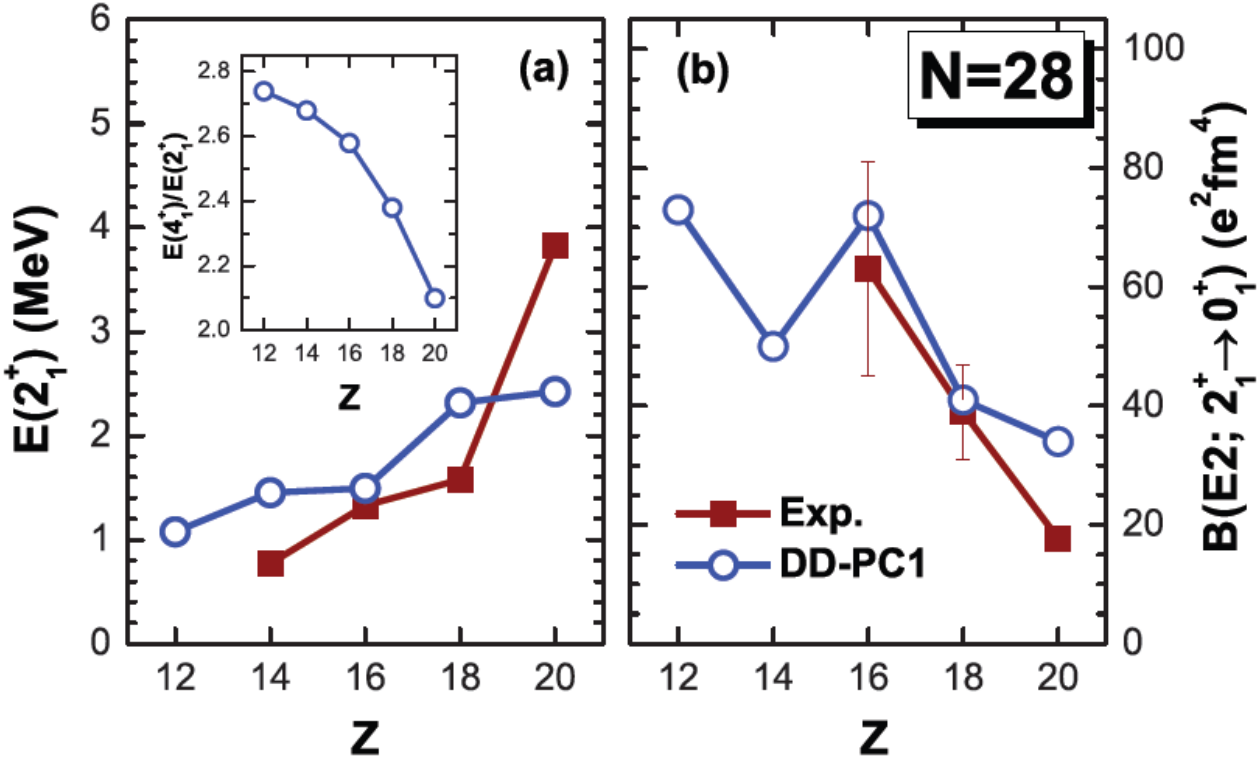




T.Niksic (2011)

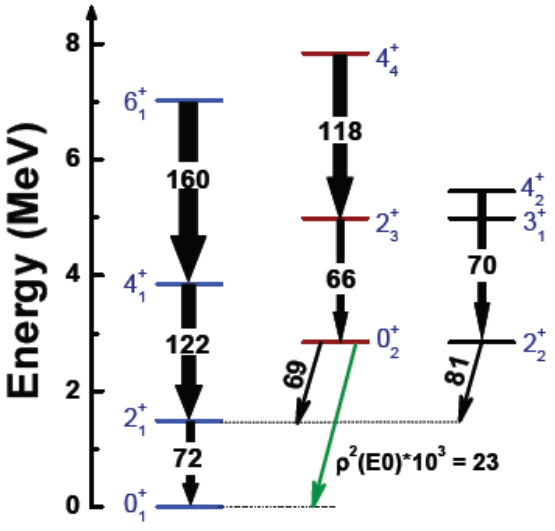
$N \approx 28$ observables

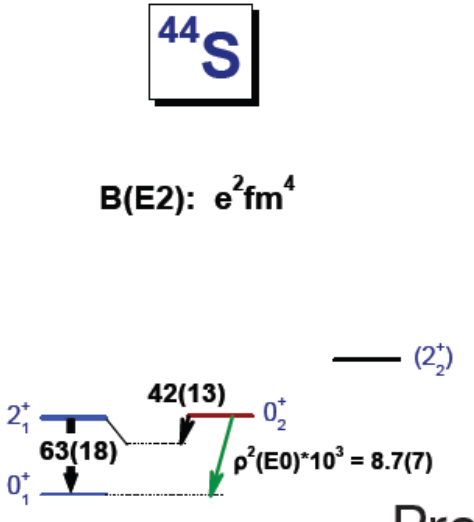
- excitation energies and reduced electric quadrupole transition probabilities
- full configuration space, no need for effective charges

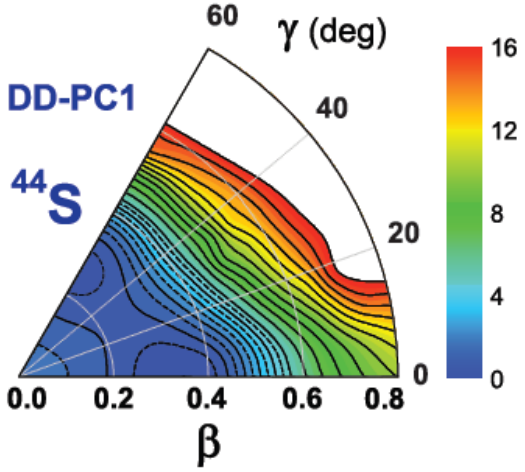


T.Niksic (2011)

^{44}S isotope: level scheme

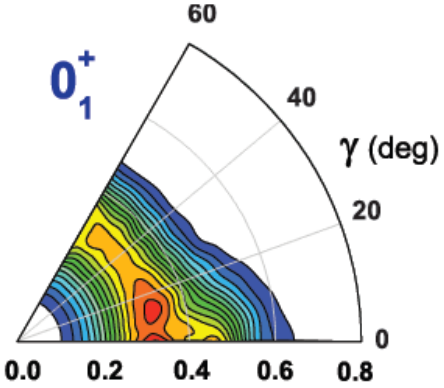


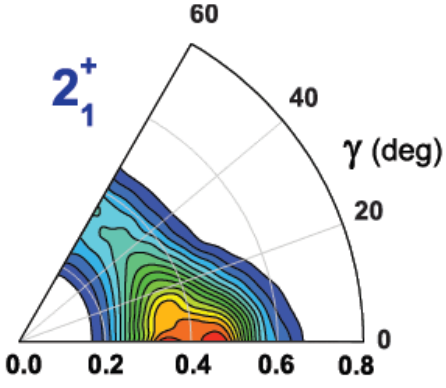


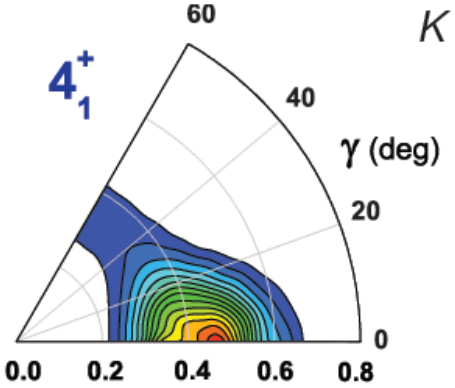


Probability density distribution:

$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^I_{\alpha K}(\beta,\gamma)|^2 \beta^3$$







T.Niksic (2011)

Summary and outlook:

- Present status
- Density functional theory provides a very successful and microscopic description for ground states and excited states in nuclei.
- there are non-relativistic and relativistic functionals
  there are zero-range and finite range functionals
- most of the successful functionas are present phenomenological
  modern functionals try to include microscopic „pseudodata“

- the mean field level we have no energy dependence of the self-energy
- and symmetry violations and no fluctuations
- energy dependence of the self energy can be treated by part.-vibr. Coupling
- symmeties and fluctuations can be treated by the projection and the GCM method
- The concept of a Bohr-Hamiltonian simplifies the calculations considerably

- Open problems and perspectives
  static part: we are far from a microscopic derivation
  we have to improve the functionals in the ph and the pp-channel
  dynamic part: PVC so far restricted to spherical systems
  GCM is restricted to very few degrees of freedom
  concept of GCM violates the local density approximation