



Microscopic Description of Quantum Phase Transitions in Nuclei

Cocoyoc, May. 17, 2012

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UNIVERSITÄT
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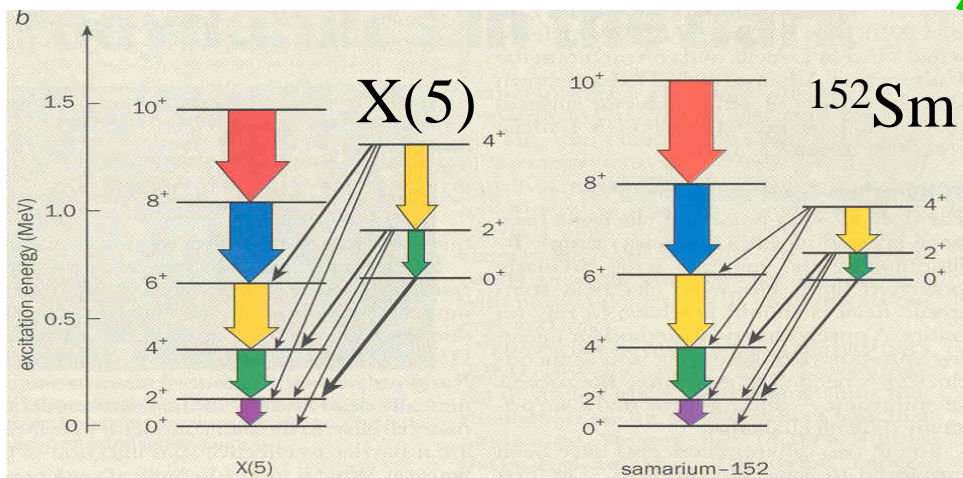
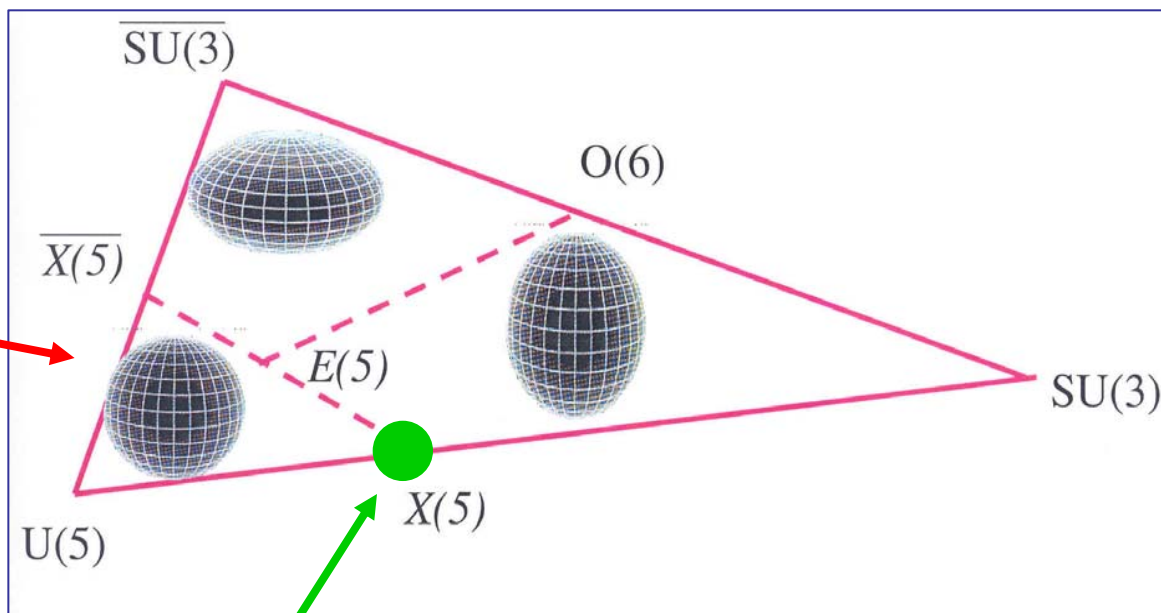
Content:

- **Quantum phase transitions**
- **Covariant density functional theory**
- **Calculations of Spectra**
 - Generator Coordinate Method
 - axial symmetric calculations of the Ne-chain
 - 5-dimensional Bohr Hamiltonian
- **Order parameters**
 - R42, B(E2),
 - isomer shifts,
 - E0-strength
- **Conclusions**

Quantum phase transitions and critical symmetries

Interacting Boson Model

Casten Triangle

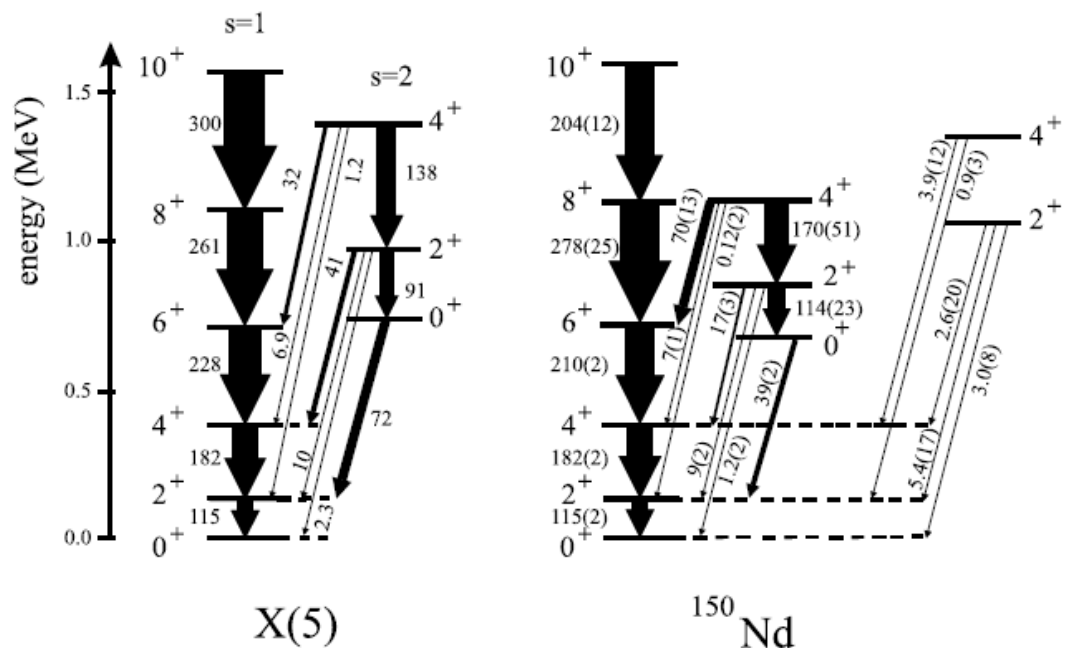


E(5): F. Iachello, PRL 85, 3580 (2000)
 X(5): F. Iachello, PRL 87, 52502 (2001)

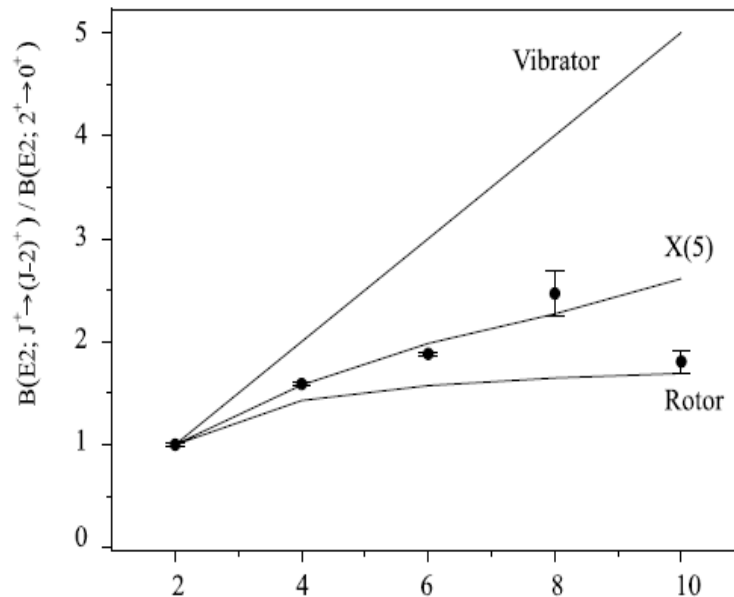
R.F. Casten, V. Zamfir, PRL 85 3584, (2000)

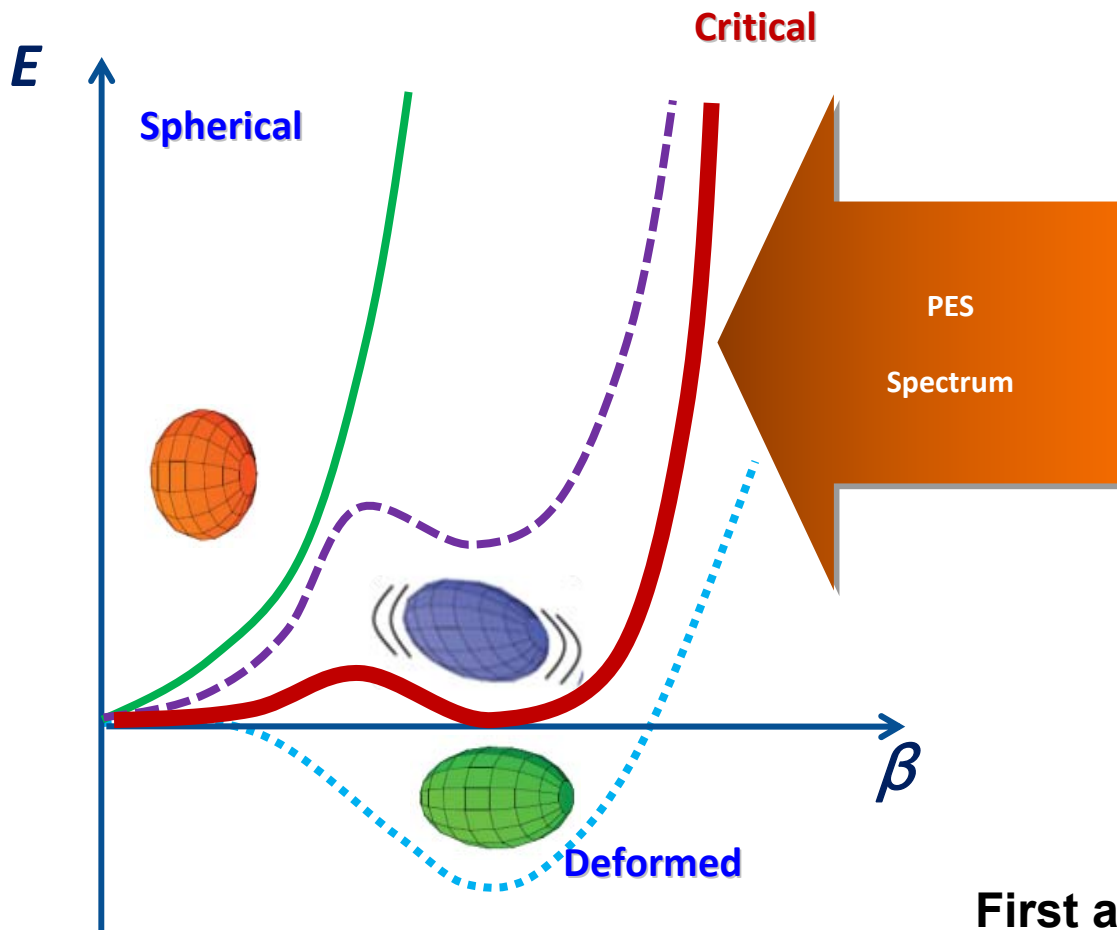
Transition U(5) \rightarrow SU(3) in Nd-isotopes

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



$$R = \frac{B(E2; J \rightarrow J-2)}{B(E2; 2^+ \rightarrow 0^+)}$$





First and second order QPT can occur between systems characterized by different ground-state **shapes**.

Control Parameter: **Number of nucleons**

Density functional theory in nuclei:

$$E[\hat{\rho}] = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | H_{eff}(\rho) | \Phi \rangle$$

Skyrme
Gogny
RMF

$|\Phi\rangle$ Slater determinant $\iff \hat{\rho}$ density matrix

$$|\Phi\rangle = \mathcal{A}\{\varphi_1(\mathbf{r}_1) \dots \varphi_A(\mathbf{r}_A)\} \iff \hat{\rho}(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^A |\varphi_i(\mathbf{r})\rangle \langle \varphi_i(\mathbf{r}')|$$

Mean field:

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Eigenfunctions:

$$\hat{h}|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle$$

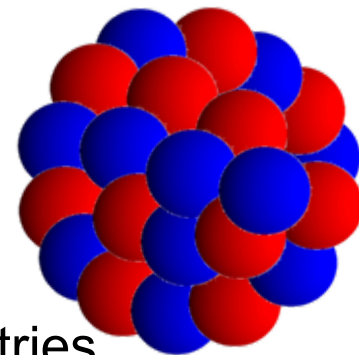
Interaction:

$$\hat{V} = \frac{\delta^2 E}{\delta \hat{\rho} \delta \hat{\rho}}$$

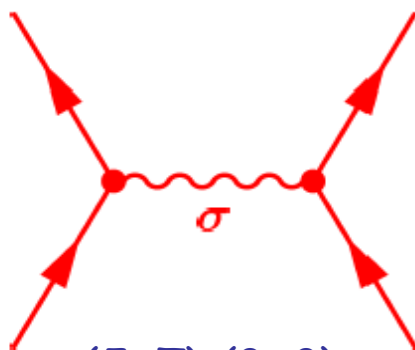
Extensions: Pairing correlations, Covariance
Relativistic Hartree Bogoliubov (RHB) theory

$$E[\rho]$$

Walecka model:



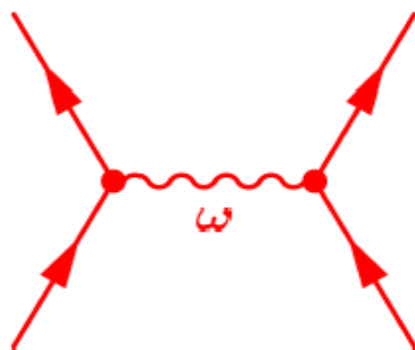
- the basis is an **effective Lagrangian** with all relativistic symmetries
- it is used in a **mean field concept** (Hartree-level)
- with the **no-sea approximation**



$$(J^\pi, T) = (0^+, 0)$$

$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r})$$

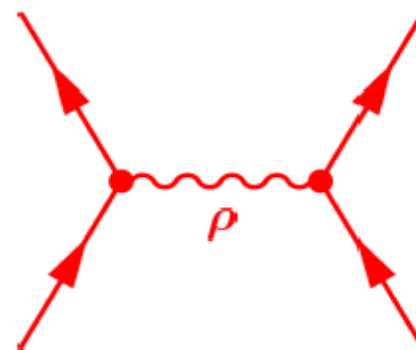
Sigma-meson:
attractive scalar field



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

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

Omega-meson:
short-range repulsive



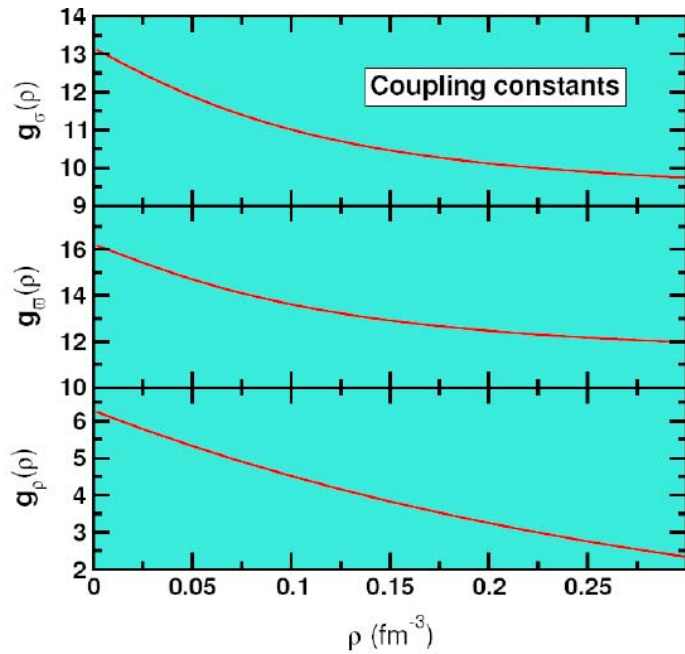
$$(J^\pi, T) = (1^-, 1)$$

Rho-meson:
isovector field

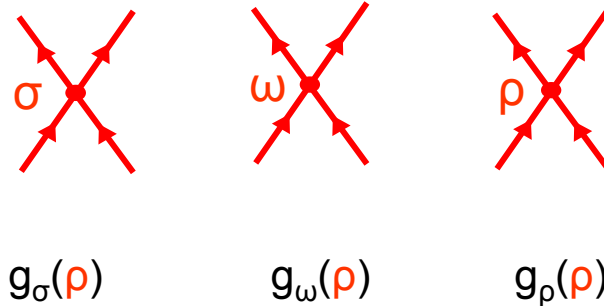
Effective density dependence:

The basic idea comes from **ab initio calculations**
density dependent coupling constants include **Brueckner correlations**
and **threebody forces**

non-linear meson coupling: **NL3**



Point-coupling models
with derivative terms:



adjusted to ground state properties of finite nuclei

Manakos and Mannel, Z.Phys. **330**, 223 (1988)

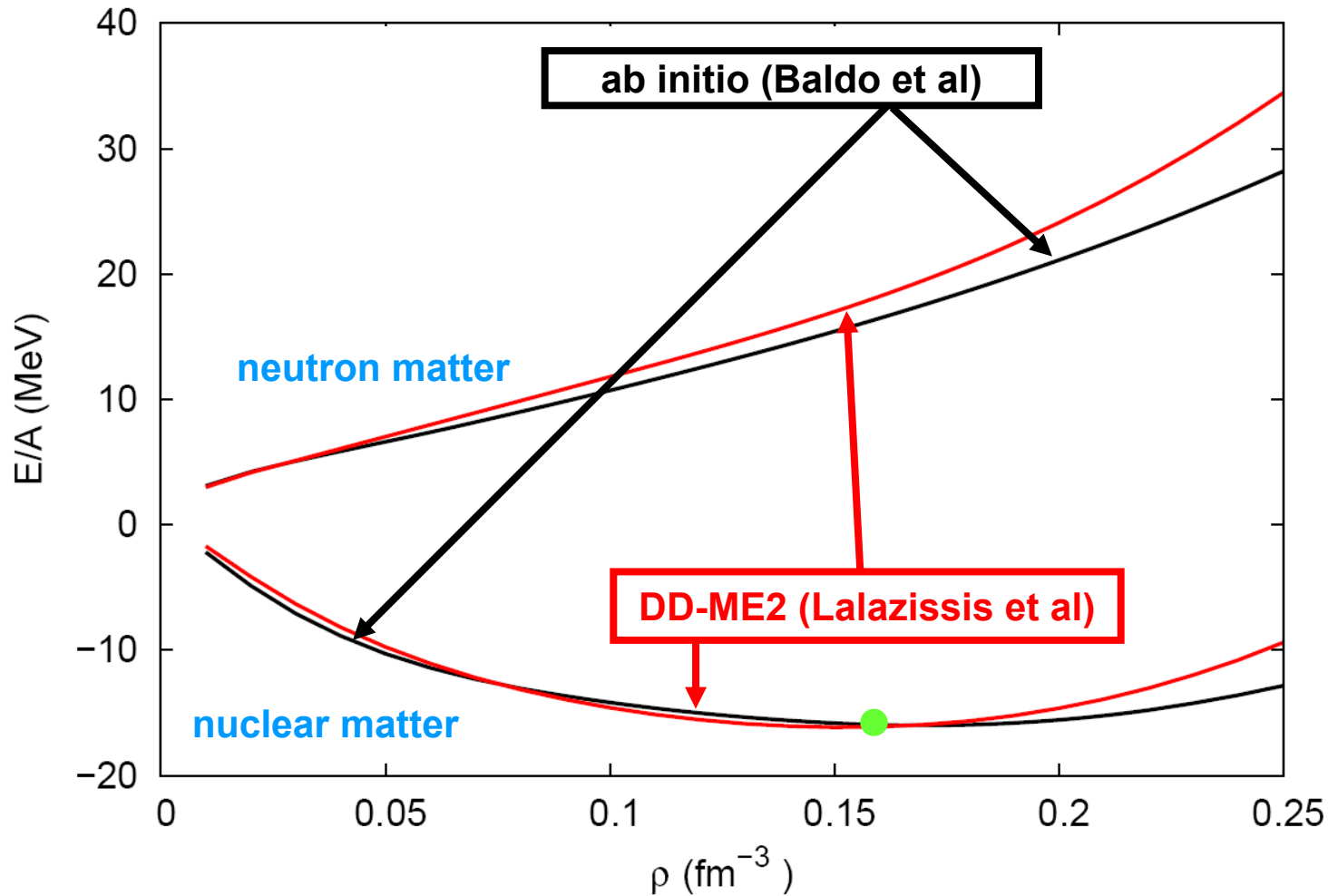
Bürvenich, Madland, Maruhn, Reinhard, PRC **65**, 044308 (2002):

Niksic, Vretenar, P.R., PRC **78**, 034318 (2008):

PC-F1

DD-PC1

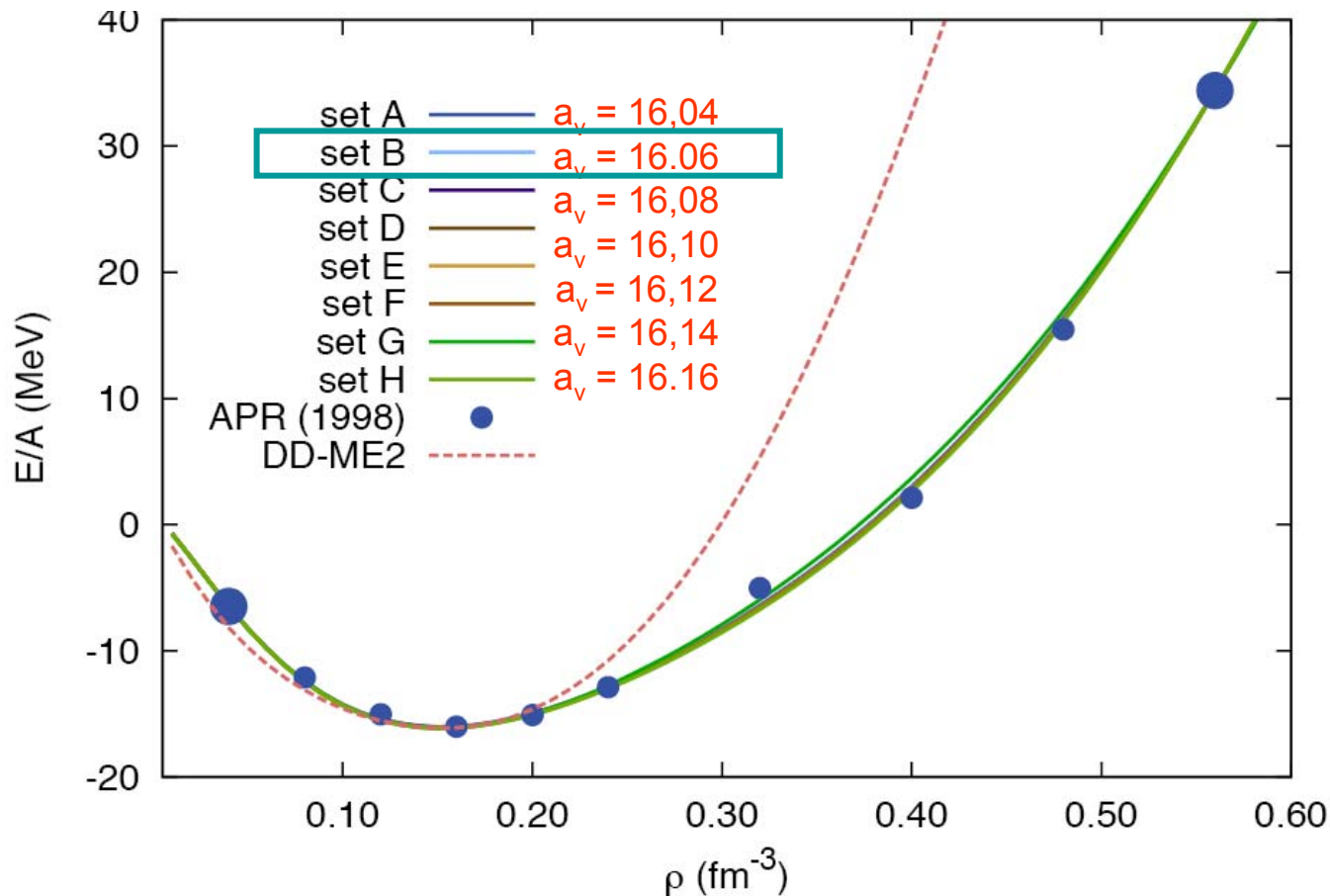
Comparison with ab-initio calculations:



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

Adjustment to ab-initio calculations:

point coupling model is adjusted to microscopic nuclear matter:



$\rho_{\text{sat}} = 0.152 \text{ fm}^{-3}$
 $m^* = 0.58m$
 $K_{\text{nm}} = 230 \text{ MeV}$

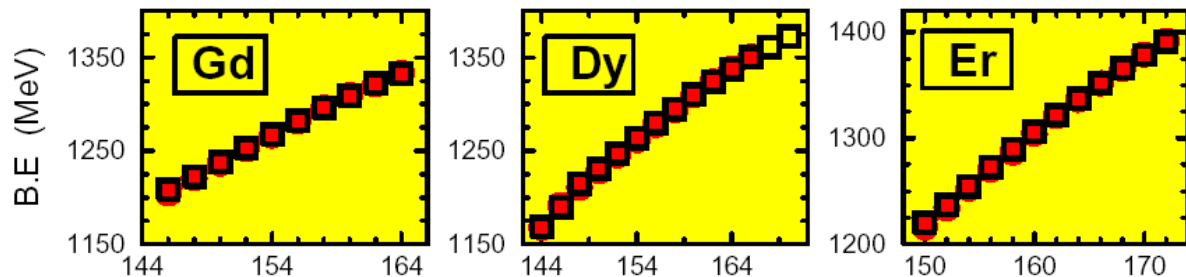
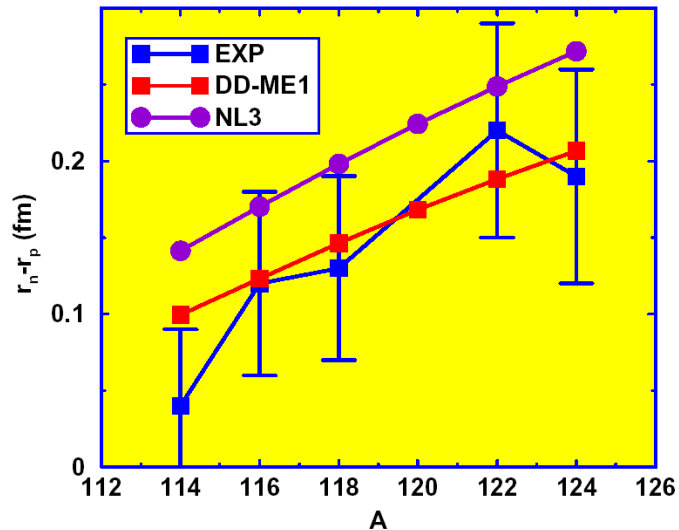
DD-PC1

● A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, PRC. 58, 1804 (1998).

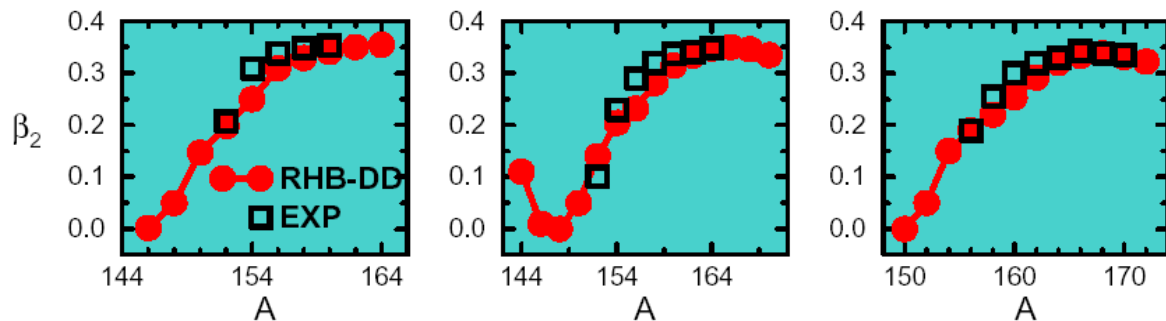
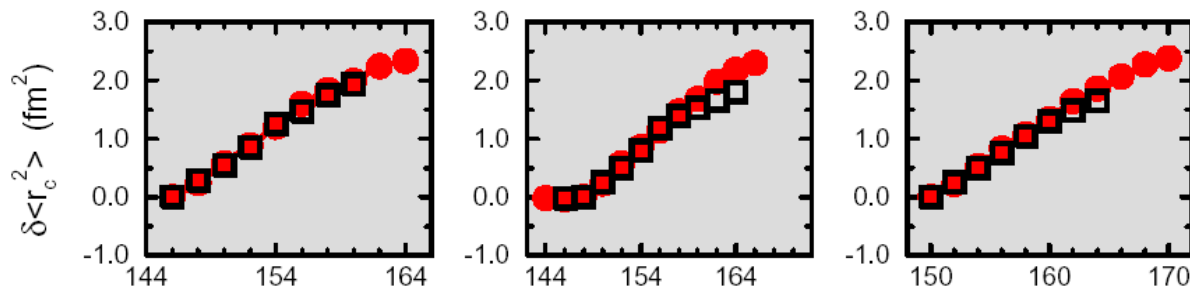
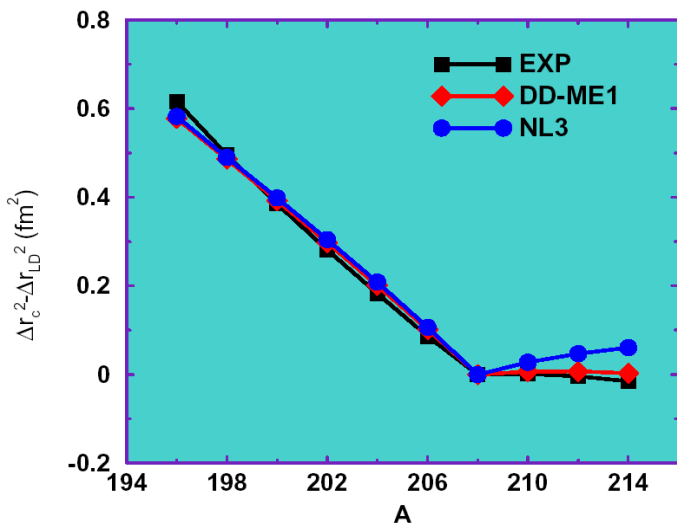
Ground state properties of finite nuclei:

DD-ME1

Binding energies, charge isotope shifts, and quadrupole Deformations of Gd, Dy, and Er isotopes.



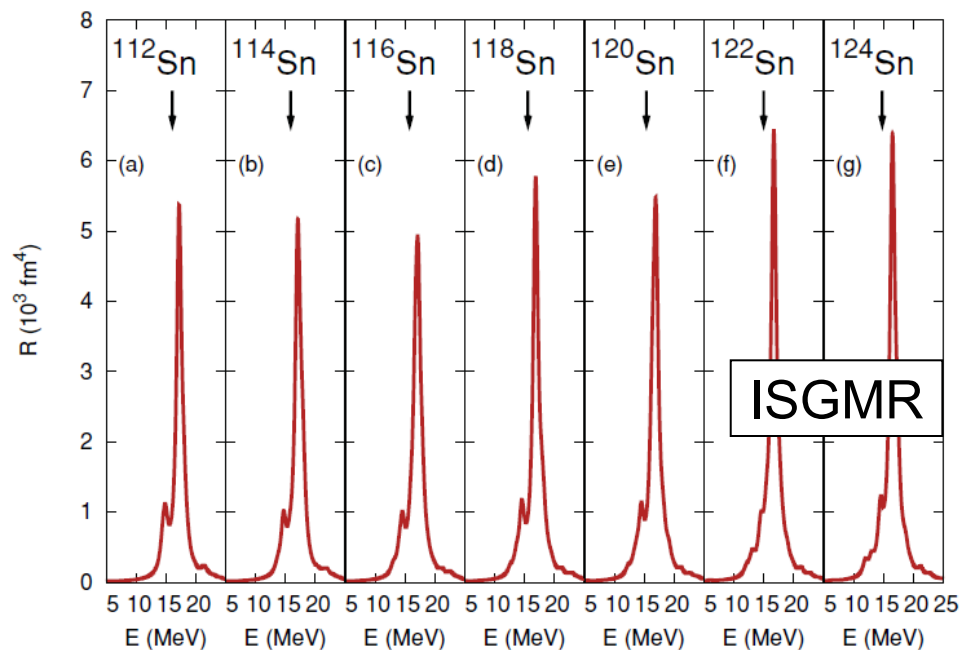
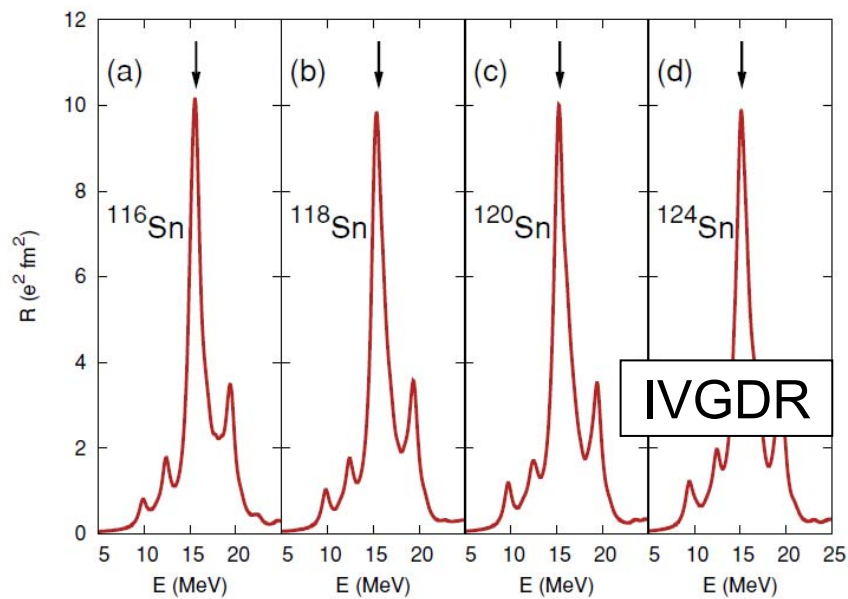
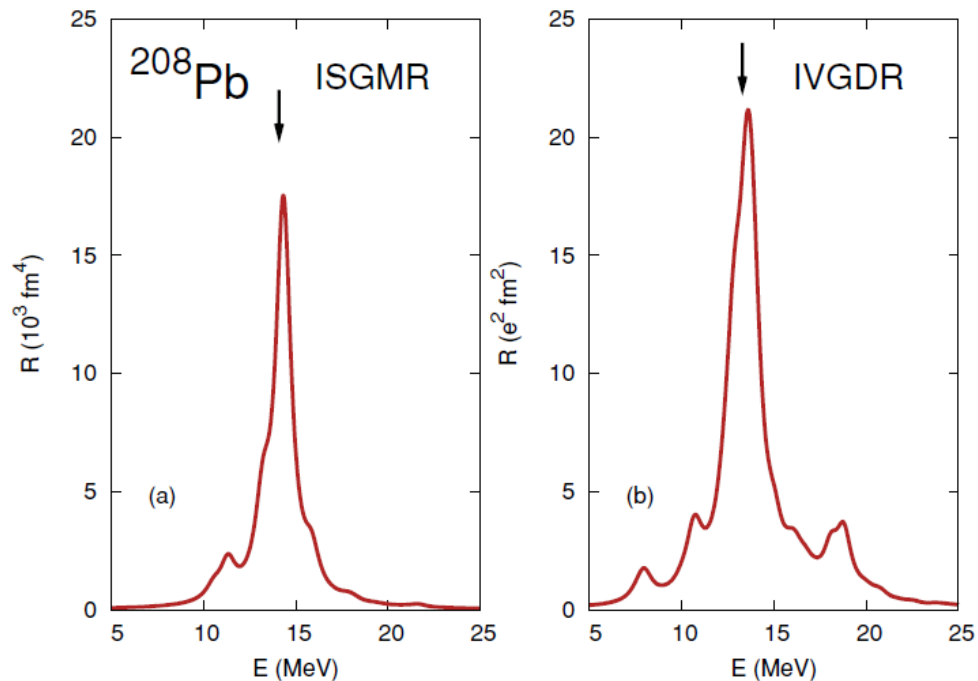
Charge isotope shifts in even-A Pb isotopes.



DD-PC1

Giant resonances:

T. Niksic et al, (2008)



Can a **universal density functional**, adjusted to ground state properties, at the same time reproduce **critical phenomena** in spectra ?

We need a method to derive spectra:

Generator coordinate method (GCM),

Adiabatic time-dependent relativistic mean field (ATDRMF)

We consider the chain of Ne-isotopes with a phase transition from **spherical (U(5))** to **axially deformed (SU(3))**

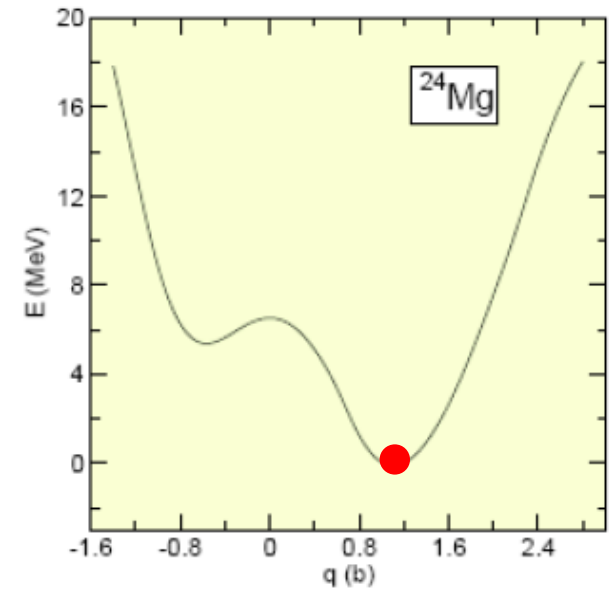
The generator coordinate method:

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



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

Constraint relativistic mean field produces wave functions depending on a **generator coordinate** q



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

the GCM wave function is a **superposition of Slater determinants**

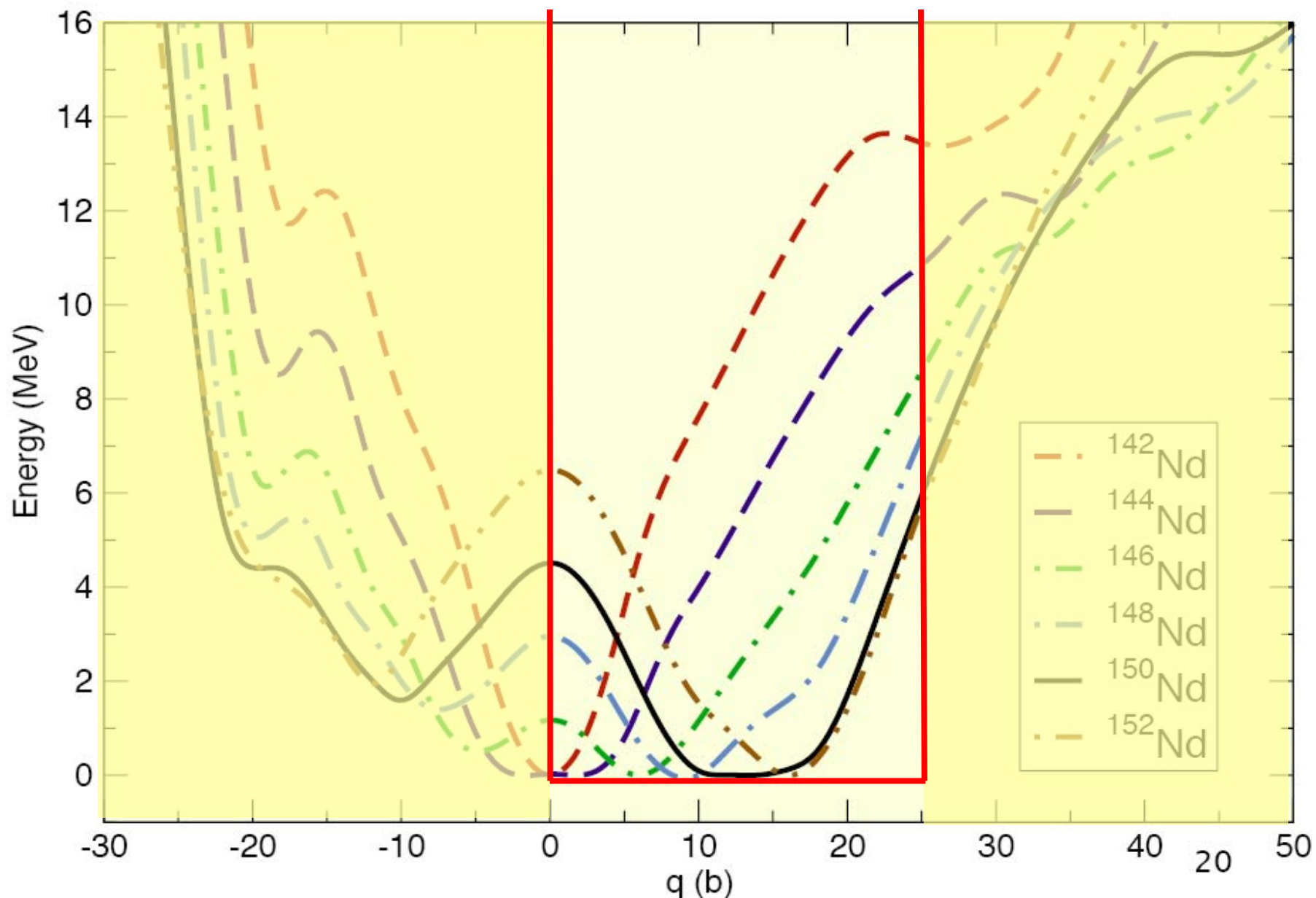
$$\int dq' [\langle q | H | q' \rangle - E \langle q | q' \rangle] f(q') = 0$$

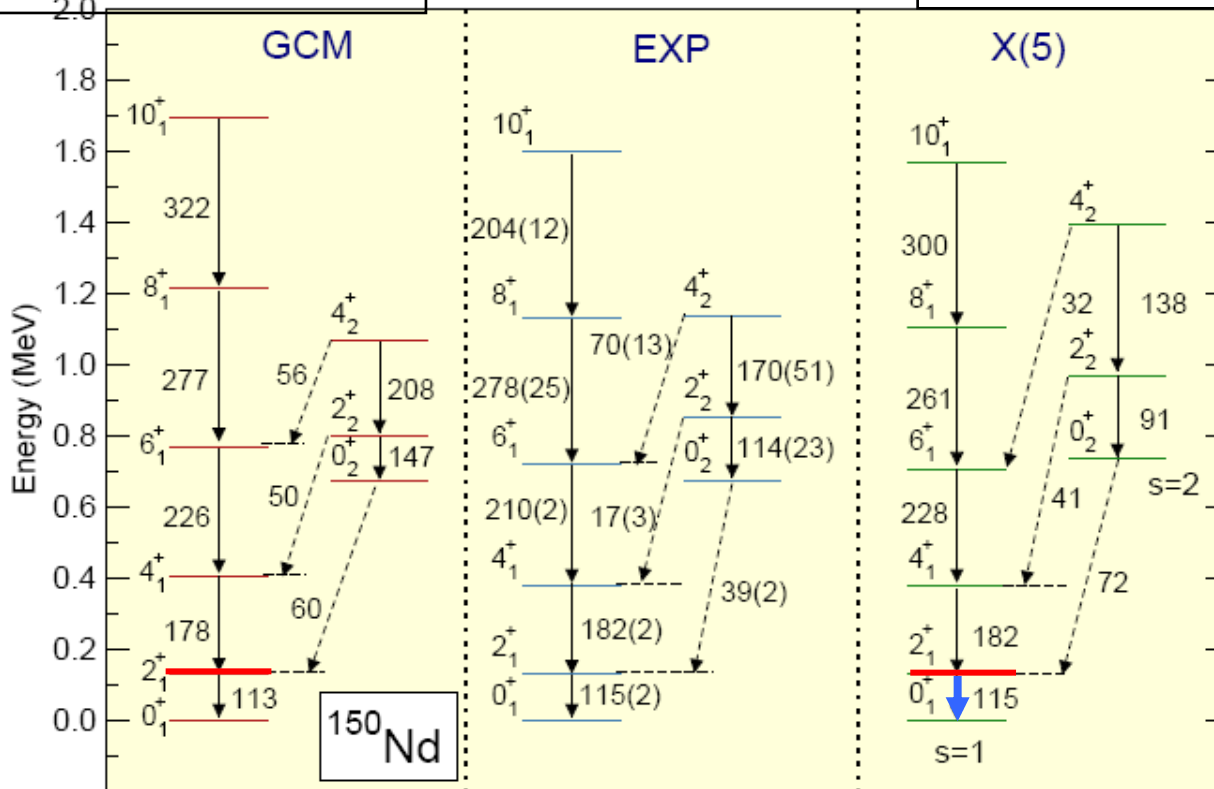
Hill-Wheeler equation:

with projection:

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

Self-consistent RMF plus Lipkin-Nogami BCS binding energy curves of $^{142-152}\text{Nd}$, as functions of the mass quadrupole moment.





GCM: only one scale parameter:

$E(2_1)$

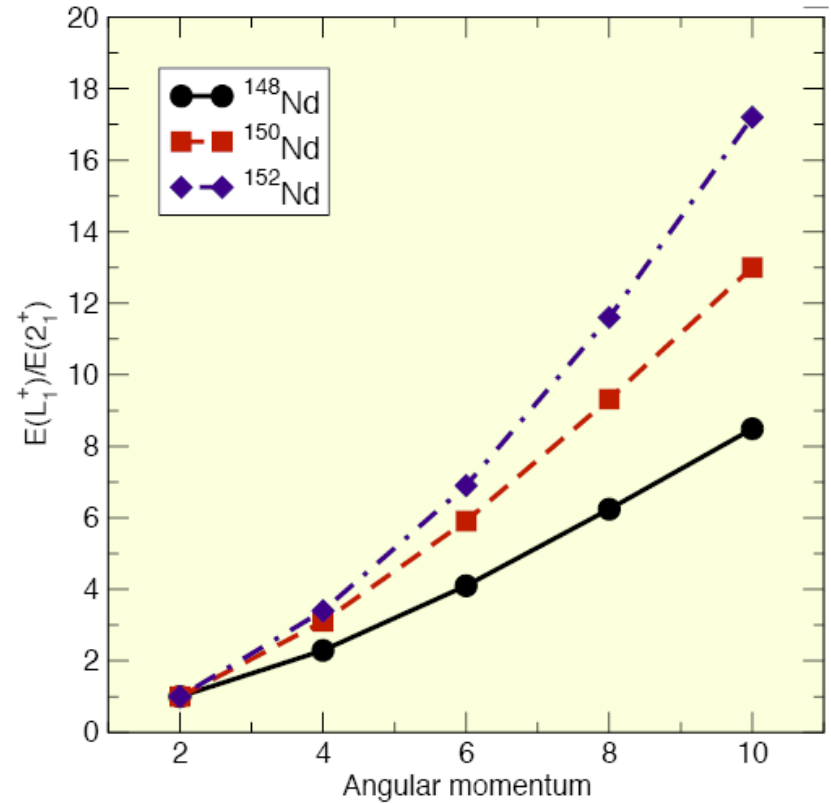
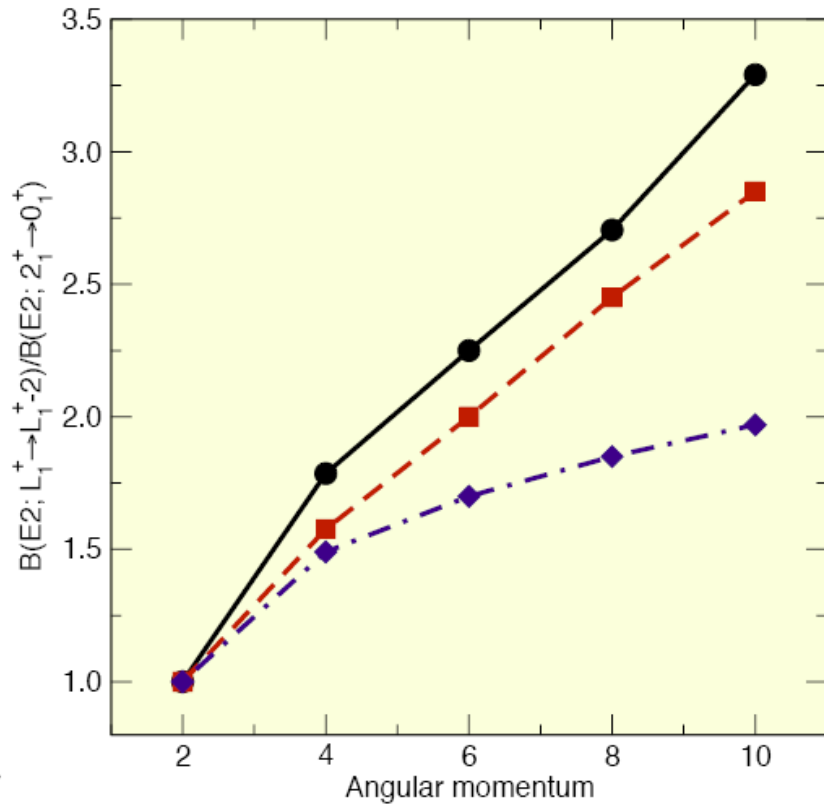
X(5): two scale parameters:

$E(2_1)$, $BE2(2_2 \rightarrow 0_1)$

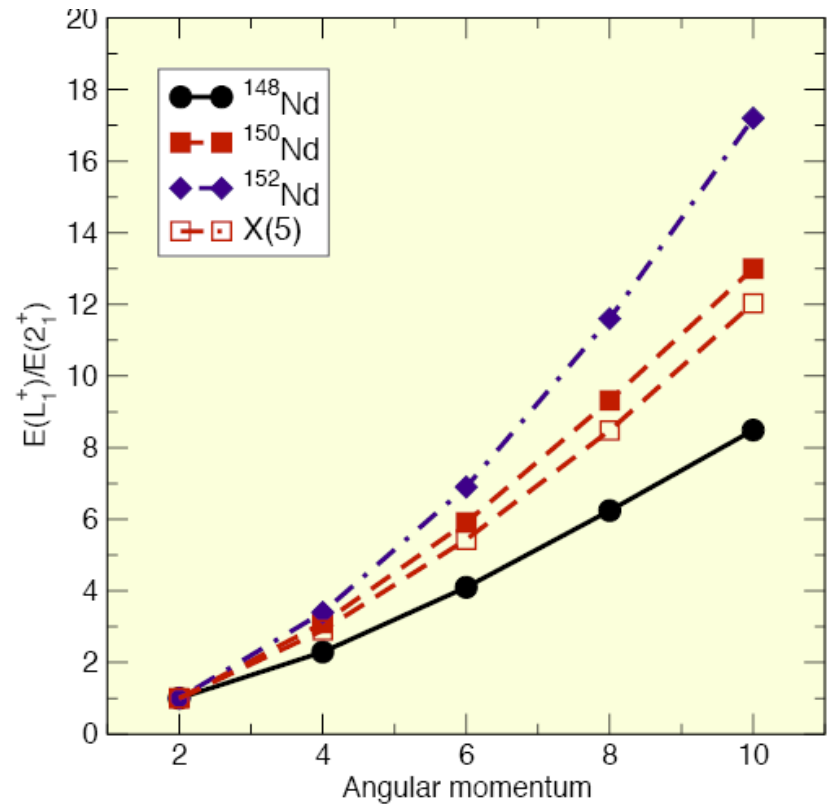
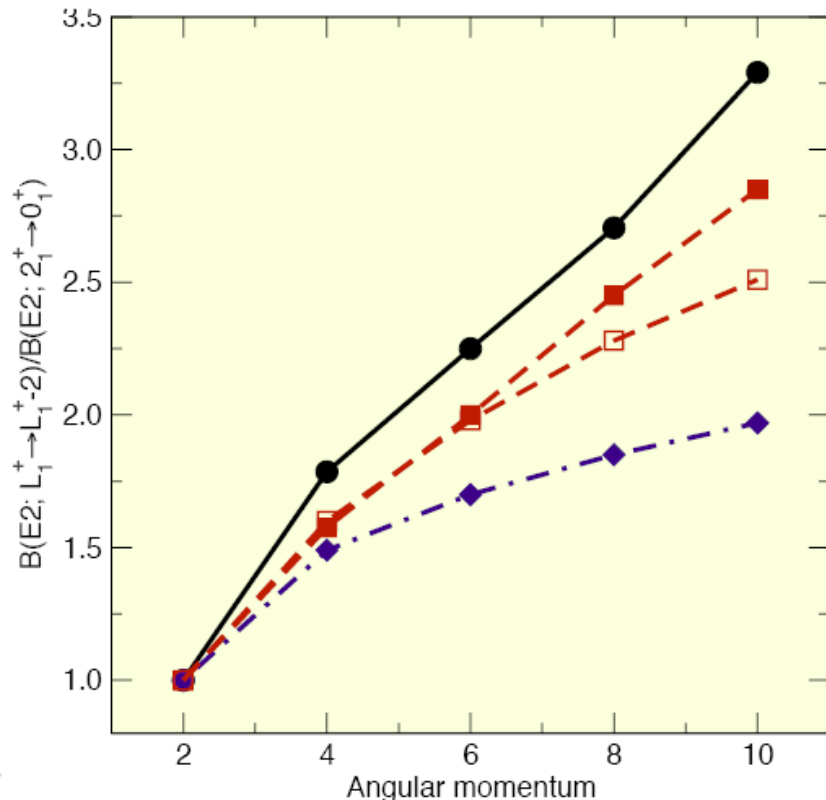
Problem of GCM at this level:

restricted to $\gamma=0$

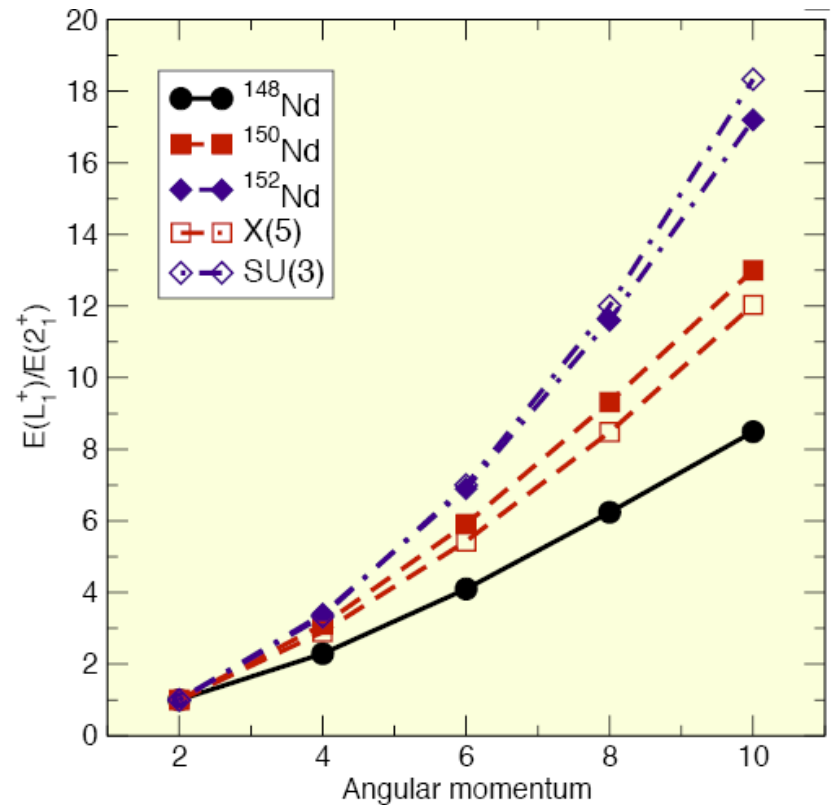
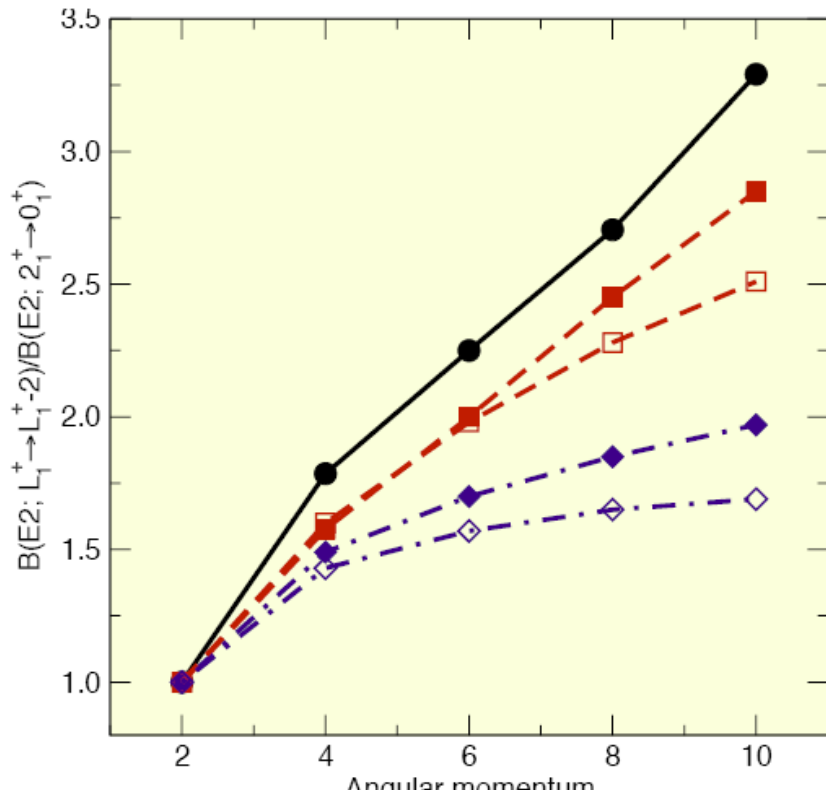
$B(E2; L \rightarrow L-2)$ values and excitation energies for the yrast states: ^{148}Nd , ^{150}Nd , and ^{152}Nd , calculated with the GCM:



$B(E2; L \rightarrow L-2)$ 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 $X(5)$:

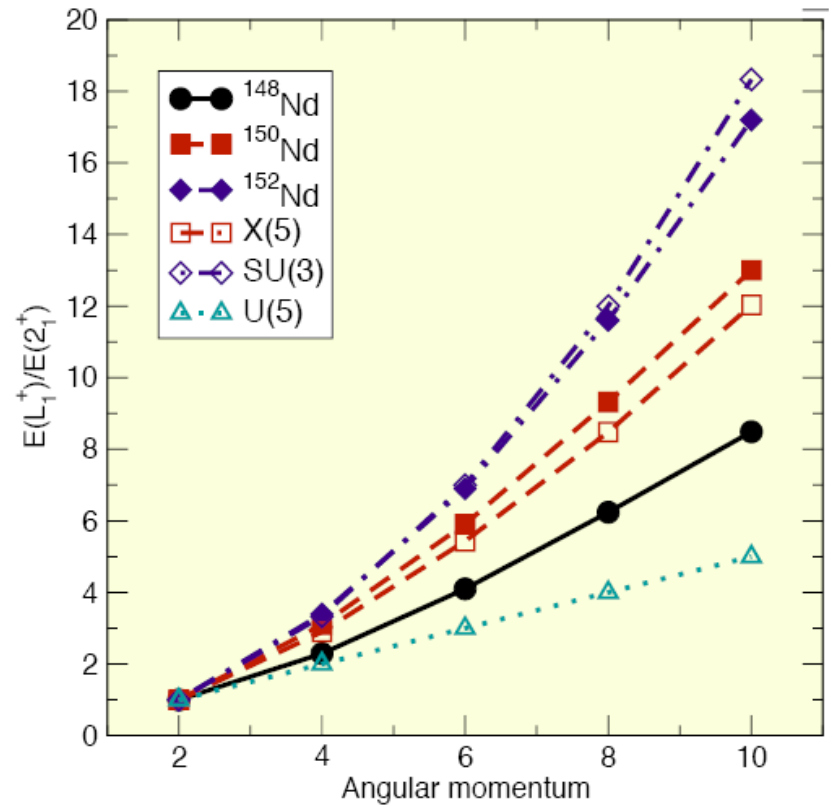
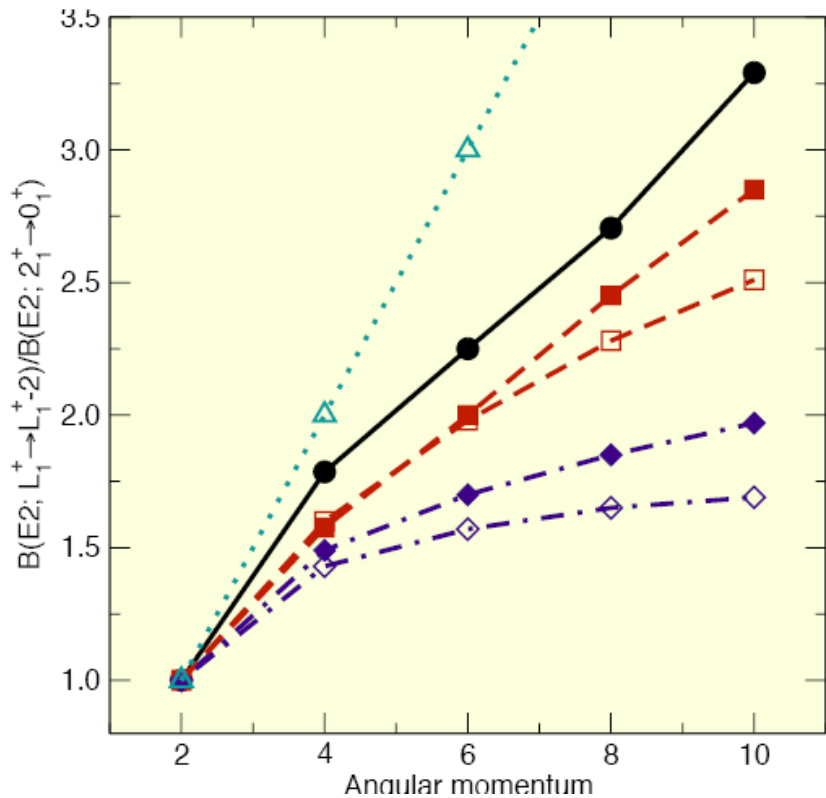


$B(E2; L \rightarrow L-2)$ values and excitation energies for the yrast states: ^{148}Nd , ^{150}Nd , and ^{152}Nd , calculated with the GCM and compared with those predicted by the **X(5)**, **SU(3)**

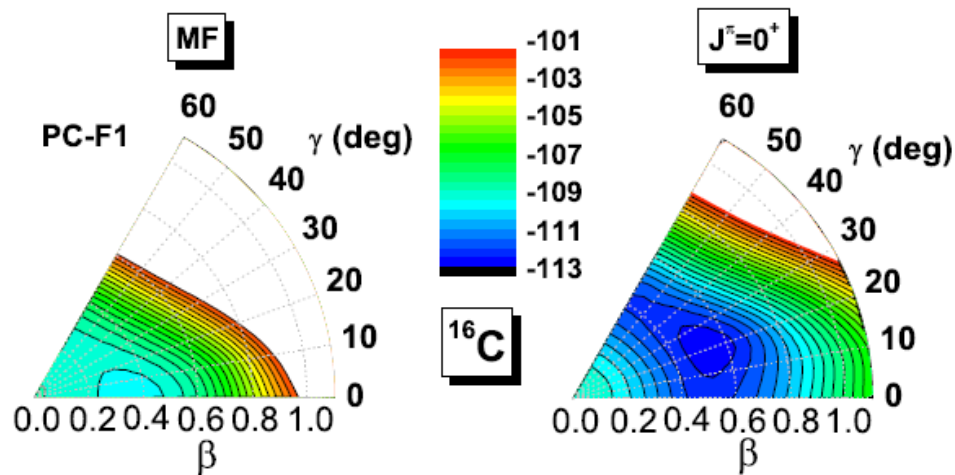


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$B(E2; L \rightarrow L-2)$ values and excitation energies for the yrast states: ^{148}Nd , ^{150}Nd , and ^{152}Nd , calculated with the GCM and compared with those predicted by the **X(5)**, **SU(3)** and **U(5)** symmetries.

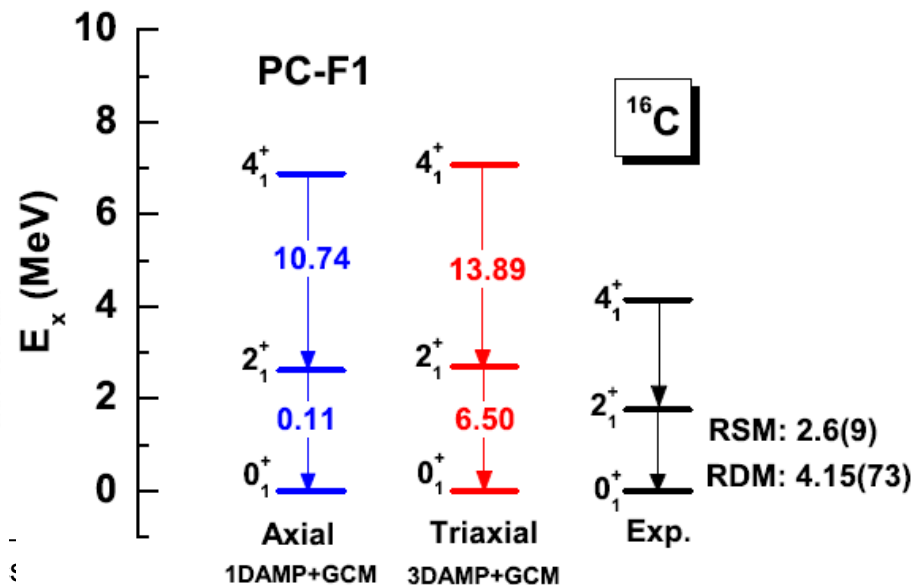
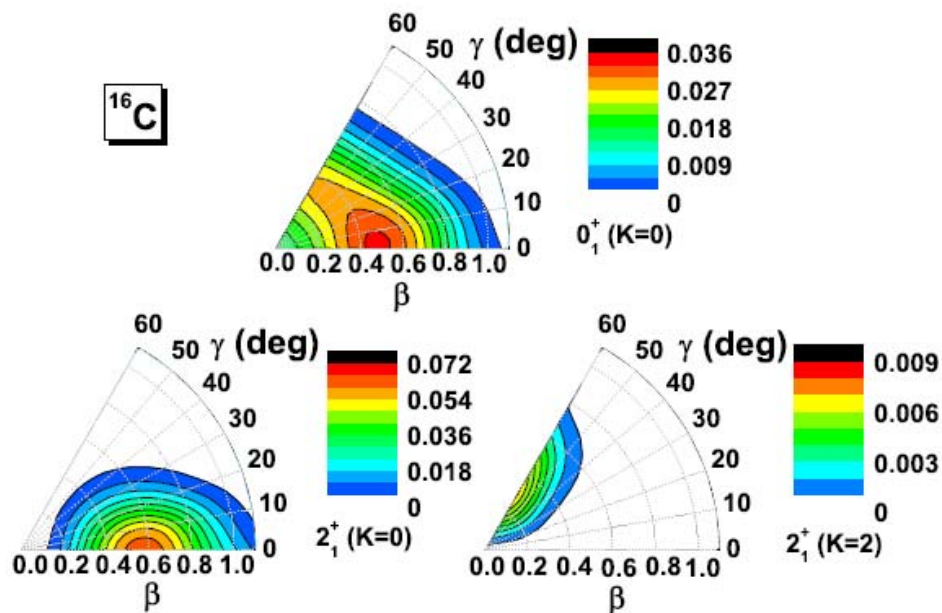


potential energy surface:



First relativistic
full 3D GCM calculations
Yao et al, PRC 81, 044311 (2010)

collective wave functions:



triaxial GCM in $q=(\beta,\gamma)$ is approximated by the diagonalization of a 5-dimensional Bohr Hamiltonian:

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

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

Theory:	Banerjee and Brink (1973)	(from GCM)
	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)	
Gogny	DelaRoche et al (2010)	

Inertia parameters:

$$B_{\mu\mu'}(\mathbf{q}) = \frac{1}{\hbar^2} \begin{pmatrix} P^* & -P \end{pmatrix}_{\mu} \mathcal{M} \begin{pmatrix} P \\ -P^* \end{pmatrix}_{\mu'}$$

$$\mathcal{M}^{-1} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} = \mathcal{M}_0^{-1} + \mathcal{V}$$

$$(\mathcal{M}_0^{-1})_{php'h'} = (\epsilon_p - \epsilon_h) \delta_{pp'} \delta_{hh'}$$

$$\mathcal{M} = \mathcal{M}_0 [\mathbb{1} + \mathcal{V}\mathcal{M}_0]^{-1}$$

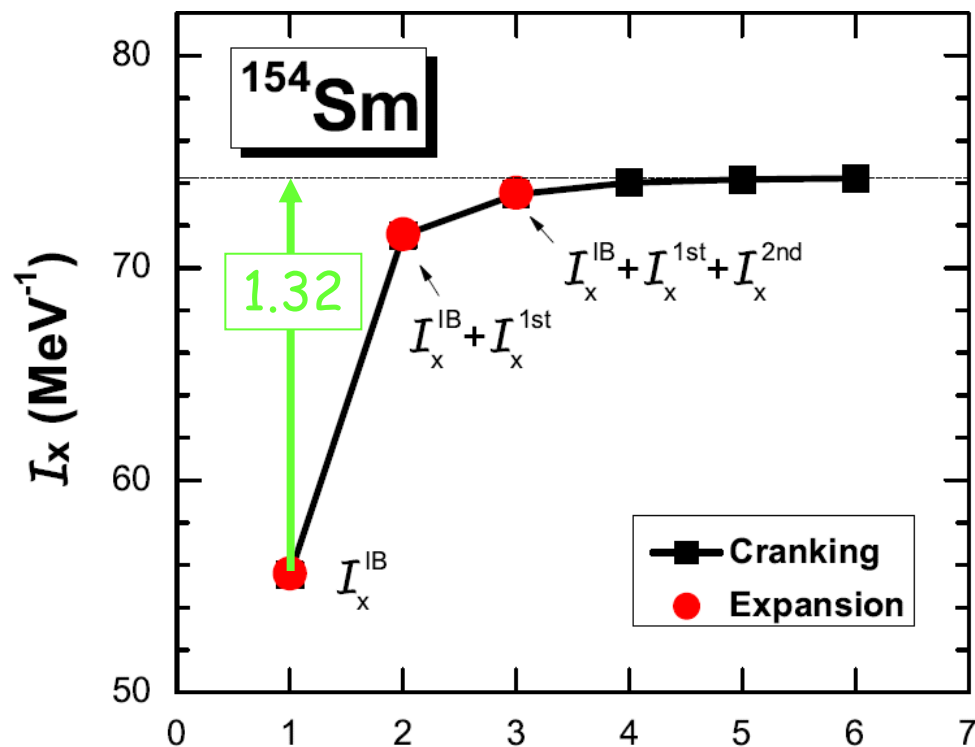
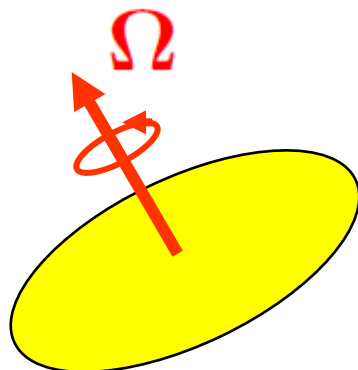
Thouless-Valatin mass

$$\mathcal{M} = \mathcal{M}_0 - \mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \mathcal{M}_0\mathcal{V}\mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \dots$$

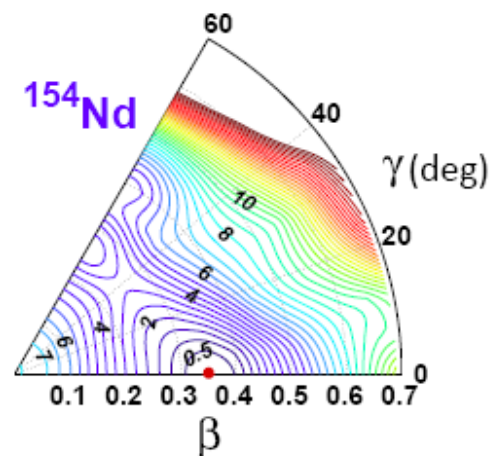
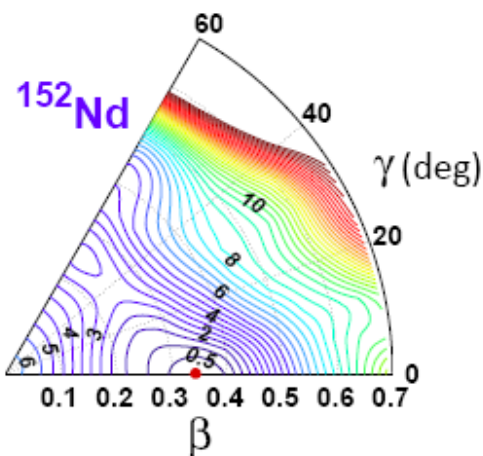
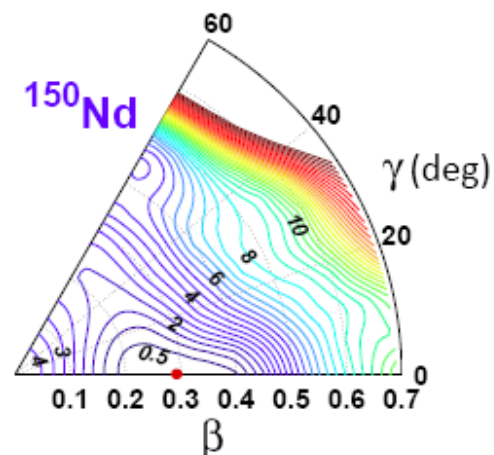
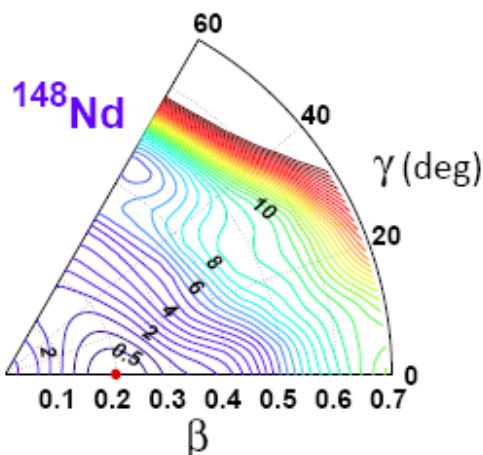
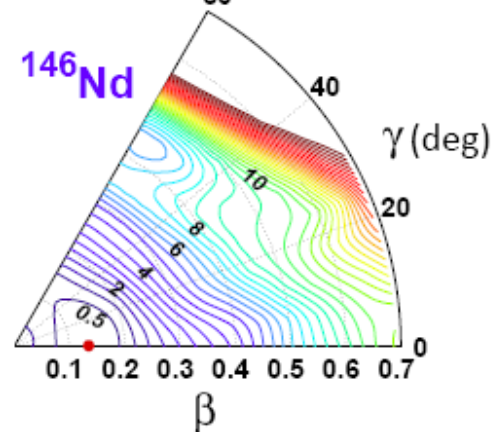
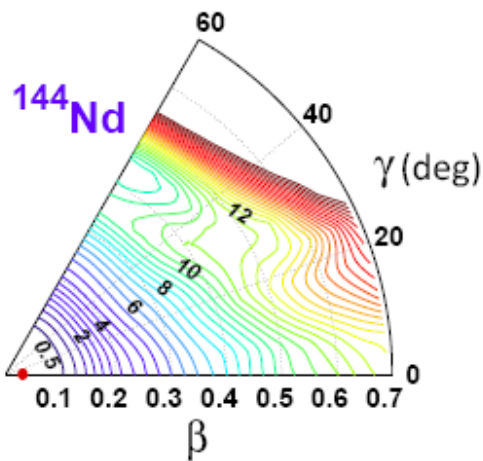
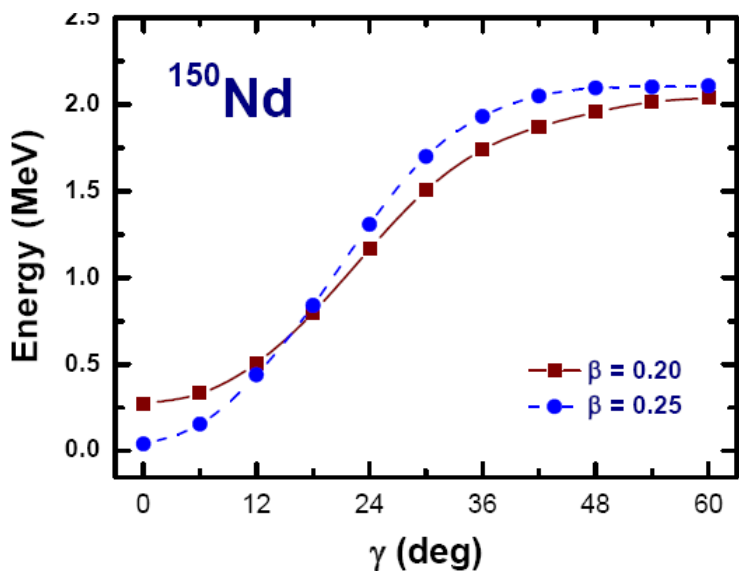
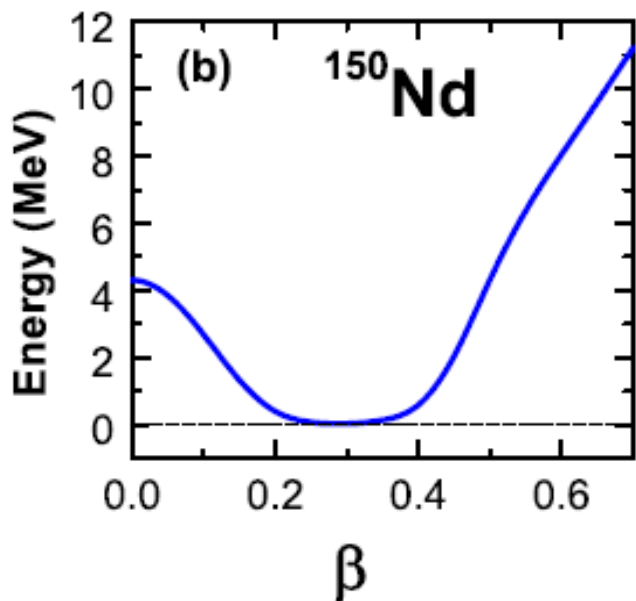
An example:

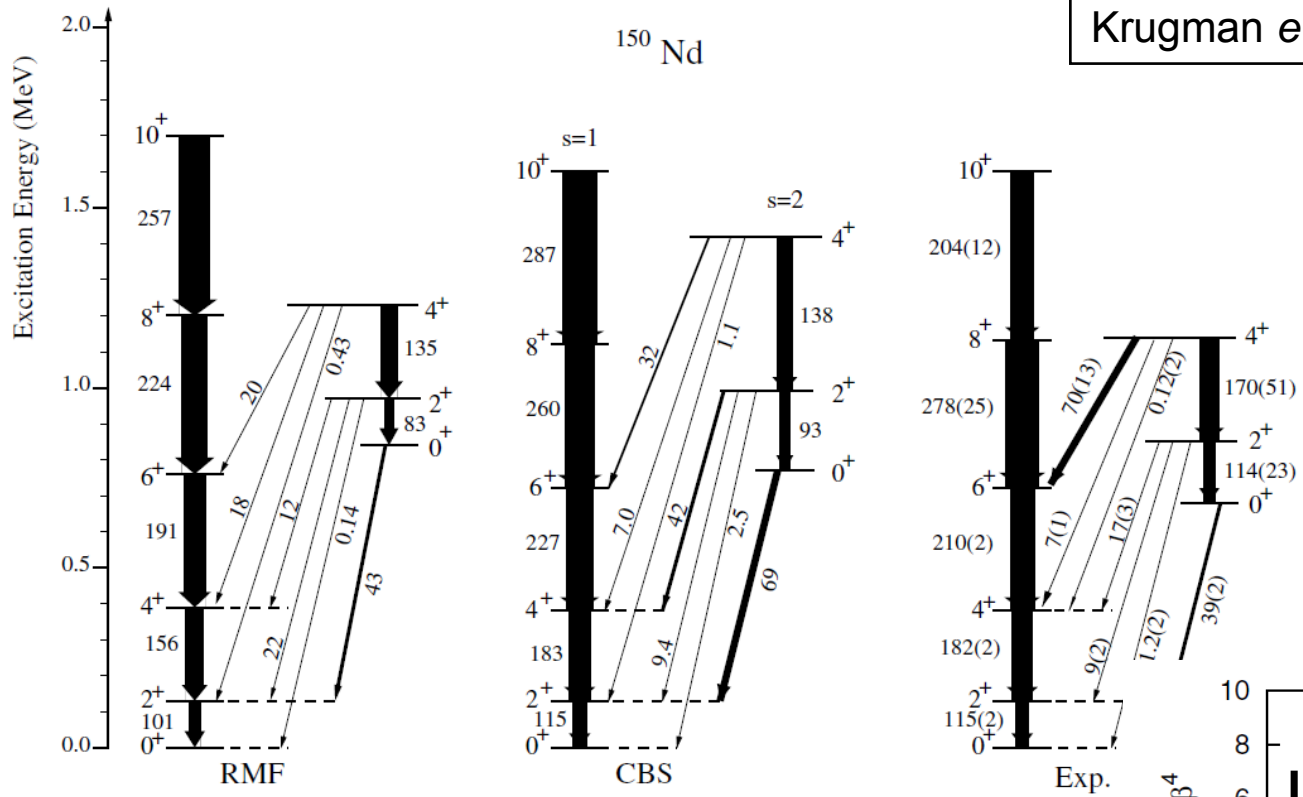
Rotational inertia

here we can use the self-consistent cranking model

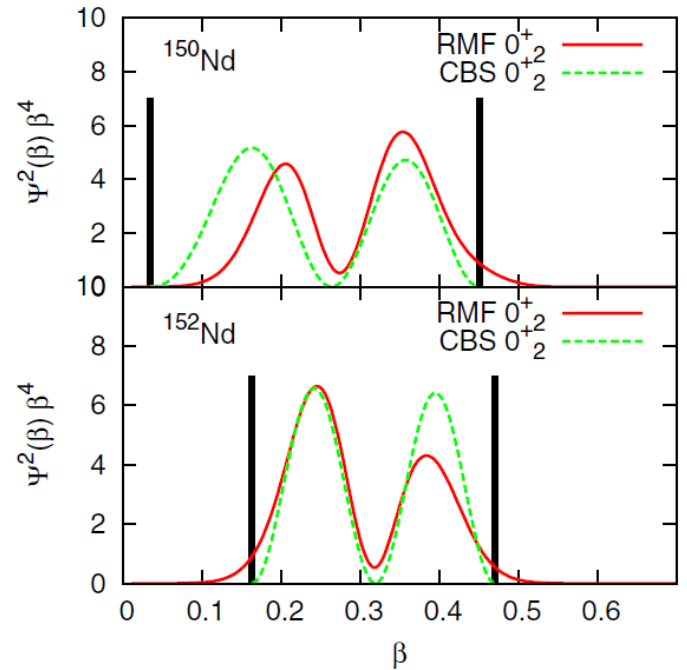


Potential energy surfaces:

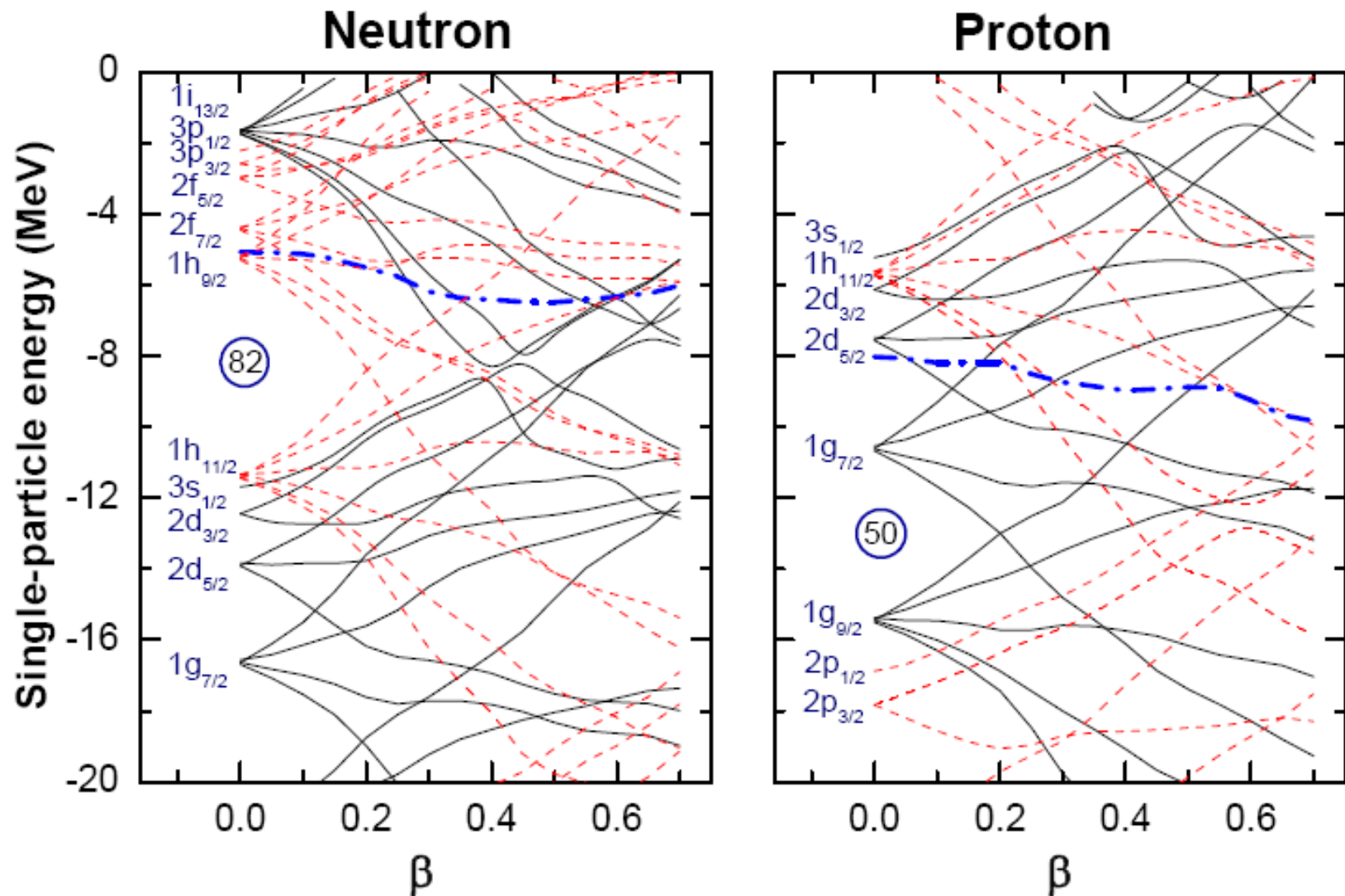




Comparison: β -soft rotor (CBS)



neutron and proton levels for ^{150}Nd



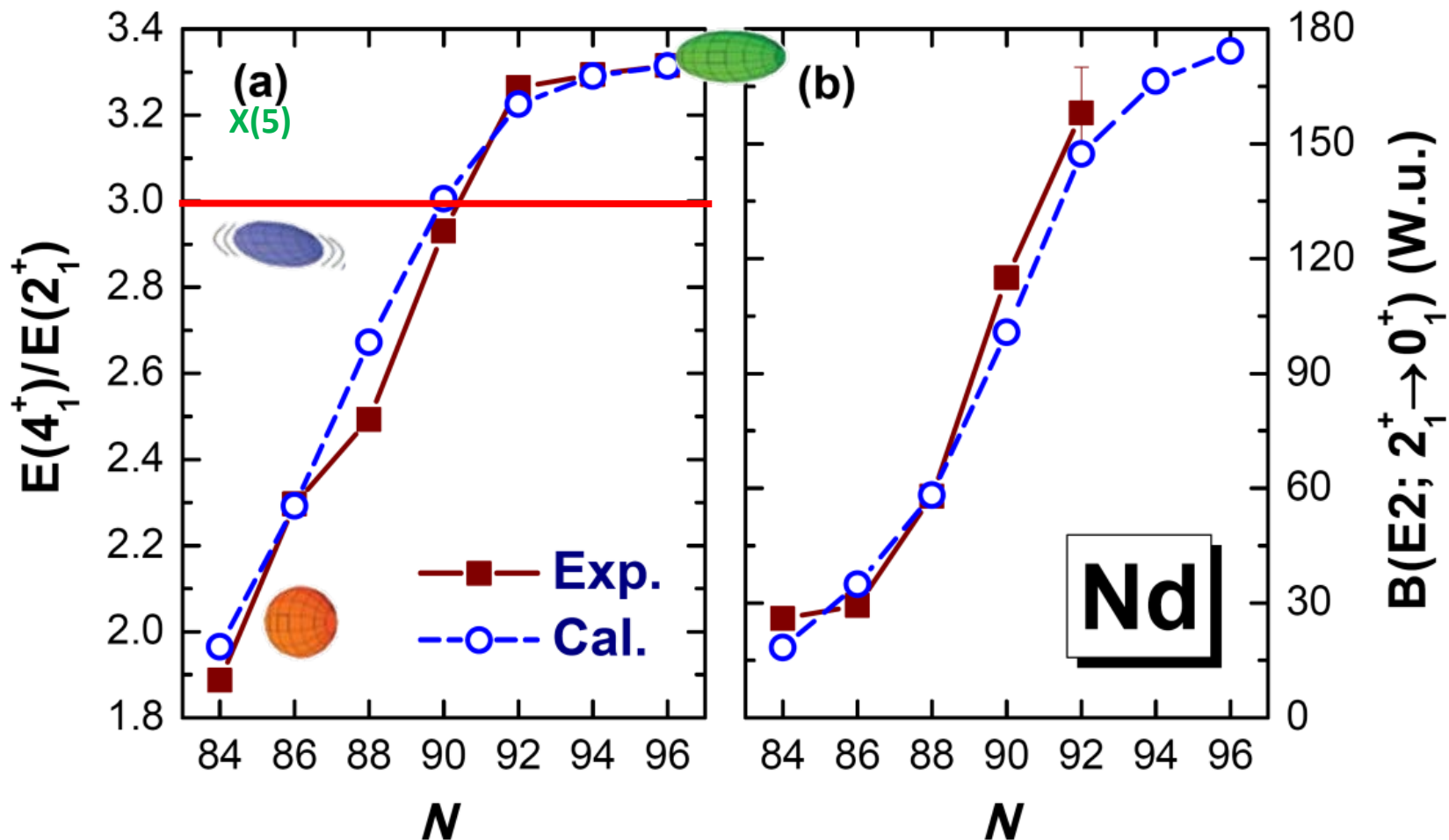
Questions:

- How much are the discontinuities **smoothed out** in finite systems ?
- How well can the phase transition be associated with a certain value of the control parameter that takes **only integer values** ?
- Which experimental data show discontinuities in the phase transition?

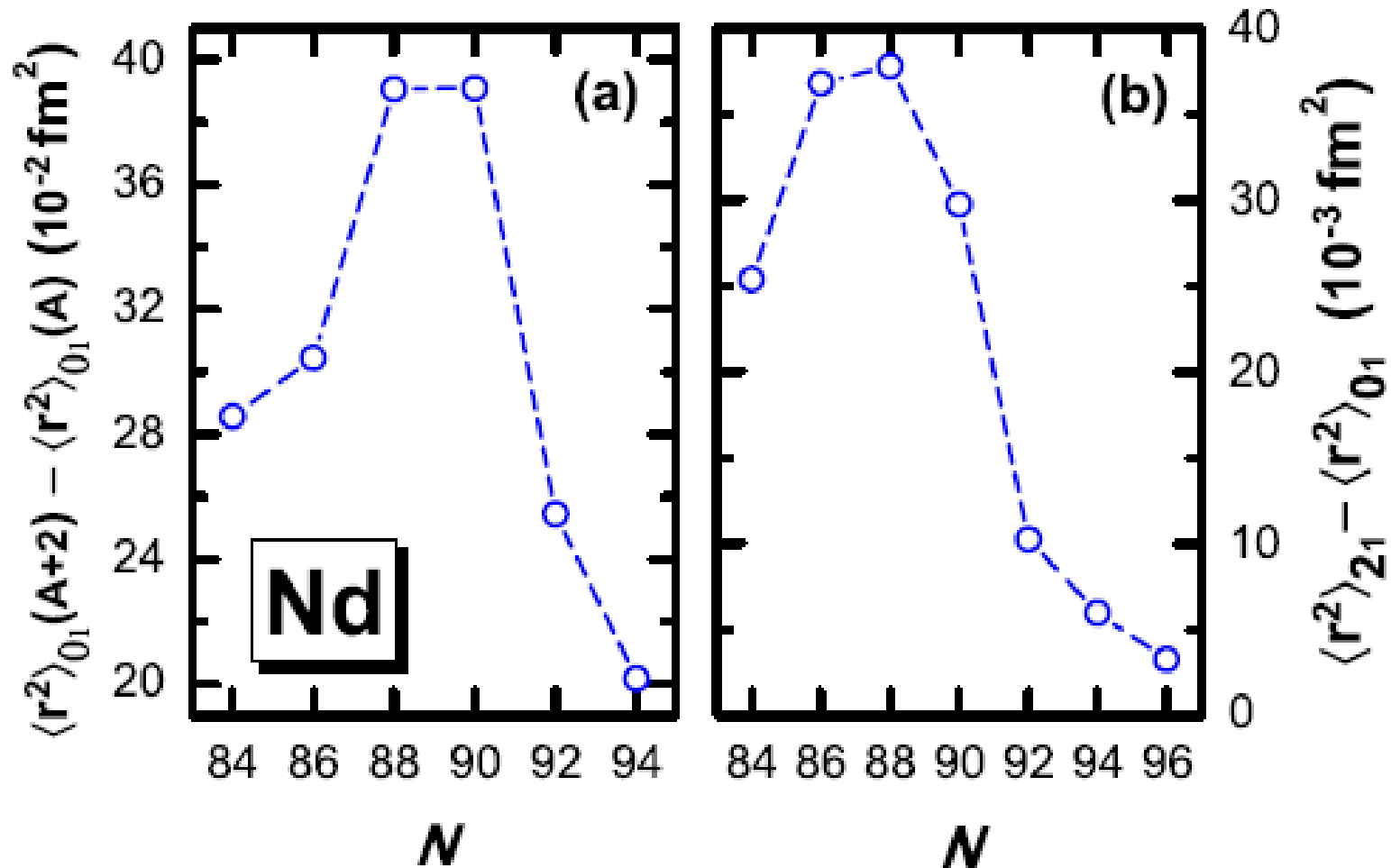
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- **Conclusions**

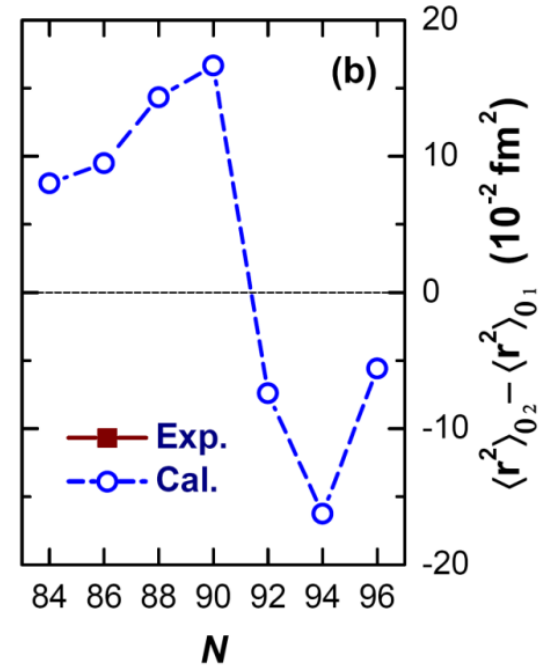
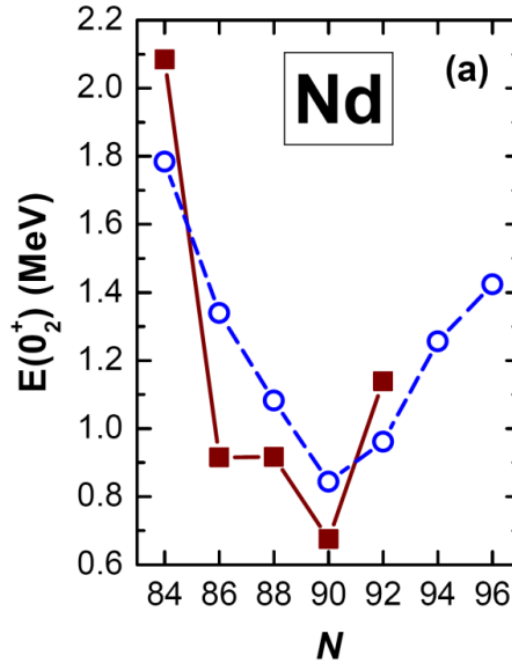
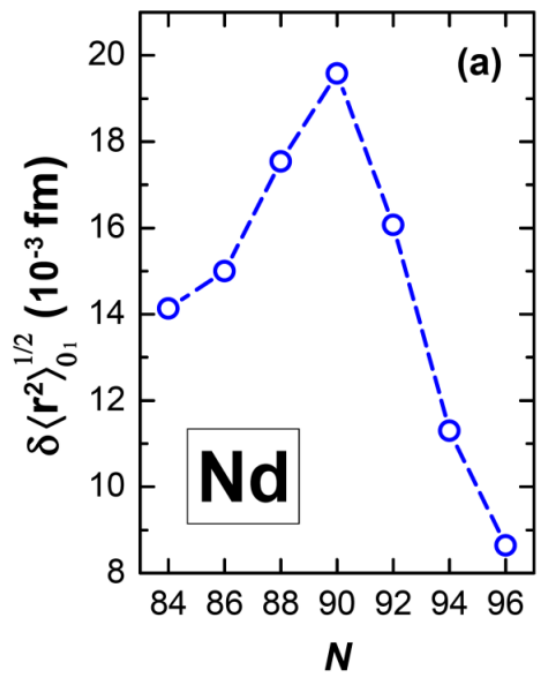
Sharp increase of $R_{42}=E(4_1)/E(2_1)$ and $B(E2;2_1-0_1)$:



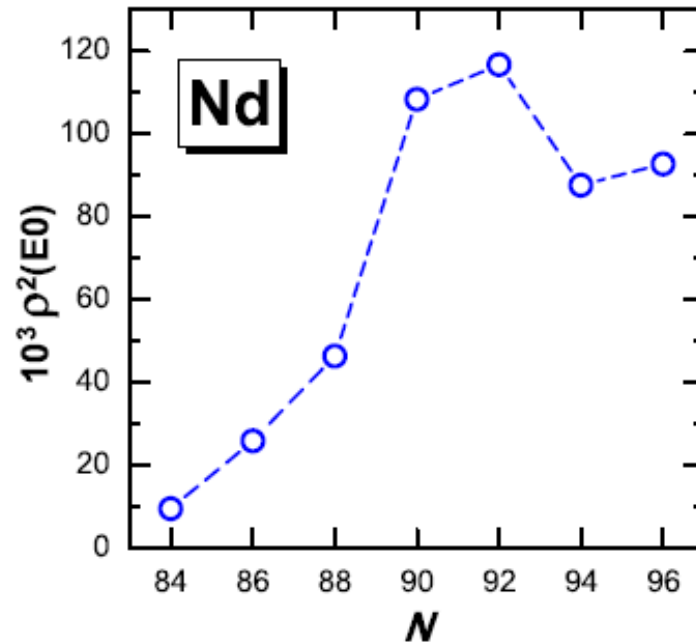
Isomeric shifts in the charge radii:

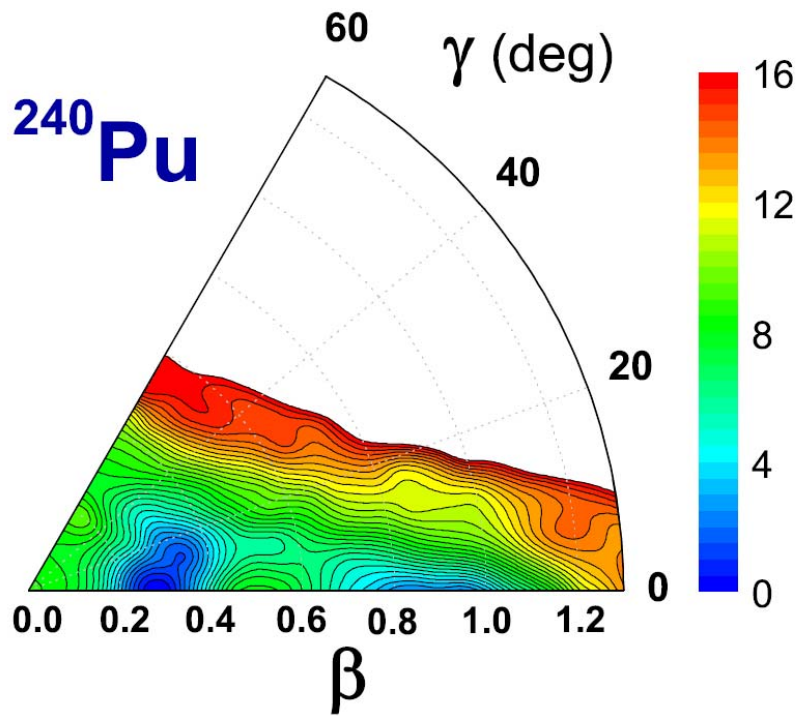


Properties of 0^+ excitations



Monopole transition strength $\rho(E0; 0_2 - 0_1)$

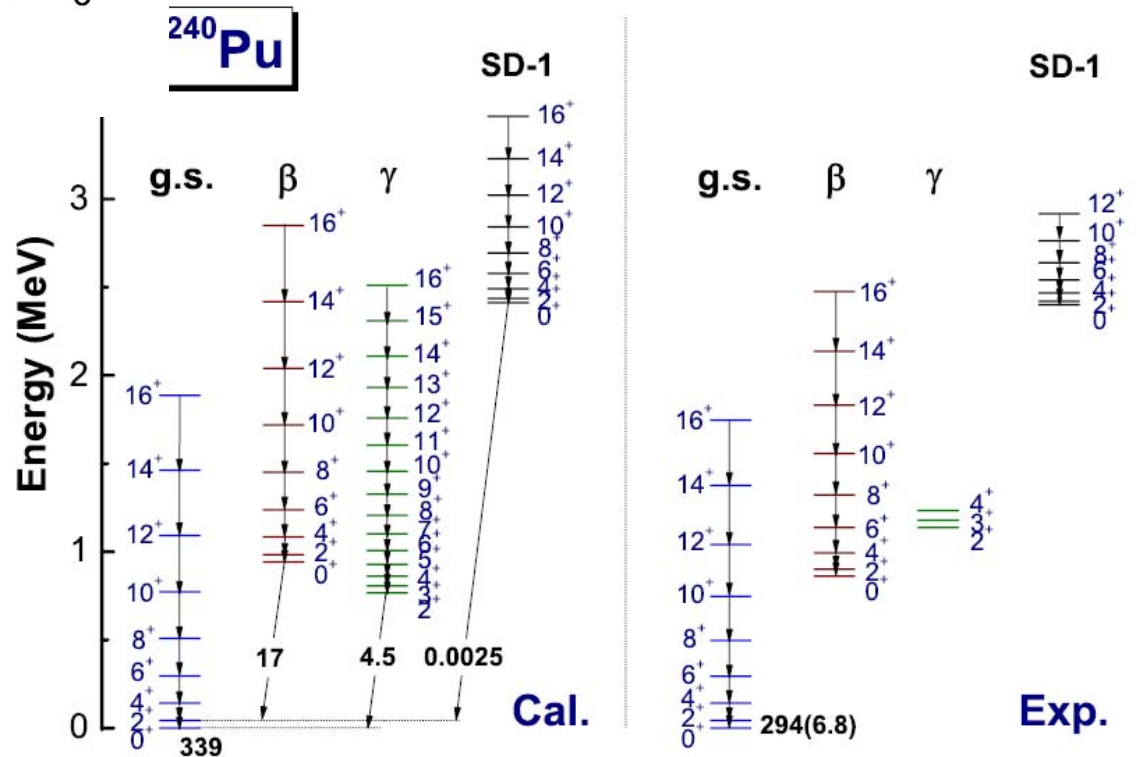
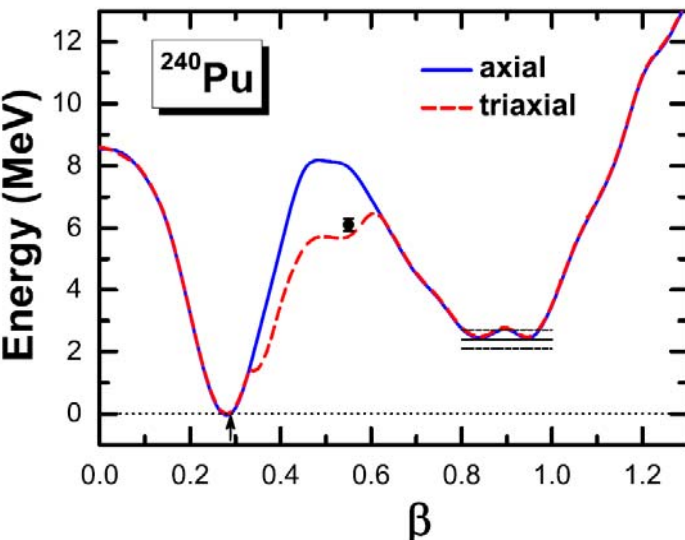




Fission barrier and super-deformed bands in ^{240}Pu

Niksic *et al* PRC 79 (2009)

DD-PC1



Conclusions:

GCM calculations for spectra in transitional nuclei

- J+N projection is important,
- triaxial calculations so only for very light nuclei possible
- **microscopic theory of quantum phase transitions**

Derivation of a collective Hamiltonian

- allows triaxial calculations
- nuclear spectroscopy based on density functionals
- open question of inertia parameters

The microscopic framework based on universal density functionals provides a consistent and (nearly) parameter free description of quantum phase transitions

The finiteness of the nuclear system does **not seem to smooth** out the discontinuities of these phase transitions

Collaborators:

T. Niksic (Zagreb)

D. Vretenar (Zagreb)

G. A. Lalazissis (Thessaloniki)

L. Prochniak (Lublin)

Z.P. Li (Beijing)

J.M. Yao (Chonqing)

J. Meng (Beijing)

Thank you

and

Happy Birthday
to you, Franco