Recent developments in Covariant density functional theory beyond mean field

Kyoto, Oct. 23, 20

Peter Ring

Technical University Munich

Excellence Cluster "Origin of the Universe"

Peking University, Beijing

Density functional theory (DFT) for manybody quantum systems

The manybody problem is mapped onto a one-body problem:

Density functional theory starts from the

Hohenberg-Kohn theorem:

„The exact ground state energy E[ρ] is a universal functional for the local density ρ(r)“

Kohn-Sham theory starts

with a density dependent self-energy:

$$h(\mathbf{r}) = \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})}$$

and the single particle equation:

$$h(\mathbf{r})|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle$$

with the exact density:

$$\rho(\mathbf{r}) = \sum_i^A |\varphi_i(\mathbf{r})|^2$$

In Coulombic systems the functional is derived *ab initio*

Density functional theory in nuclei:

- **more degrees of freedom**: spin,isospin,pairing,relativistic
- Nuclei are **selfbound systems**
- **Symmetry breaking** is important:

Advantage:
Correlations can be
taken into account
in simple wave functions

Janus

Problems:
no good quantum numbers
no spectroscopy
projection required

translational,	rotational,	gauge symmetry,	…….
momentum P	spin J	particle number N	

- **Shape coexistence**: transitional nuclei, shape transitions
- **Energy dependence** of the self energy
- at present all successful functionals are **phenomenological**

Density Functional Theory: mean field and beyond

- **Mean Field Level:** static DFT: $h[\rho(r)] = \dfrac{\delta E}{\delta \rho}$

  Static DFT: ground state properties

  constraint mean field: fission landscapes

  rotating mean field: rotational spectra

  adiabatic DFT: $h[\rho_t(r)]$ time-dependent mean field: RPA, QRPA

- **Beyond Mean Field:** time-dep. DFT

  Energy dependent self energy $\boxed{h[\rho(r,t)] \rightarrow h(\omega)}$

  Small amplitudes: coupling to vibrations PVC (model)

- **Beyond Mean Field:** Configuration Mixing:

  Large amplitudes: Generator coordinate (GCM) $|\Psi\rangle = \int dq\ f(q)|q\rangle$

  Collective Hamiltonian

Content:

- **Generator-Coordinate Method (GCM)**
- Applications:

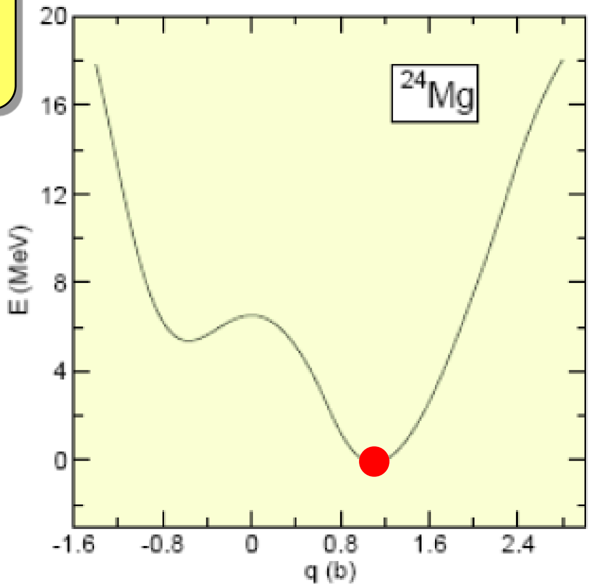
  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure N=28 isotones

  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- Benchmark calculations (full GCM ↔ 5DCH)
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

DFT beyond mean field: GCM-method

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



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

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

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

GCM wave function is a
superposition of Slater determinants

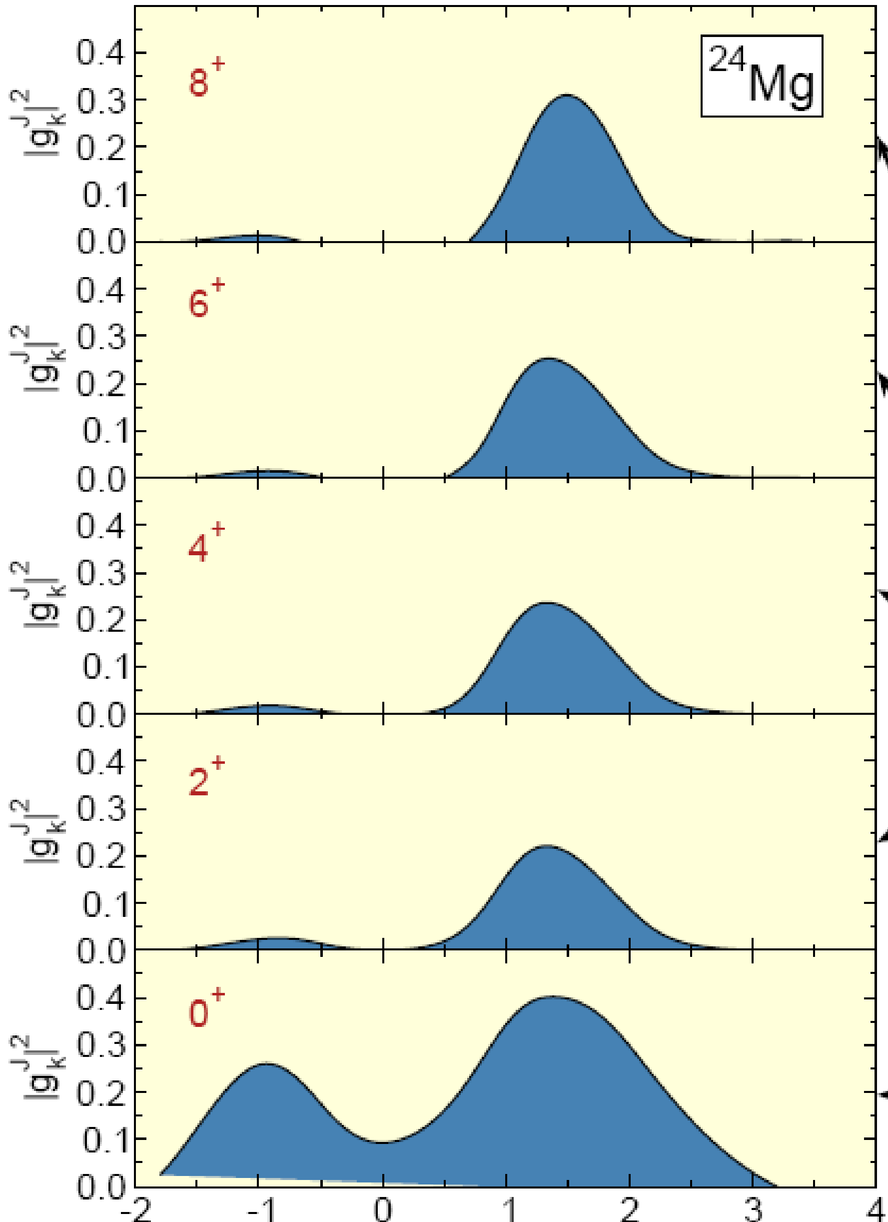
$$\int dq' \left[\langle q | H | q' \rangle - E \langle q | q' \rangle \right] f(q') = 0$$

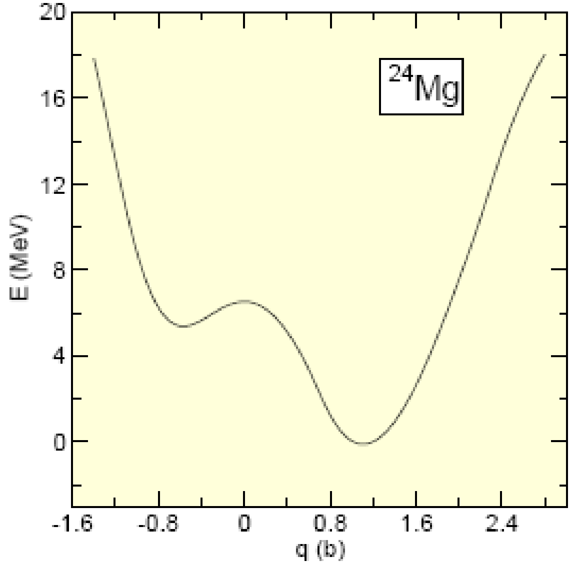
Hill-Wheeler equation:

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

with projection:

GCM:

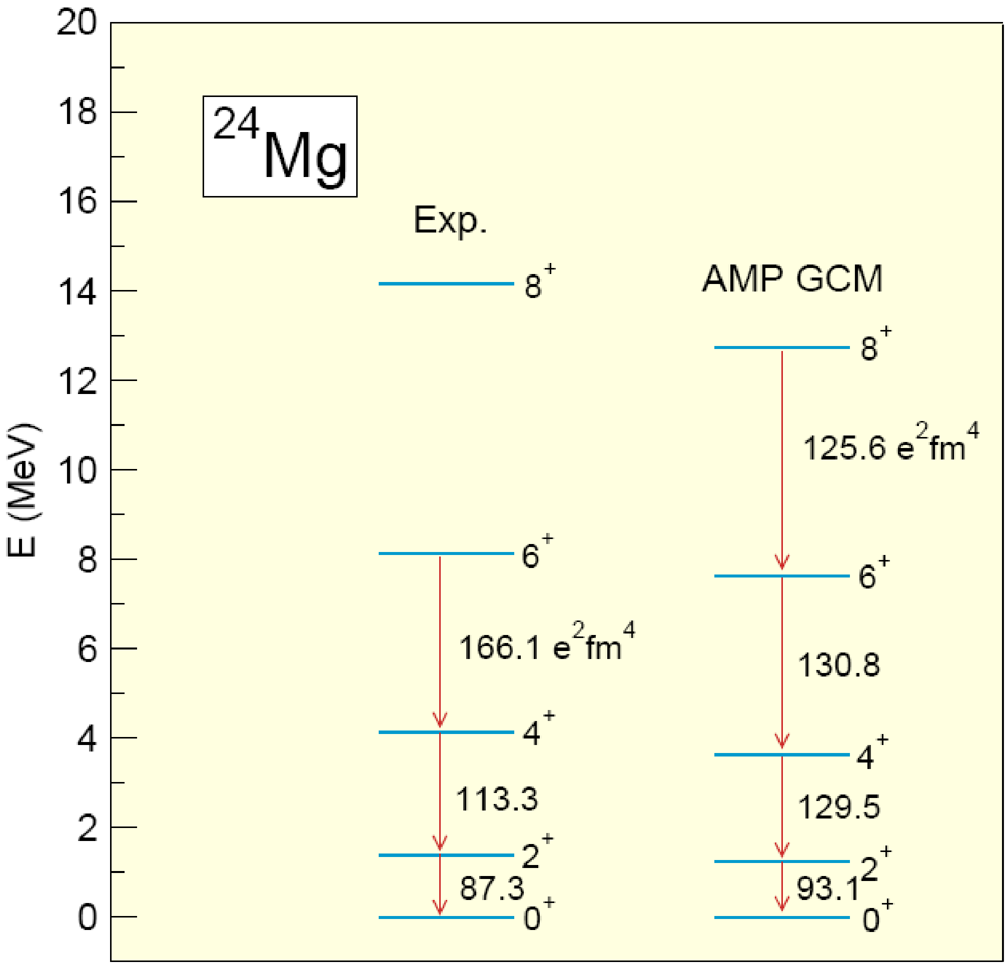




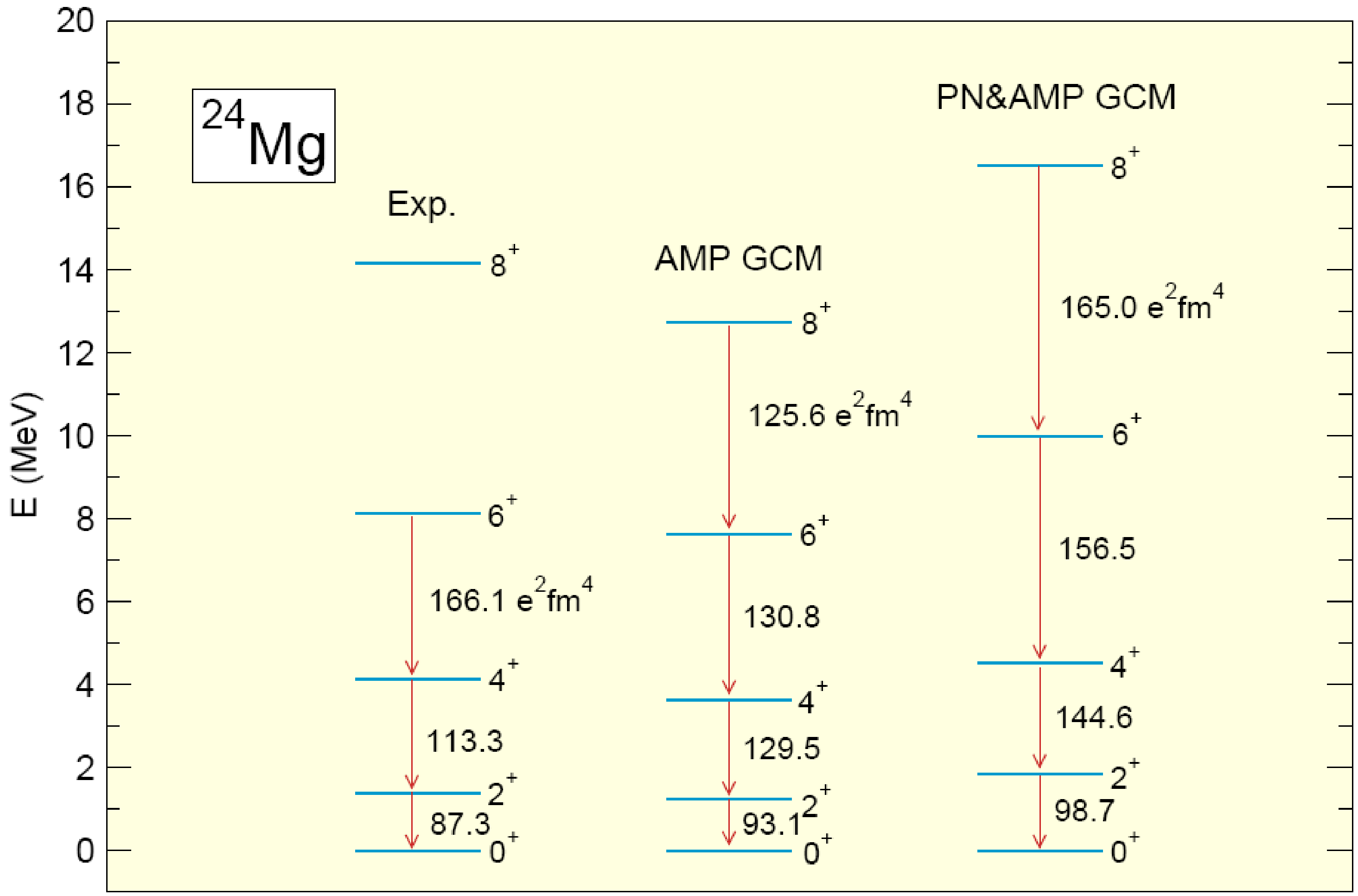
The amplitudes of states with $J \geq 2$ are concentrated in the prolate well.

Only the 0_1^+ state contains significant admixtures of oblate deformed shapes.

Spectra in ^{24}Mg



Spectra in ^{24}Mg



Content:

- Generator-Coordinate Method (GCM)
- Applications:

  Quantum Phase Transitions in finite systems (QPT)

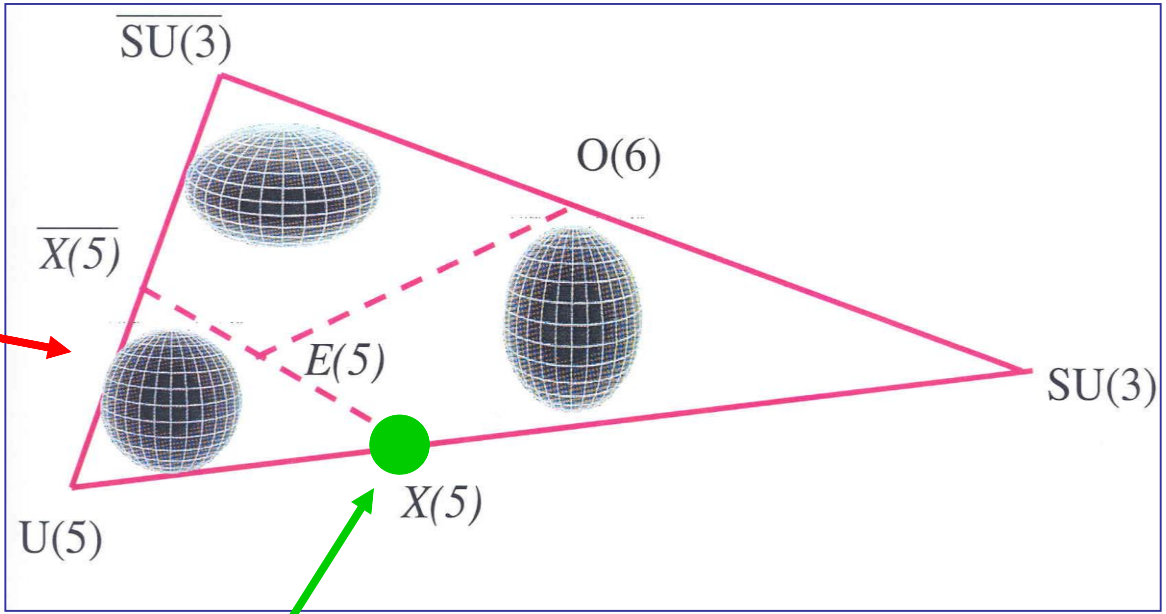
  Importance of single particle structure N=28 isotones

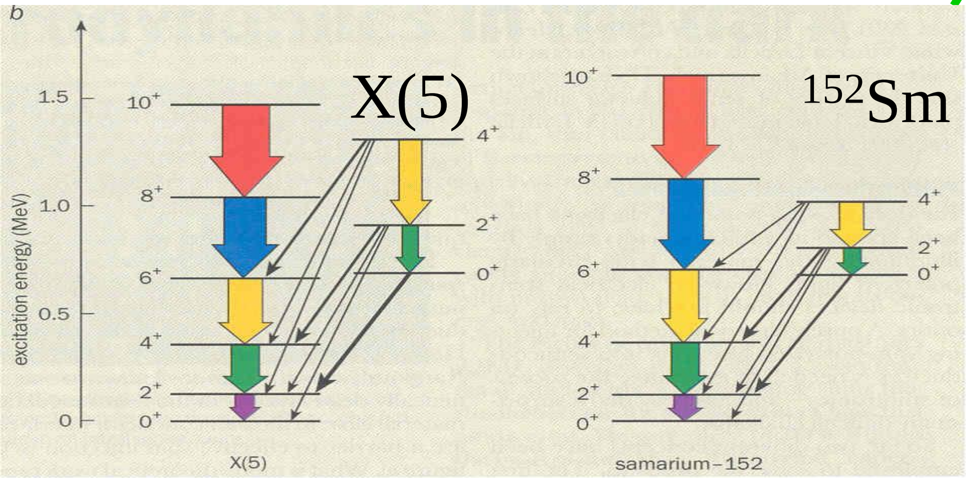
  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- Benchmark calculations (full GCM ↔ 5DCH)
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

Quantum phase transitions and critical symmetries

Interacting Boson Model

Casten Triangle



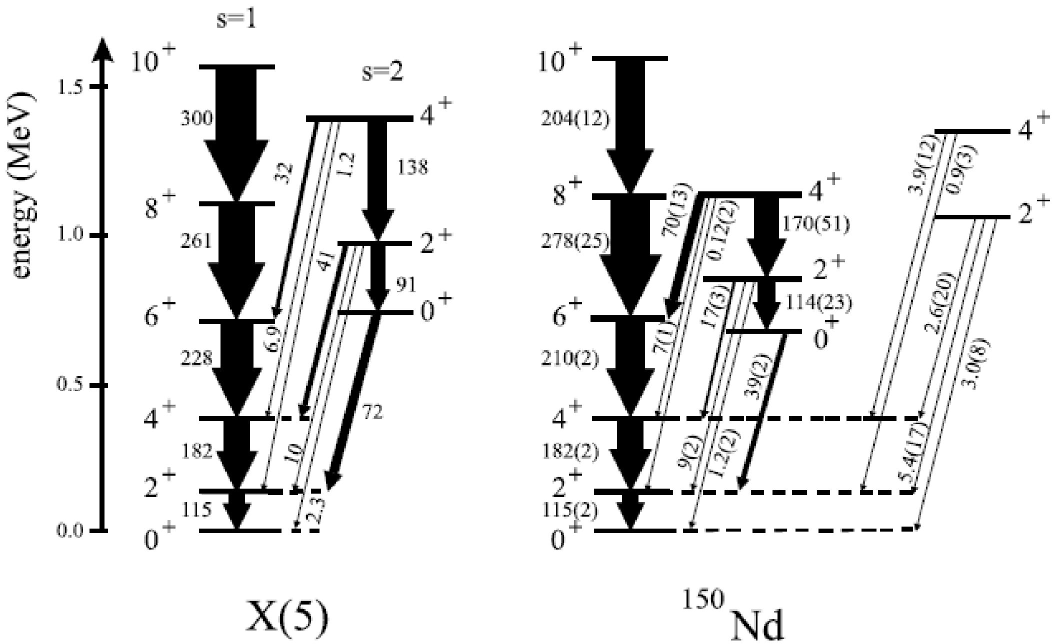


E(5): F. Iachello, PRL 85, 3580 (2000)
X(5): F. Iachello, PRL 87, 52502 (2001)

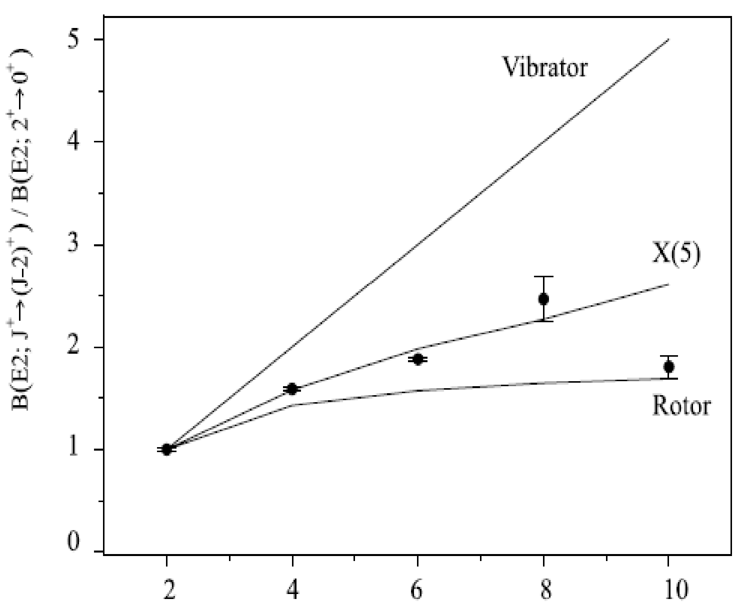
R.F. Casten, V. Zamfir, PRL 85 3584, (2000)

Transition U(5) → SU(3) in Ne-isotopes

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



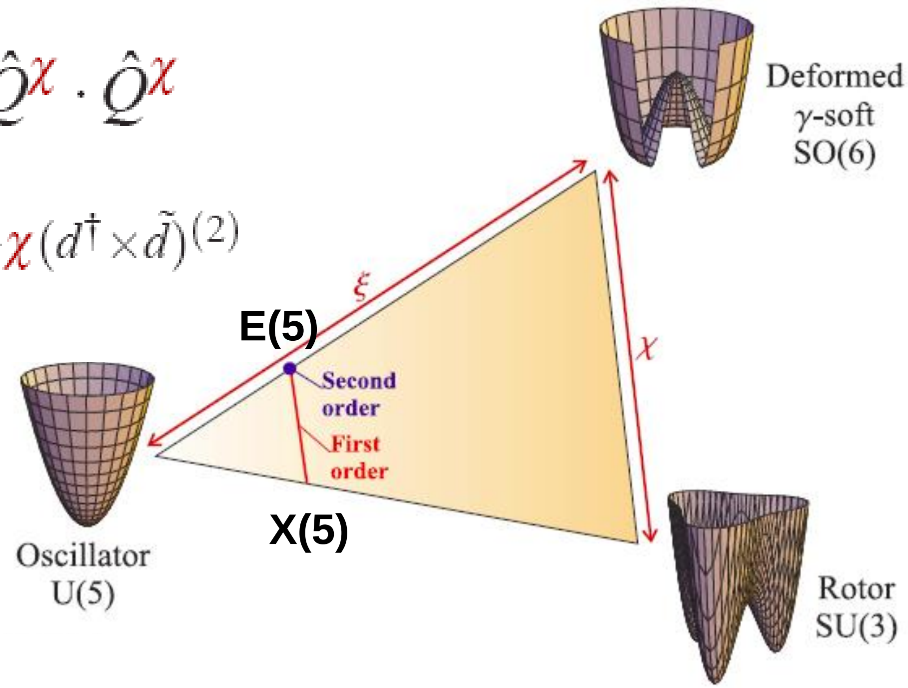
R = BE2(J→J-2) / BE2(2→0)



Quantum phase transitions in the interacting boson model:

$$H_{\mathrm{IBM}} = \frac{(1-\xi)}{N}\hat{n}_d - \frac{\xi}{N^2}\hat{Q}^{\chi}\cdot\hat{Q}^{\chi}$$

$$\hat{n}_d = d^\dagger\cdot\tilde{d} \qquad \hat{Q}^{\chi} = (s^\dagger\times\tilde{d}+d^\dagger\times\tilde{s})^{(2)} + \chi(d^\dagger\times\tilde{d})^{(2)}$$

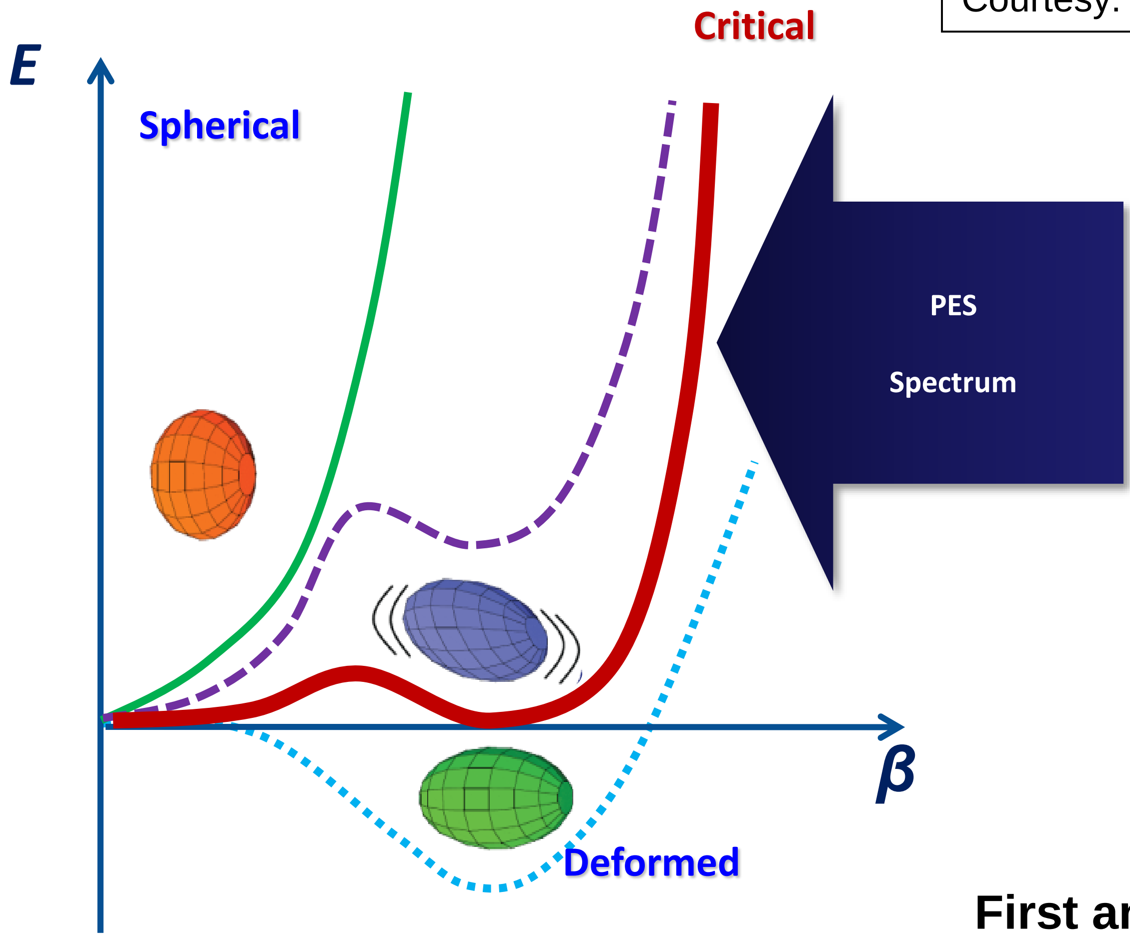


$$|\beta,\gamma;N\rangle = (N!)^{-1/2}(b_c^\dagger)^N|0\rangle ,$$

$$b_c^\dagger = (1+\beta^2)^{-1/2}[\beta\cos\gamma\, d_0^\dagger + \beta\sin\gamma\,(d_2^\dagger + d_{-2}^\dagger)/\sqrt{2} + s^\dagger]$$

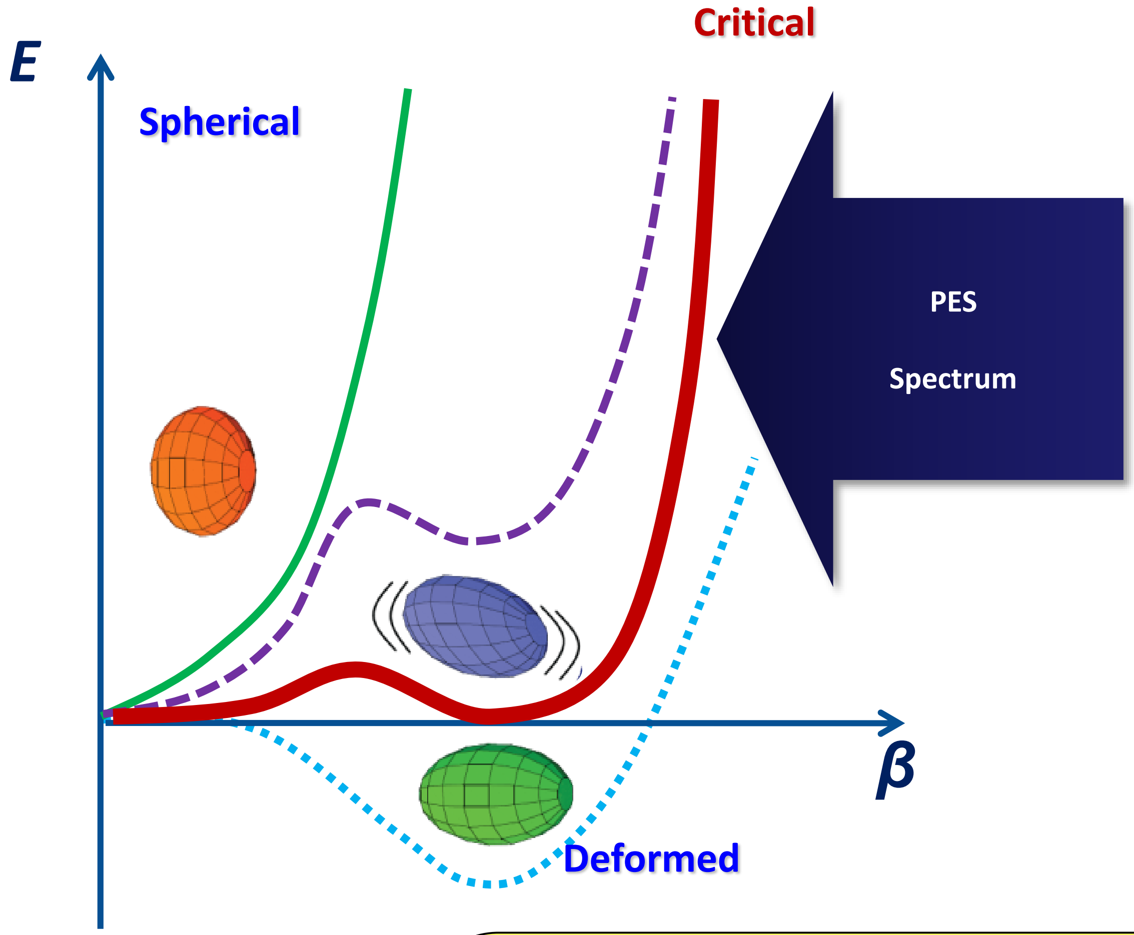
E(5): F. Iachello, PRL 85, 3580 (2000)
X(5): F. Iachello, PRL 87, 52502 (2001)

Courtesy: Zhipan Li



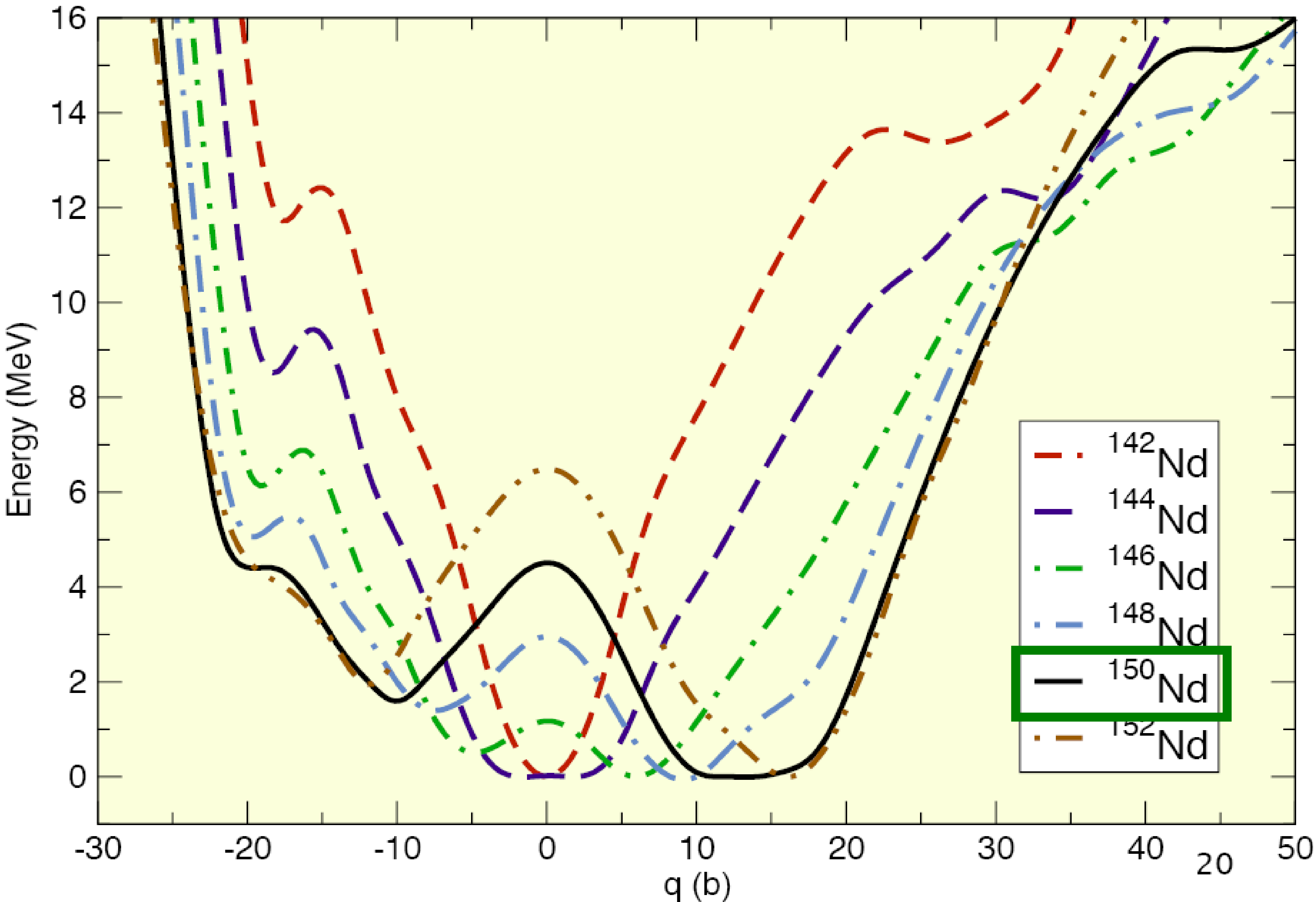
First and second order QPT can occur between systems characterized by different ground-state **shapes**.

Control Parameter: **Number of nucleons**

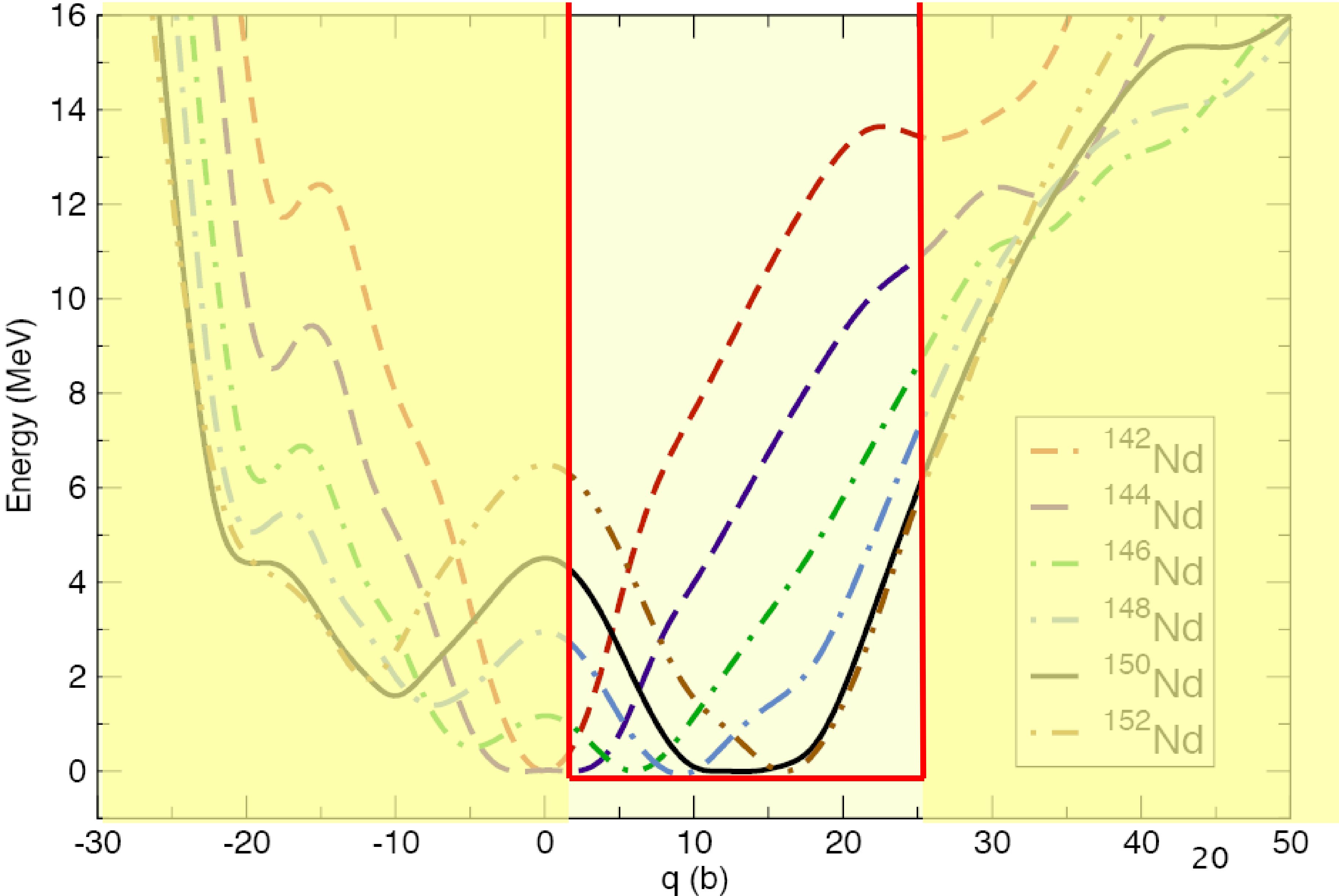


Can we descibe such phenomena
in a microscopic picture,
with nucleonic degrees of freedom,
free of phenomenological parameters?

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



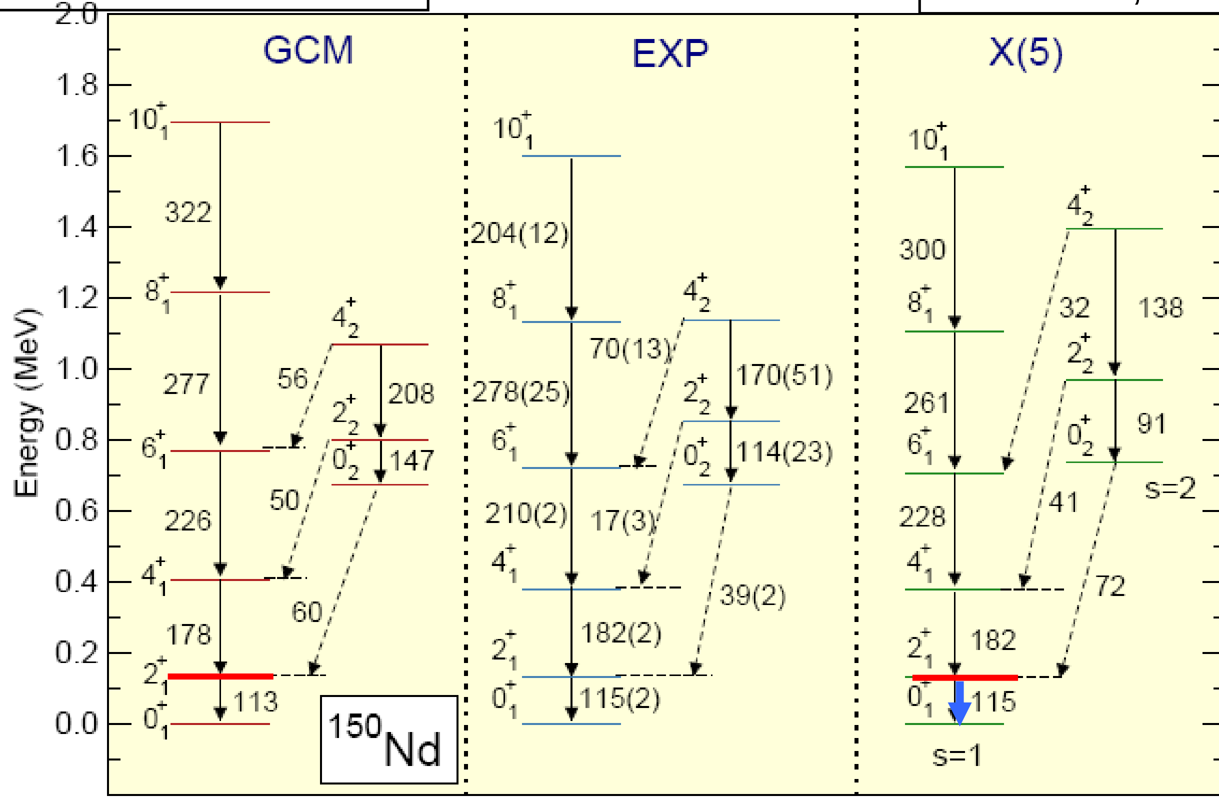
Self-consistent RMF plus Lipkin-Nogami BCS binding energy curves of $^{142-152}$Nd, as functions of the mass quadrupole moment.



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

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

F. Iachello, PRL 87, 52502 (2001)

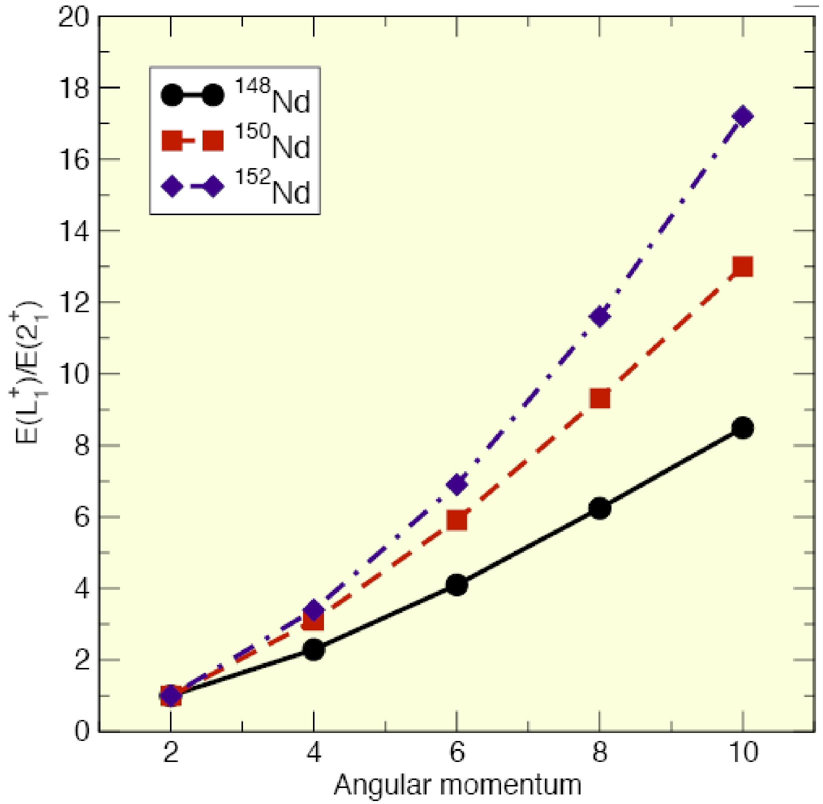


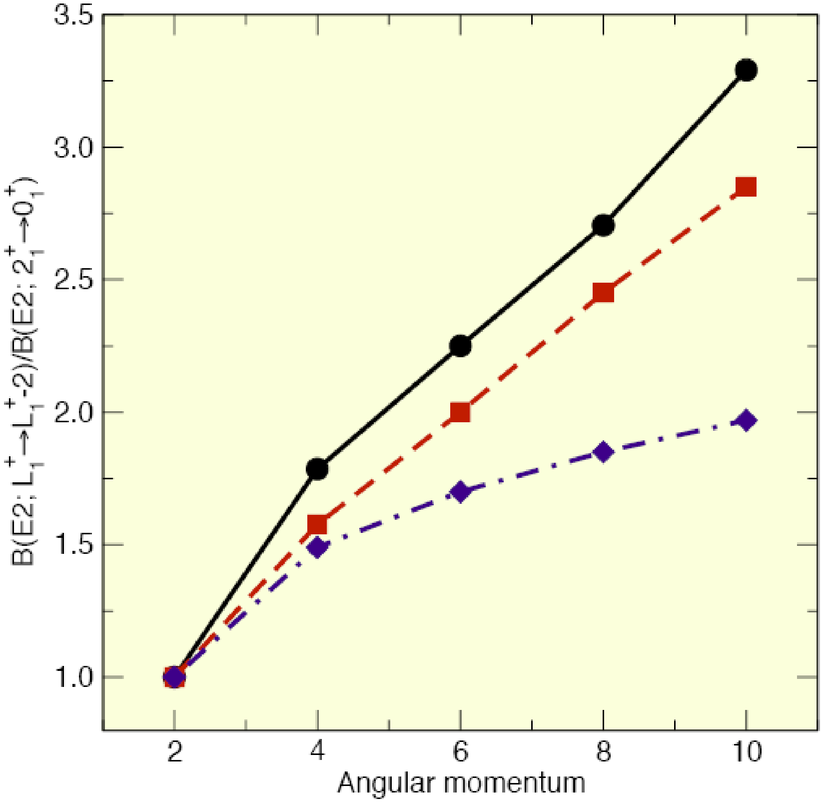
GCM: only one scale parameter: **$E(2_1)$**

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

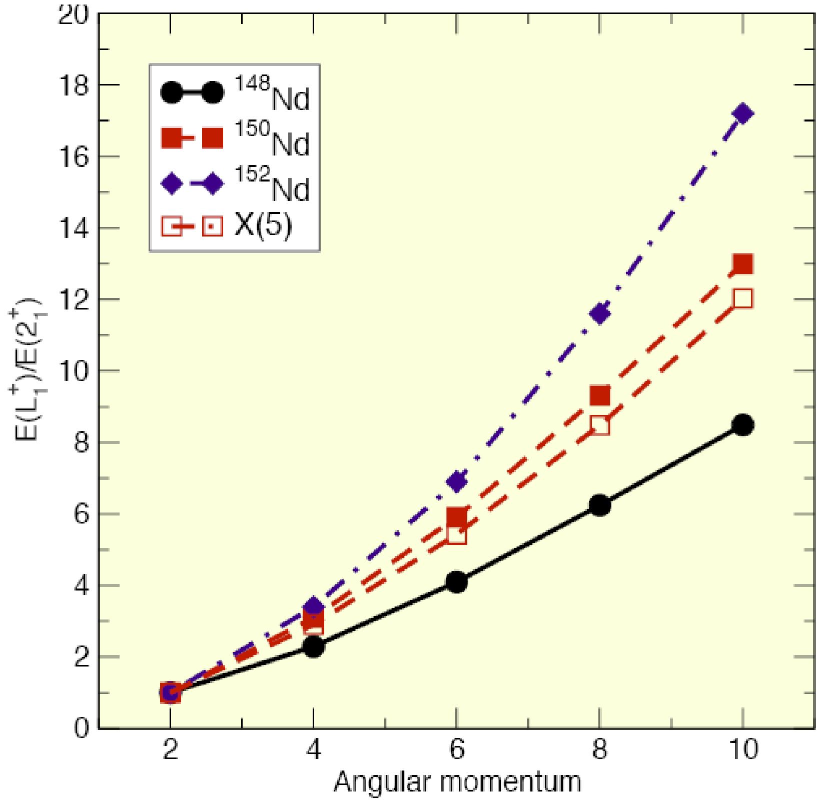
Problem of GCM at this level: **restricted to $\gamma=0$**

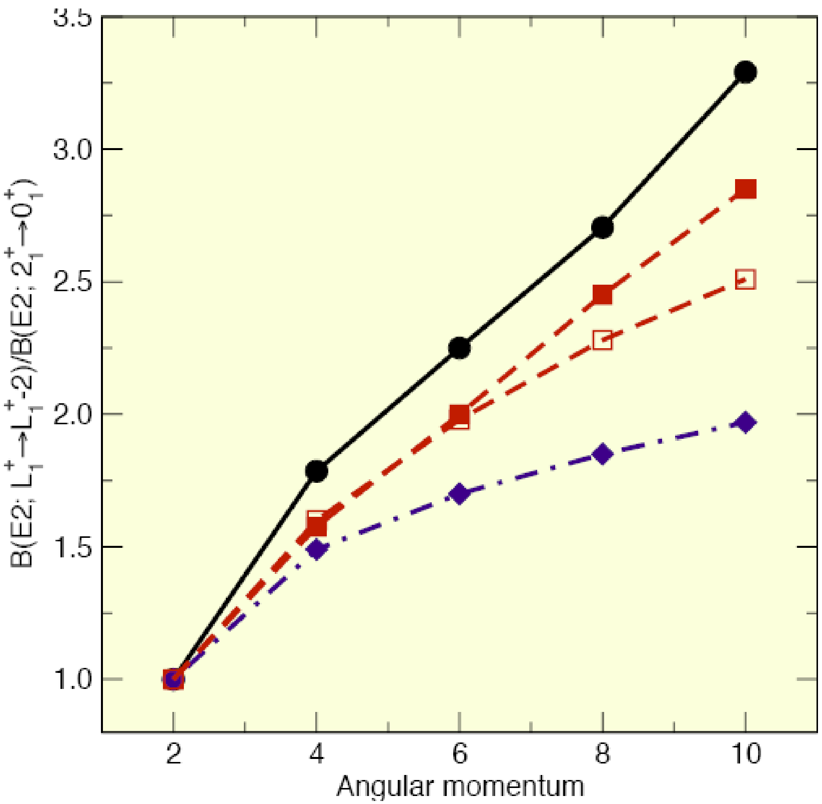
B(E2; L → L-2) values and excitation energies for the yrast states: **^{148}Nd**, **^{150}Nd**, and **^{152}Nd**, calculated with the GCM:



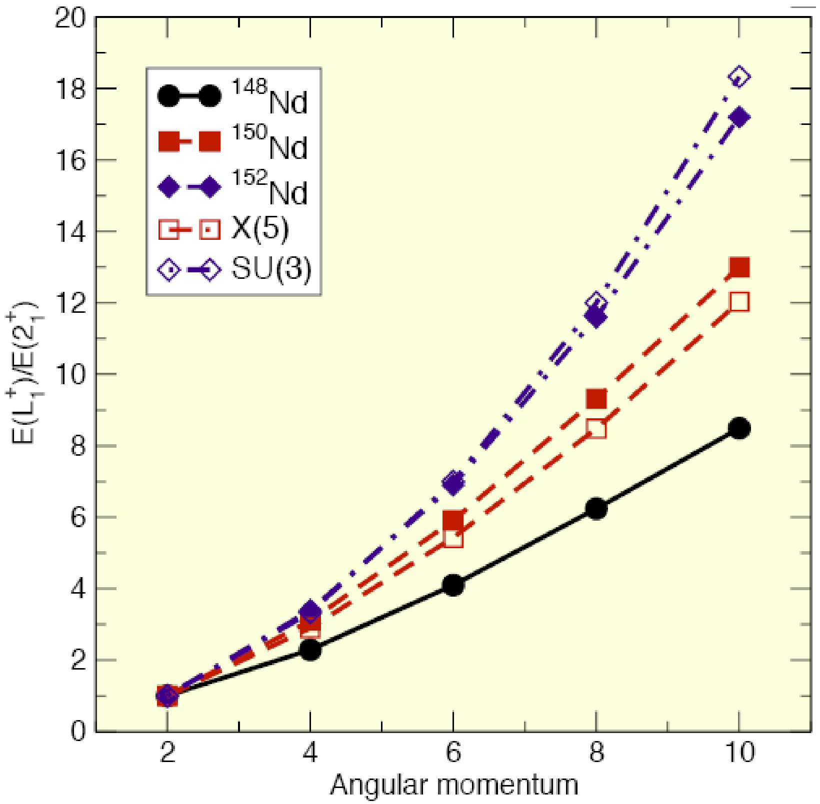


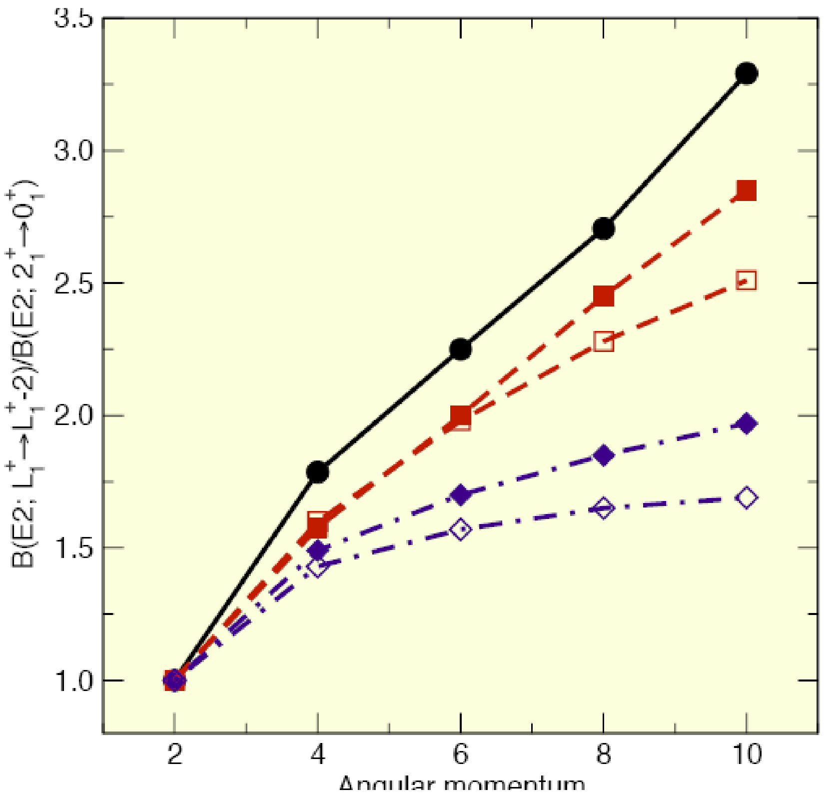
B(E2; L → L-2) values and excitation energies for the yrast states: **^{148}Nd**, **^{150}Nd**, and **^{152}Nd**, calculated with the GCM and compared with those predicted by the **X(5)**:



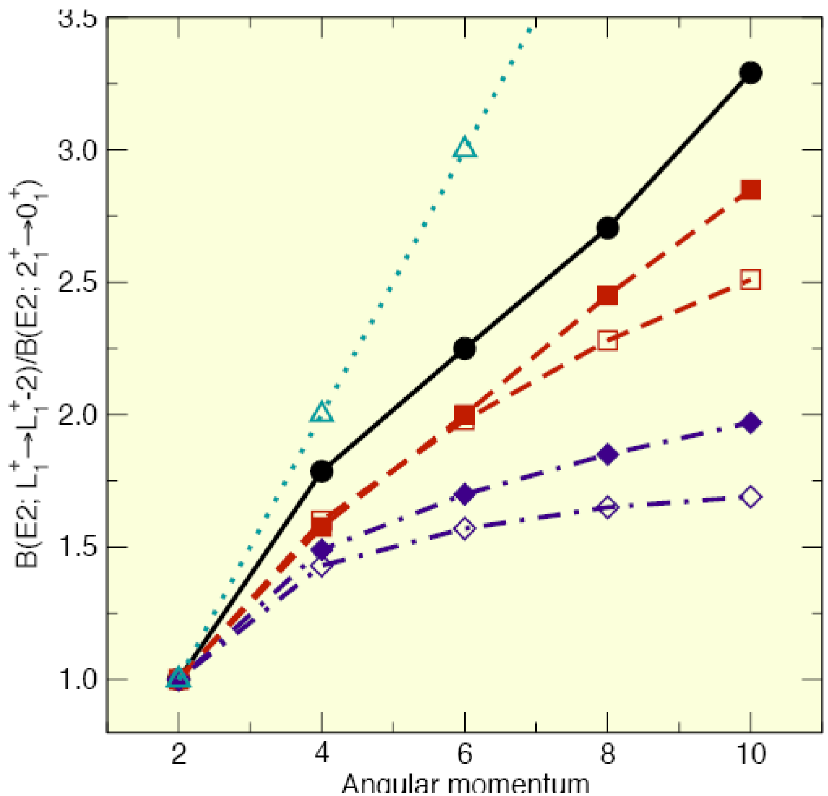


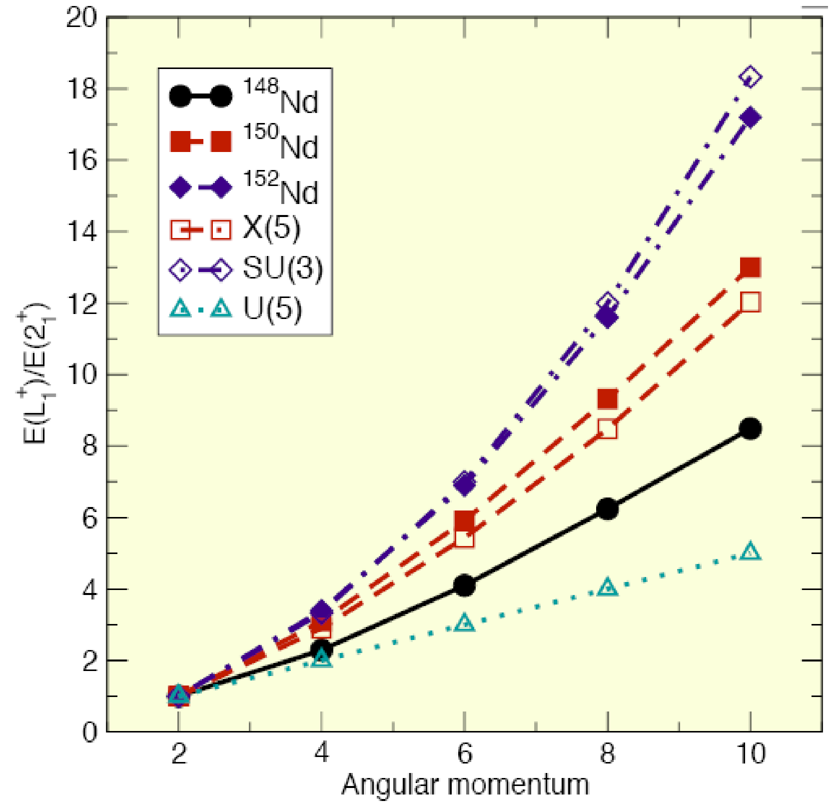
B(E2; L → L-2) values and excitation energies for the yrast states: **^{148}Nd**, **^{150}Nd**, and **^{152}Nd**, calculated with the GCM and compared with those predicted by the **X(5)**, **SU(3)**





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.





Content:

- Generator-Coordinate Method (GCM)
- Applications:

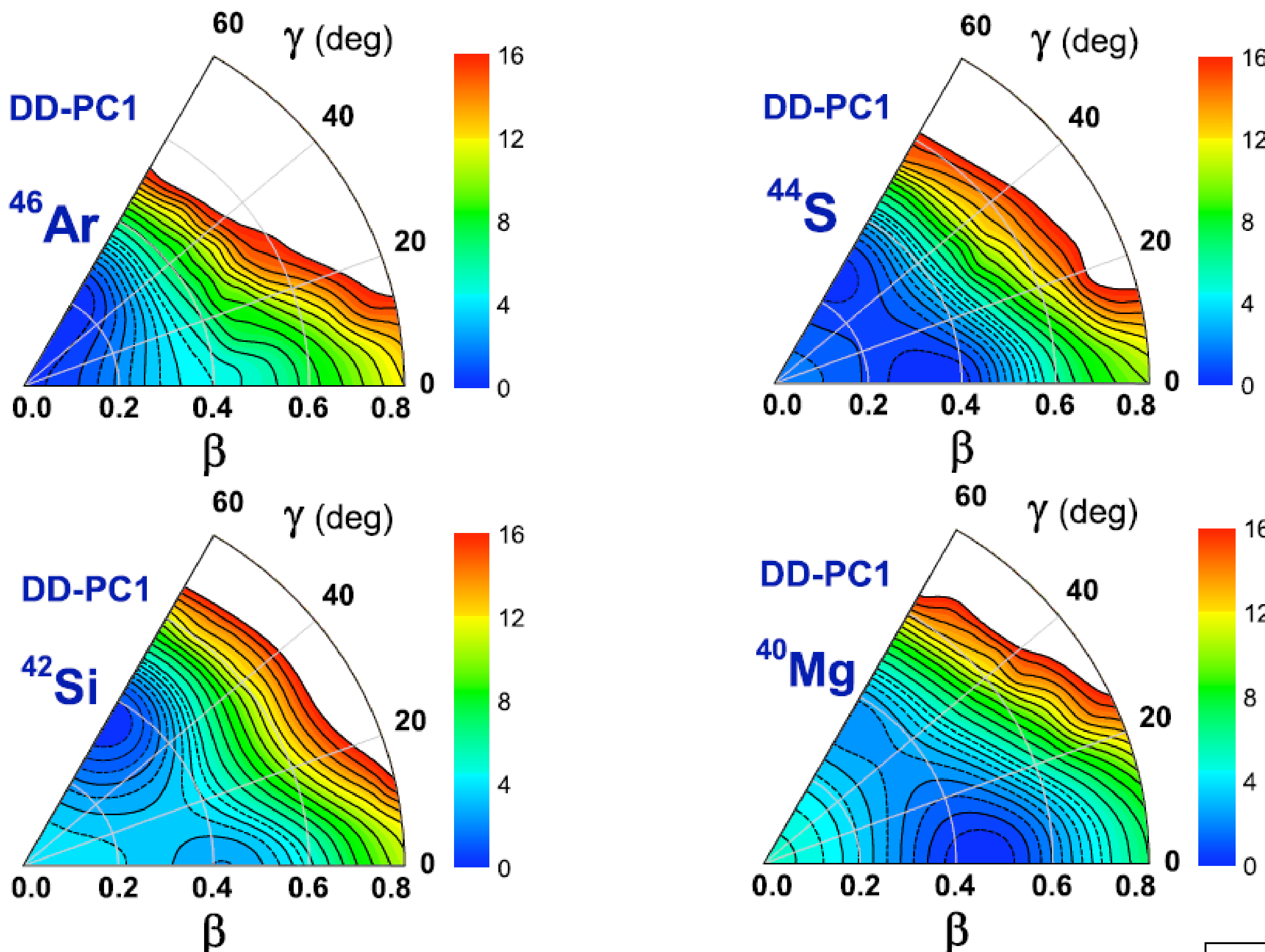
  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure: N=28 isotones

  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- Benchmark calculations (full GCM ↔ 5DCH)
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

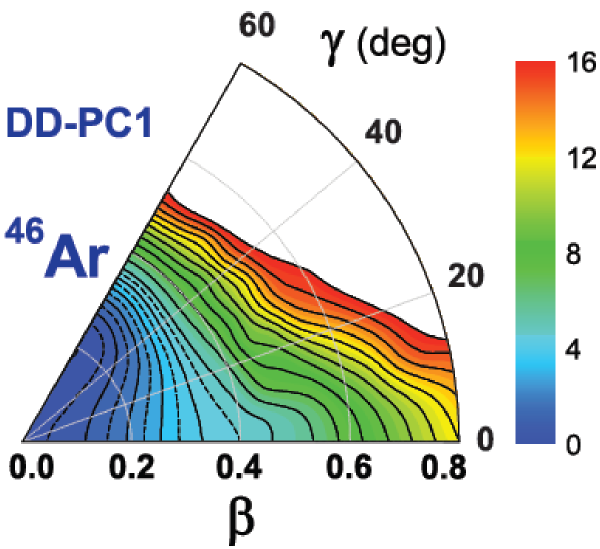
Applications: $N = 28$ isotones

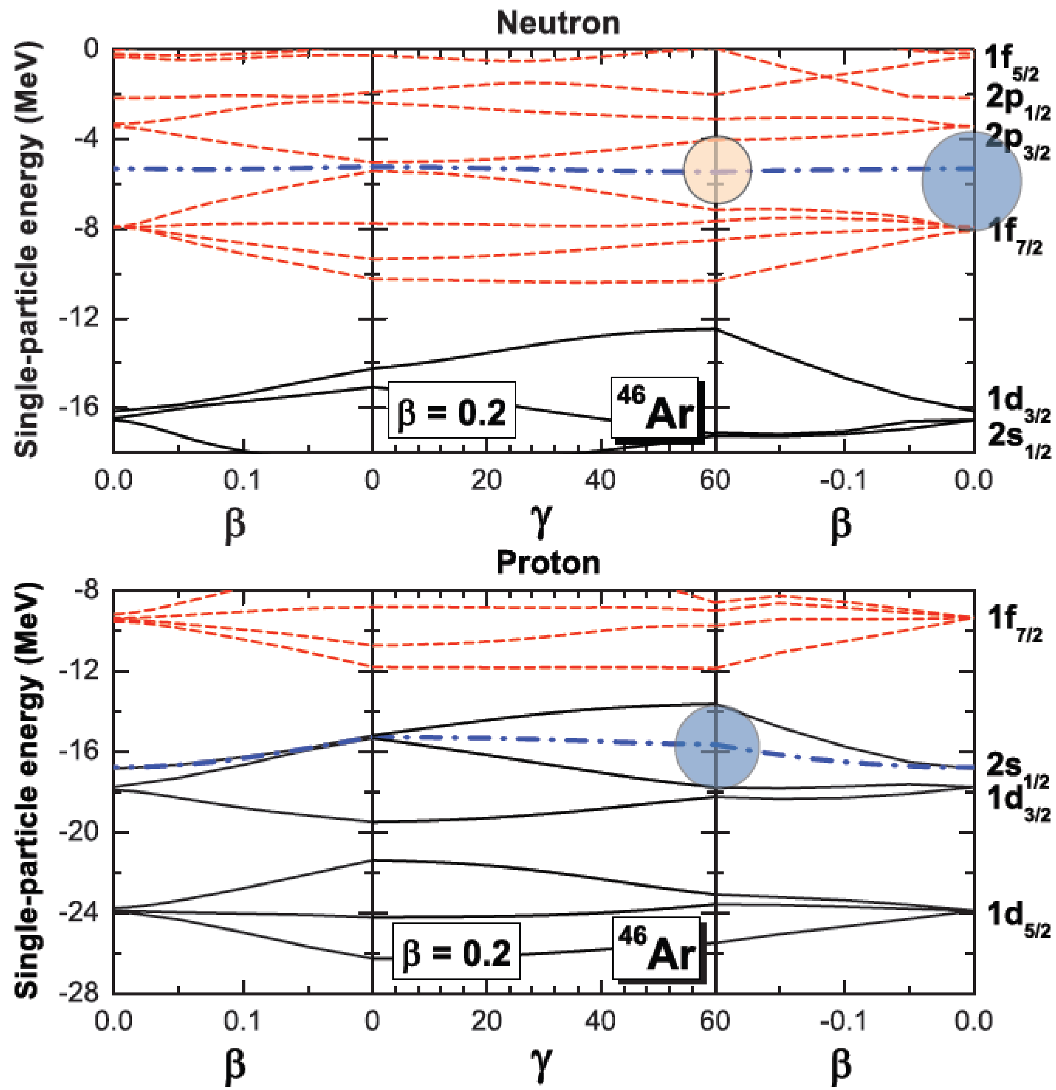
The variation of the mean-field shapes is governed by the evolution of the underlying shell structure of single-nucleon orbitals.



T.Niksic (2011)

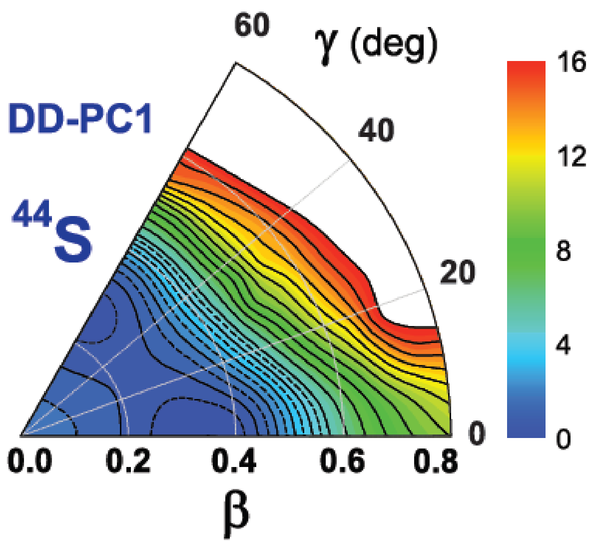
^{46}Ar isotope: single-particle levels

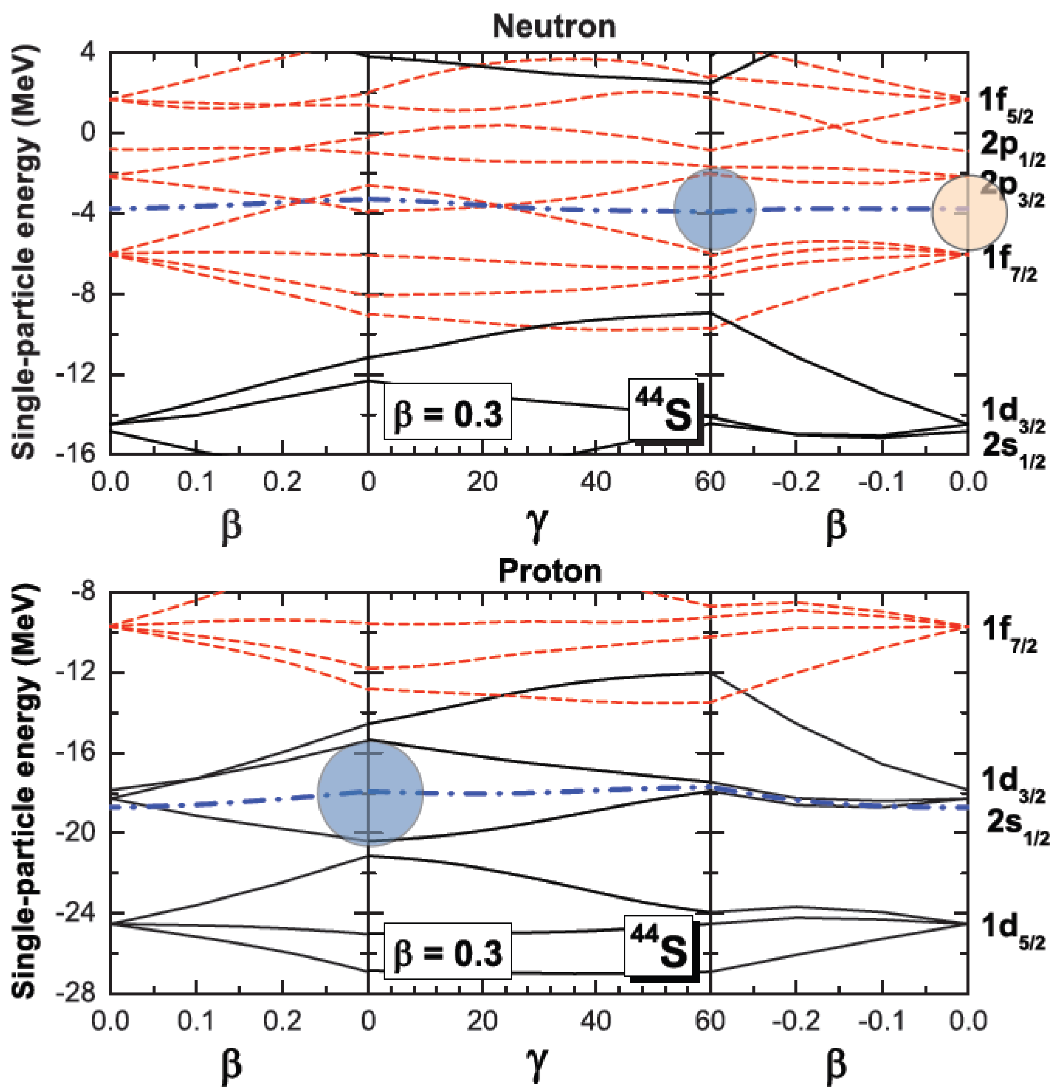




T.Niksic (2011)

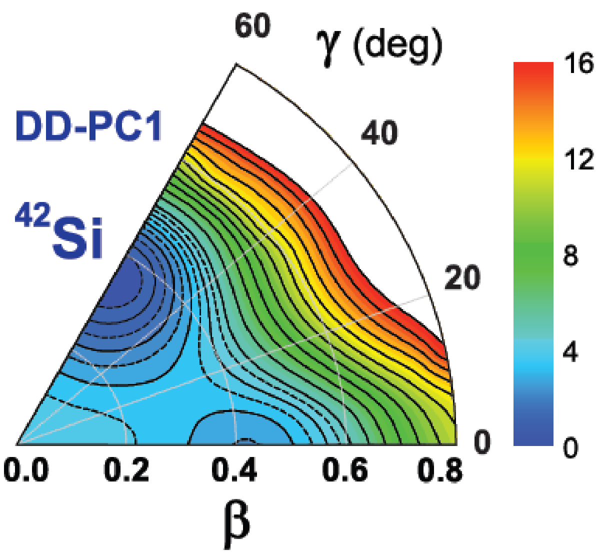
^{44}S isotope: single-particle levels

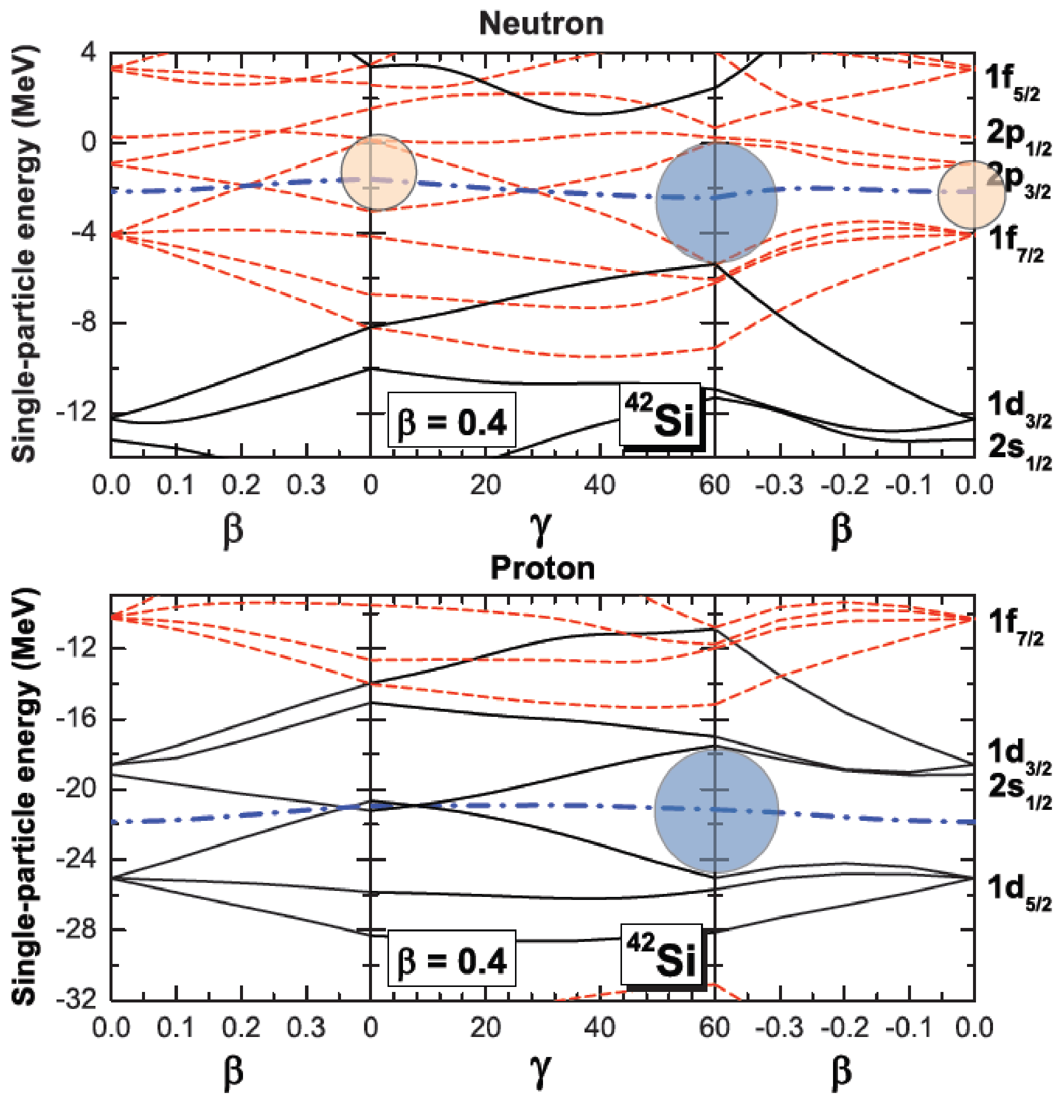




T.Niksic (2011)

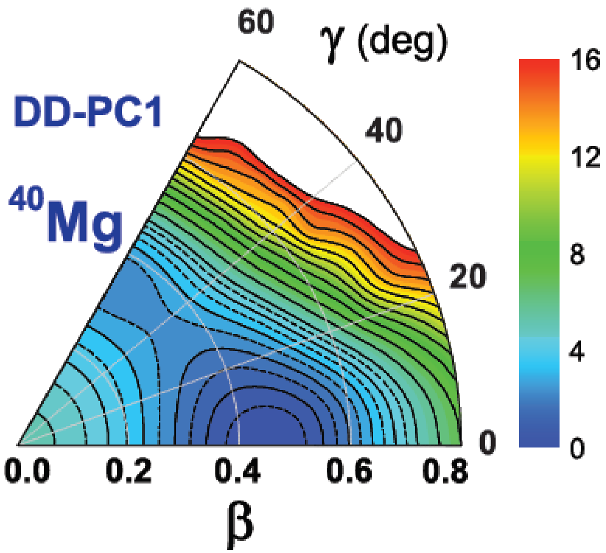
^{42}Si isotope: single-particle levels

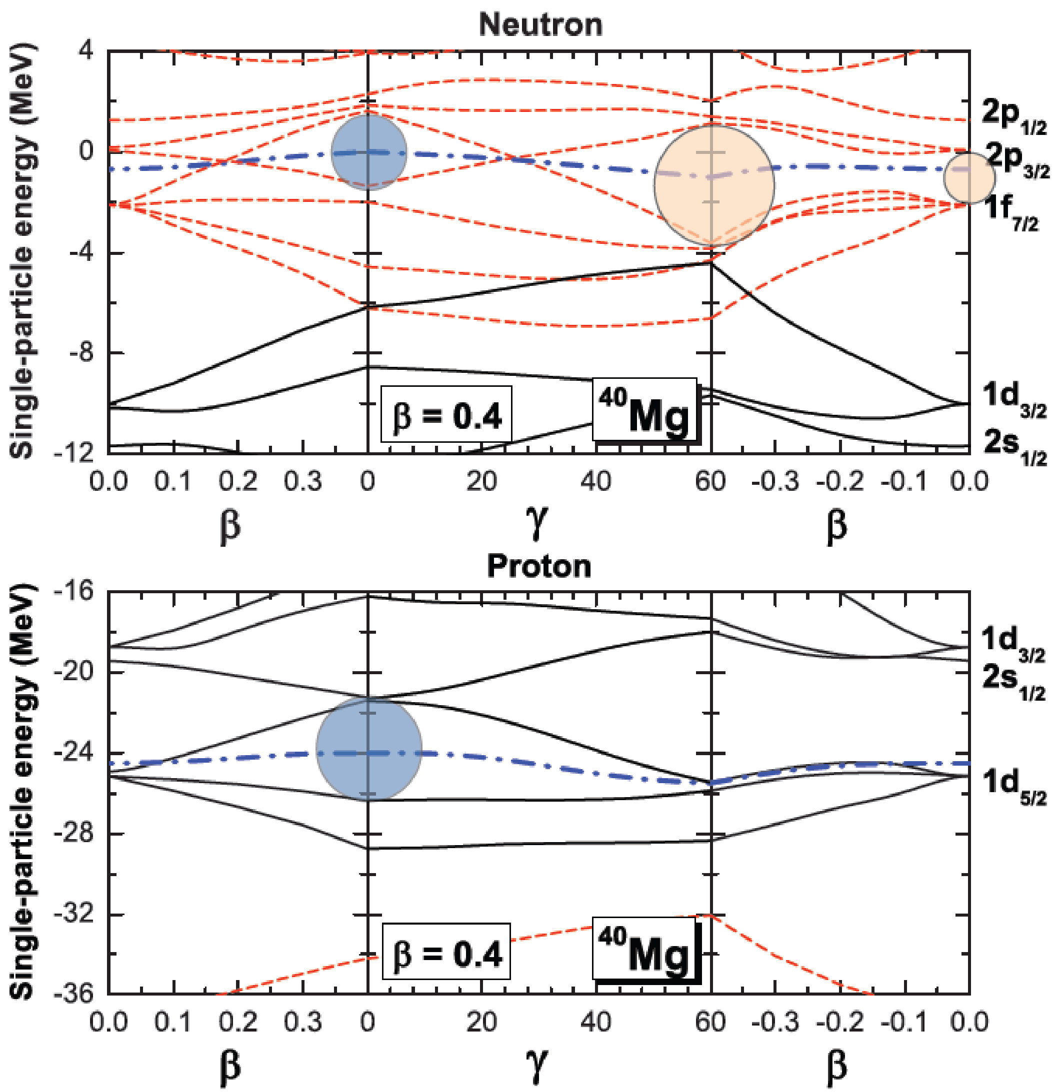




T.Niksic (2011)

^{40}Mg isotope: single-particle levels





T.Niksic (2011)

Content:

- Generator-Coordinate Method (GCM)
- Applications:

  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure: N=28 isotones

  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- Benchmark calculations (full GCM ↔ 5DCH)
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

alpha-clustering in nuclei:

- α-clustering happens mostly in excited states

  v. Oertzen et al, Phys.Rep (2006), Freer Rep.P.Phys. (2997), Kanada-En'yo et al (2012)

- light α-conjugate nuclei have duality structure
  (mean-field is mixed with α-configurations)

  Wiringa et al, PRC (2000), Chernykh et al, PRC (2011)

- ^{20}Ne: mixture between def. mean field and α+^{16}O
  with increasing spin α+^{16}O structure becomes weaker

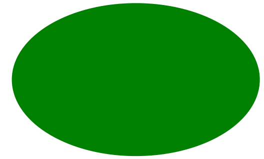
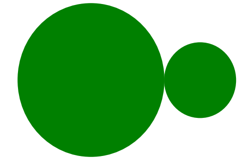
  AMD-calculations: Kanada-En'yo et al PTP (1995)

- Relativistic mean fields are deeper and favor cluster structure

  Ebran et al, Nature 2012

- Relativistic GCM provides tool for a quantitative assessment

alpha-clustering in nuclei:

^{20}Ne:  or  ?

- α-clustering happens mostly in excited states

  v. Oertzen et al, Phys.Rep (2006), Freer Rep.P.Phys. (2997), Kanada-En‘yo et al (2012)

- light α-conjugate nuclei have duality structure
  (mean-field is mixed with α-configurations)

  Wiringa et al, PRC (2000), Chernykh et al, PRC (2011)

- ^{20}Ne: mixture between def. mean field and α+^{16}O
  with increasing spin α+^{16}O structure becomes weaker

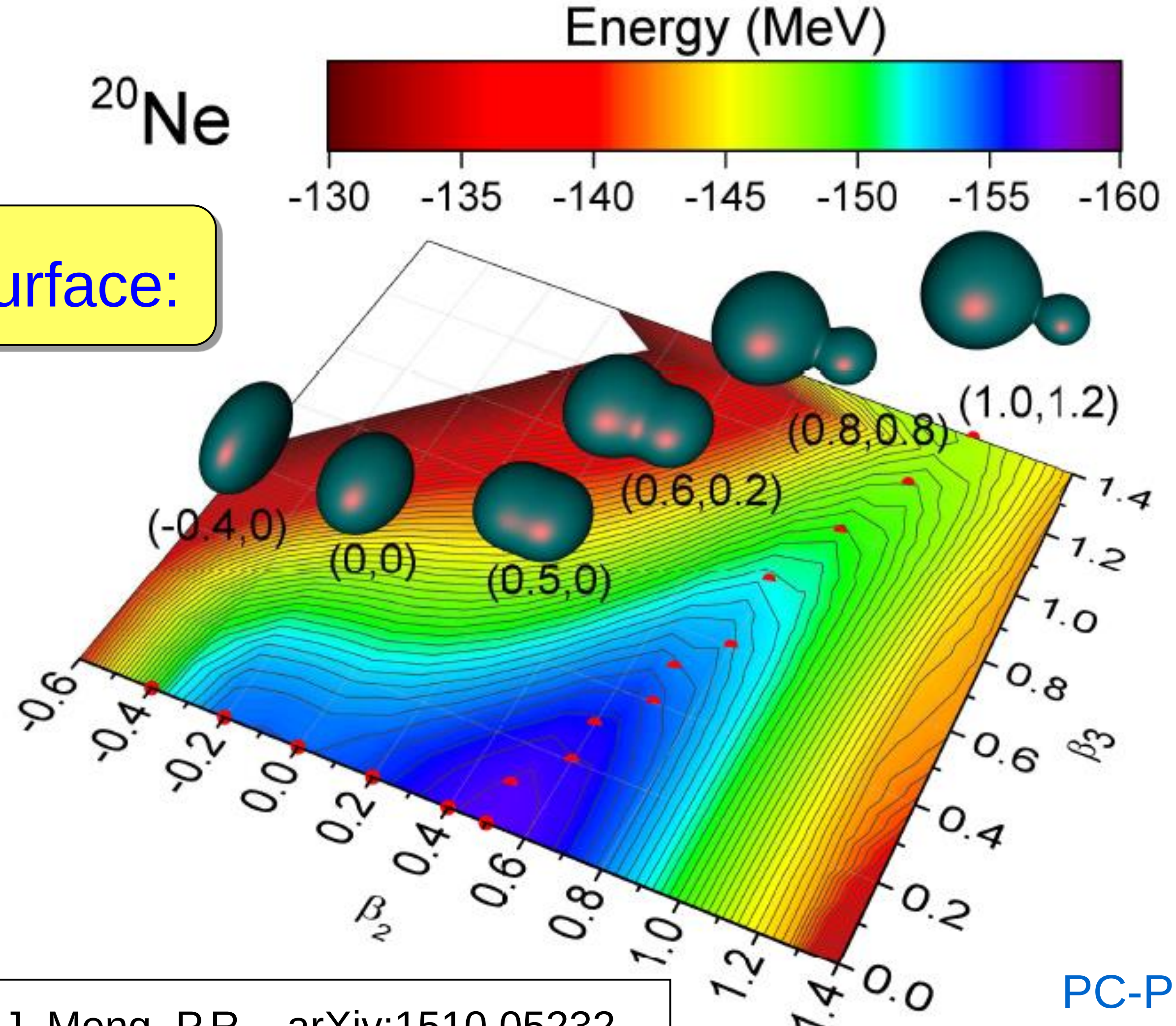
  AMD-calculations: Kanada-En‘yo et al PTP (1995)

- Relativistic mean fields are deeper and favor cluster structure

  Ebran et al, Nature 2012

- Relativistic GCM provides tool for a quantitative assessment

Mean field energy surface:



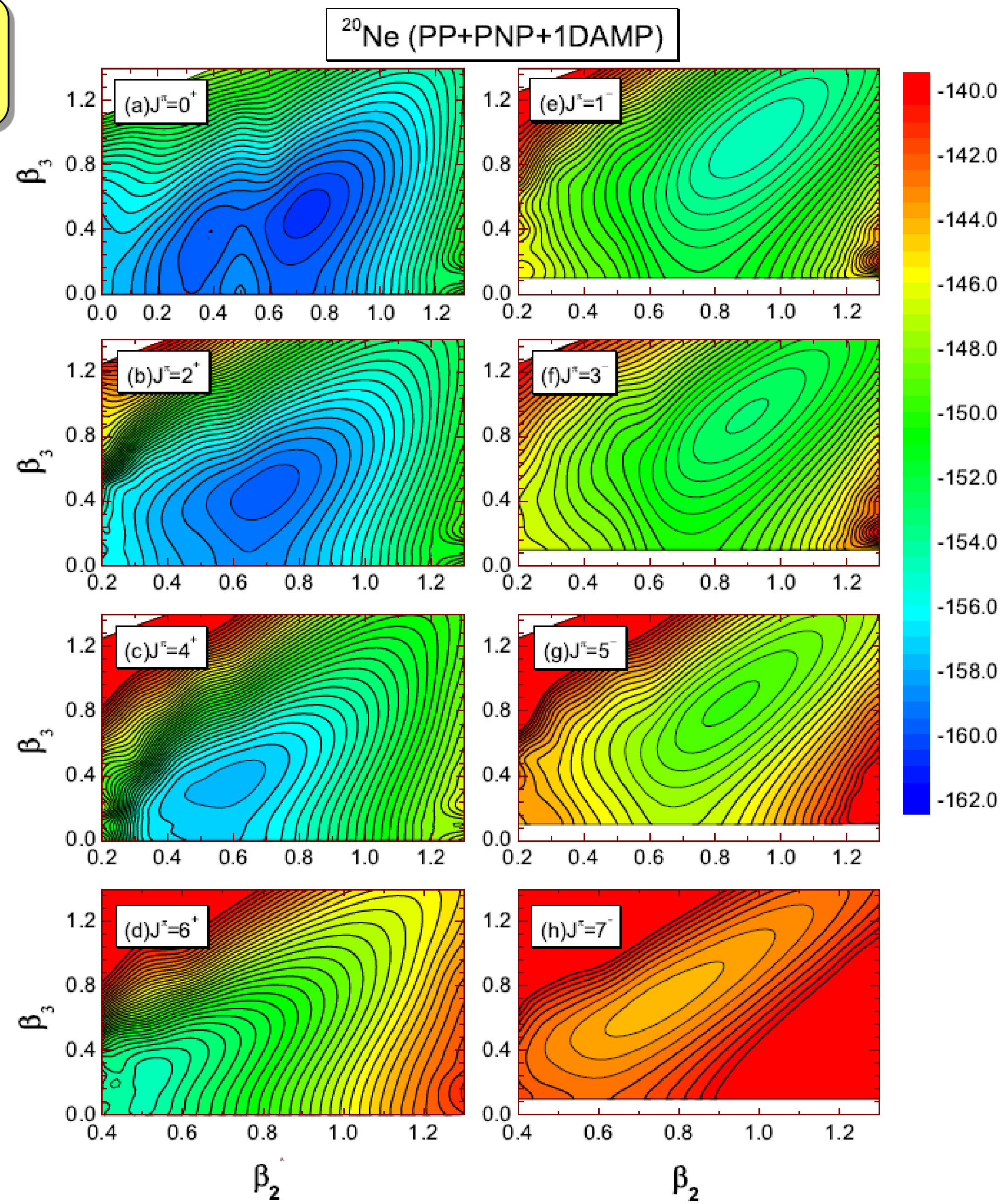
E.F. Zhou, J.M. Yao, Z.P. Li, J. Meng, P.R. arXiv:1510.05232

PC-PK1
N_f=10
N_{GCM}=54

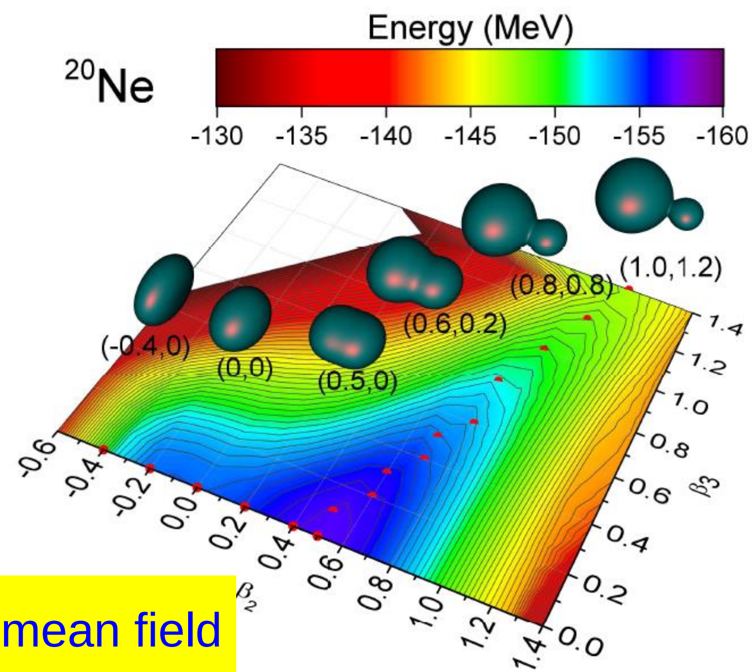
$$|J^\pi NZ;\alpha\rangle = \sum_{\kappa\in\{q,K\}} f_\kappa^{J\pi\alpha} \hat{P}^J_{MK}\hat{P}^N\hat{P}^Z\hat{P}^\pi|q\rangle, \qquad q = \{\beta_2, \beta_3\}$$

ıte, Kyoto

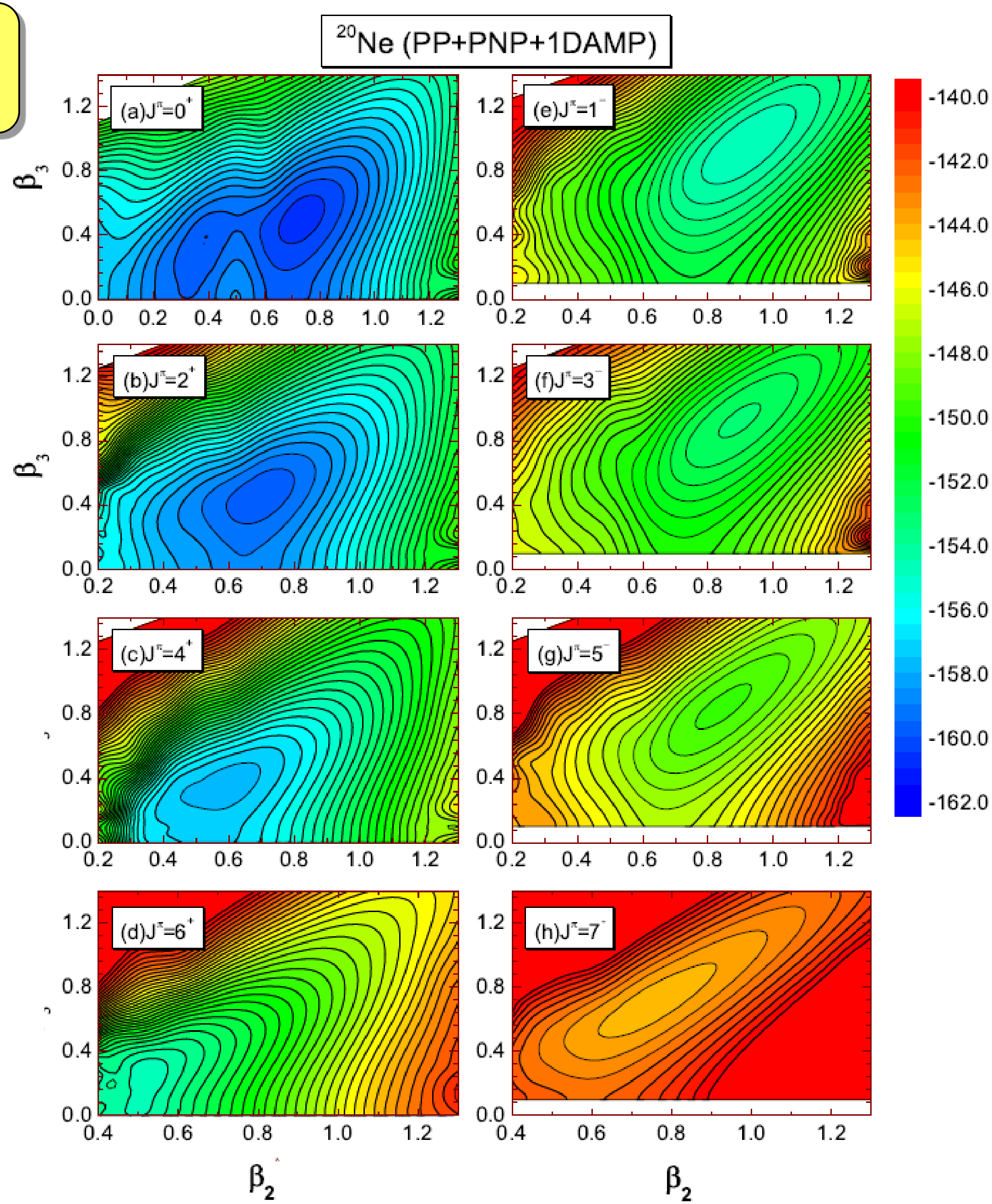
Projected energy surfaces:



Projected energy surfaces:



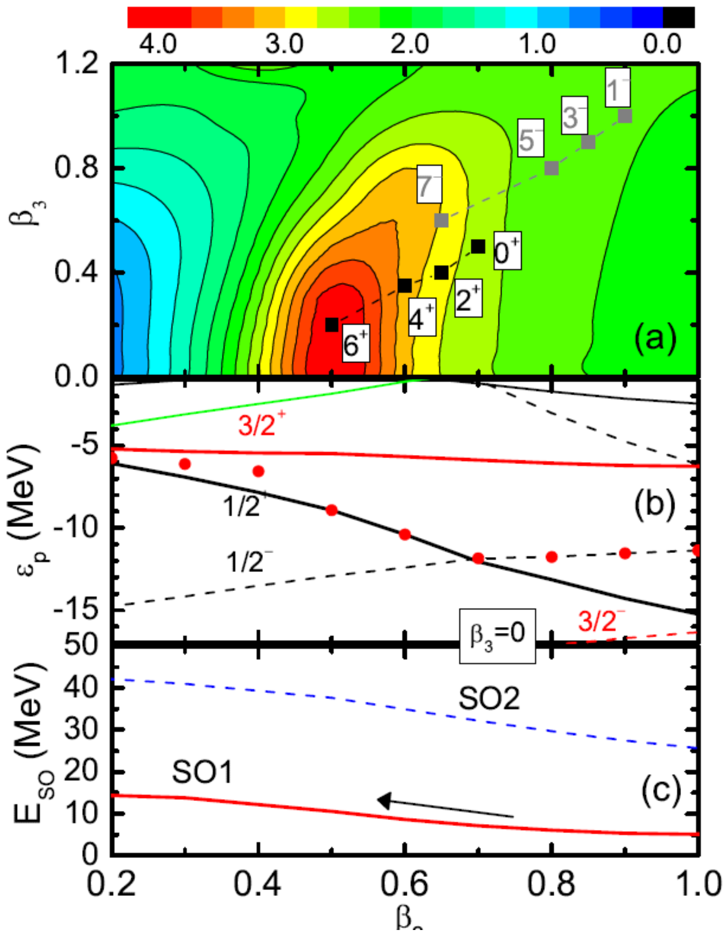
mean field

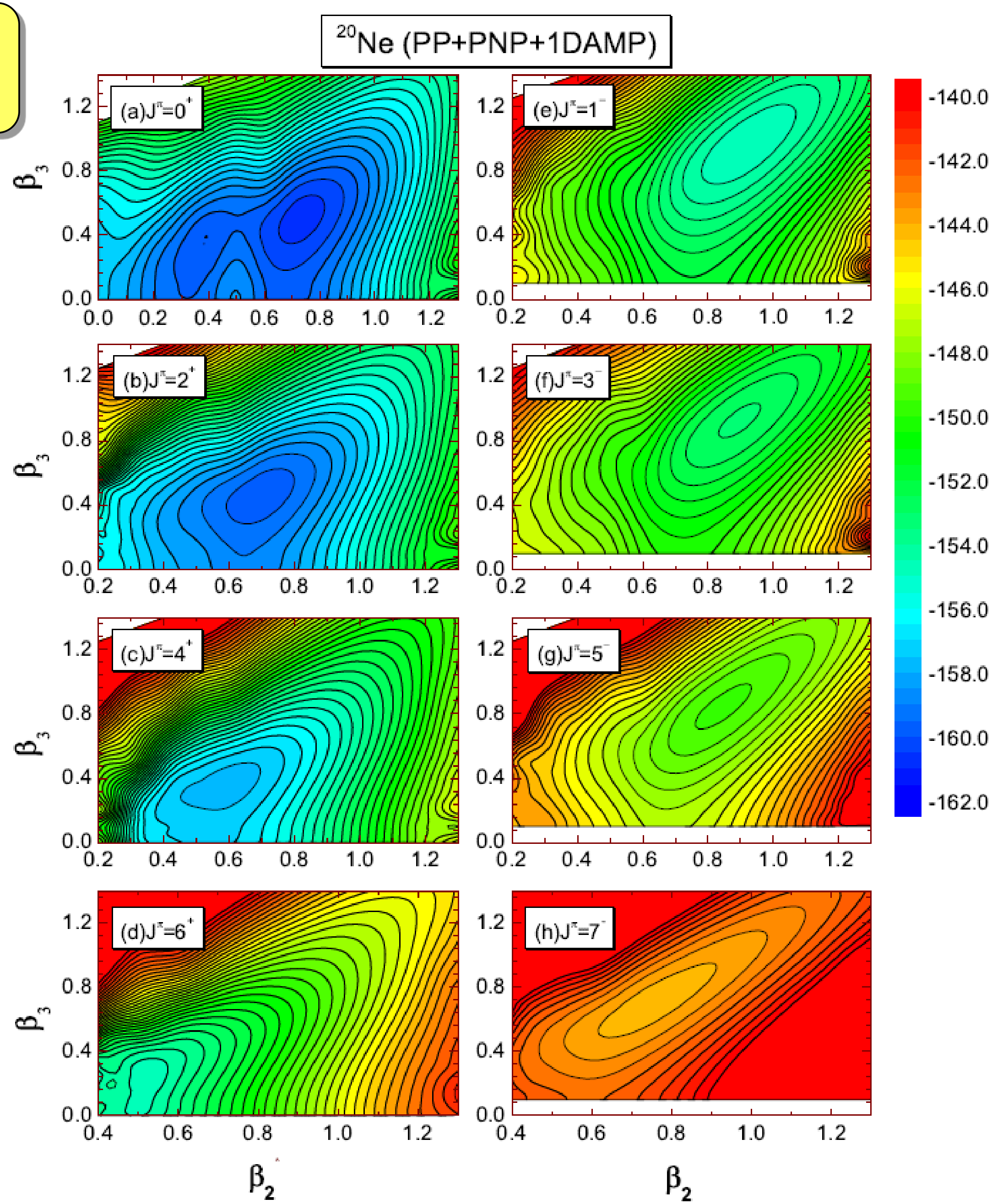


Enfu Zhou et al. 2015

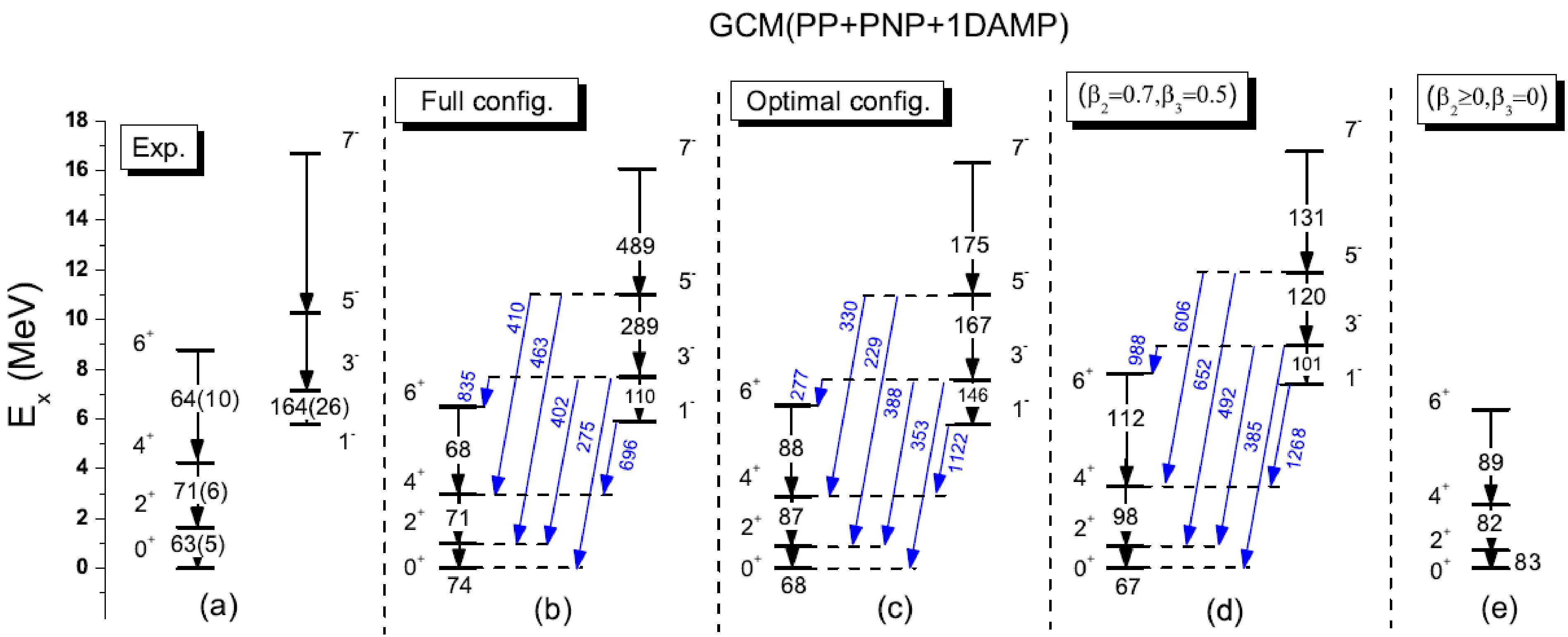
Projected energy surfaces:

Moment of inertia *J*





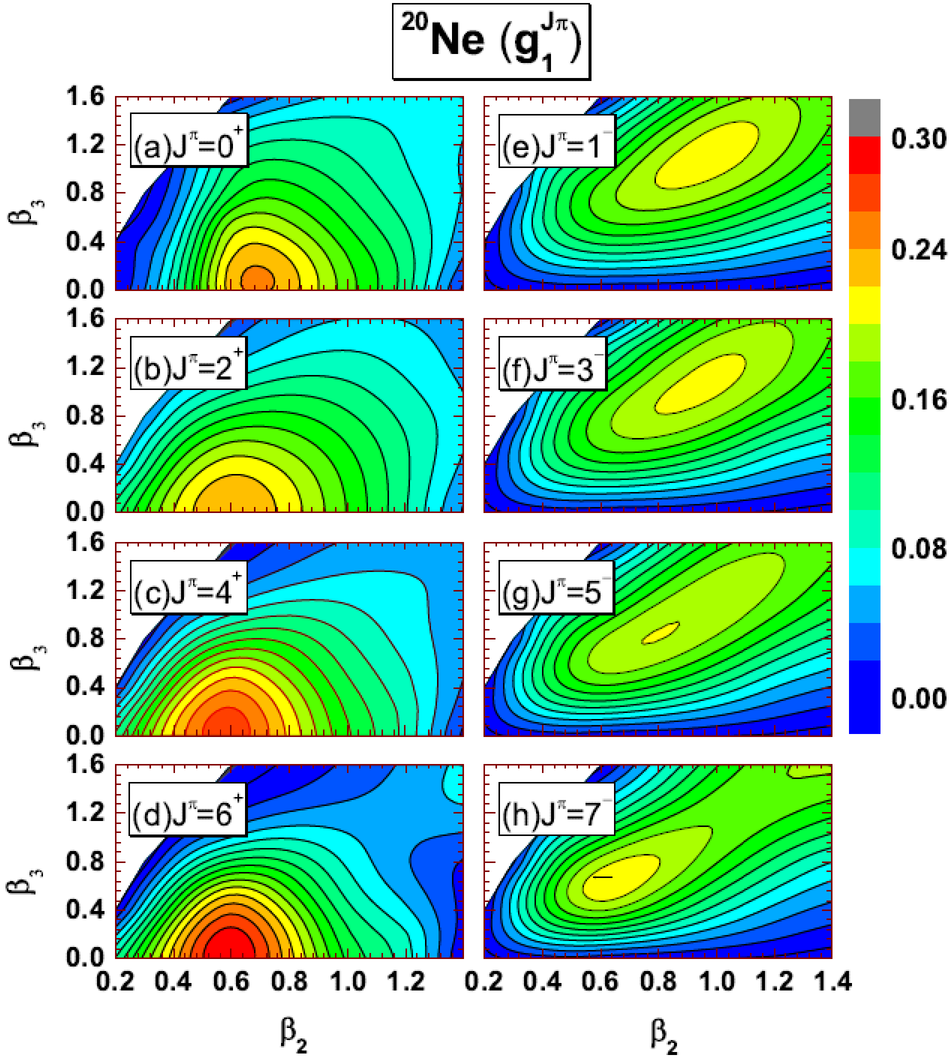
Low-lying spectra:



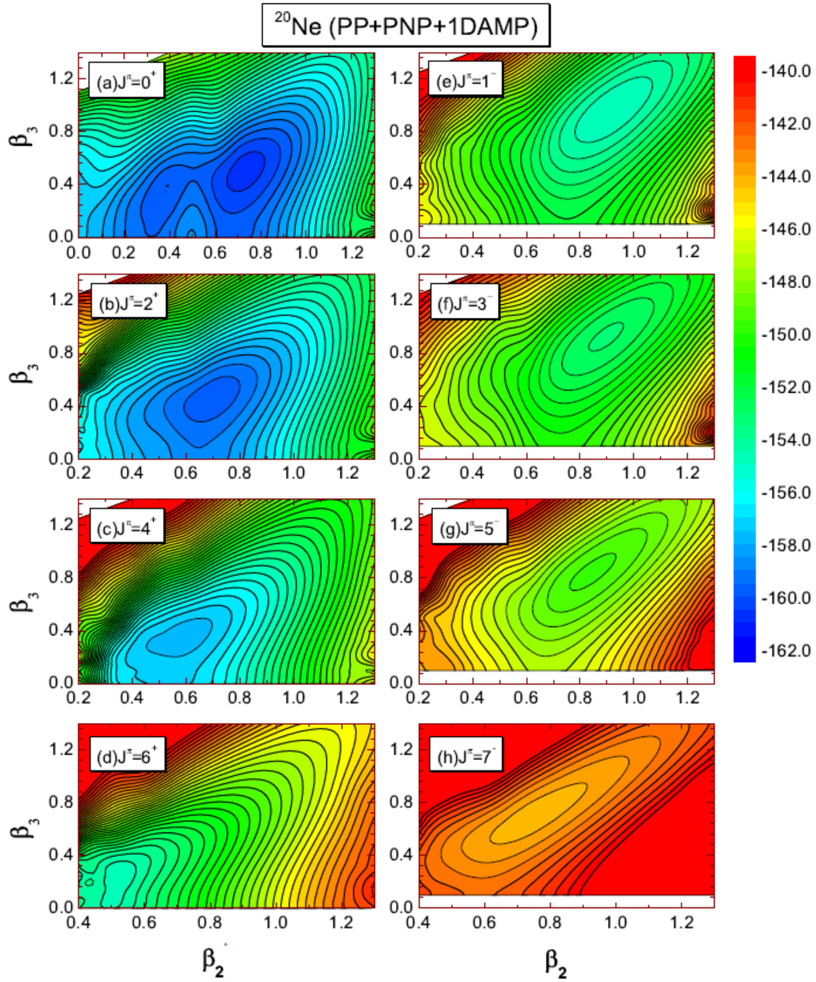
B(E2)

B(E3)

Wave functions:

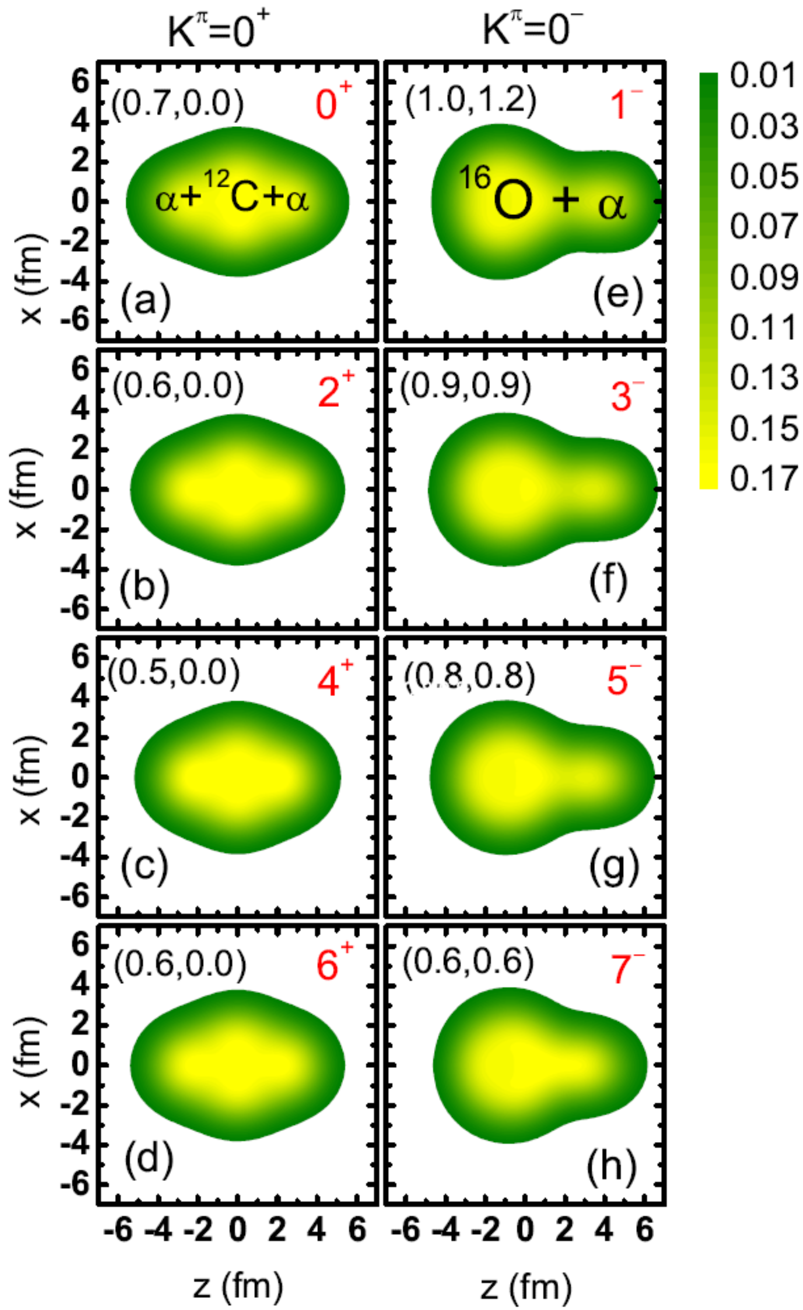


projected energy:



Enfu Zhou et al. 2015

Intrinsic density of the dominand configuration for each J^{π}-value



Enfu Zhou et al. 2015

Content:

- Generator-Coordinate Method (GCM)
- Applications:

  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure N=28 isotones

  α-clustering in light nuclei
- **Derivation of a Collective Hamiltonian (5DCH)**
- Benchmark calculations (full GCM ↔ 5DCH)
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

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)	

Inertia of Thouless Valatin:

$$\hat{P} = \frac{1}{i}\frac{\partial}{\partial q}$$

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

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

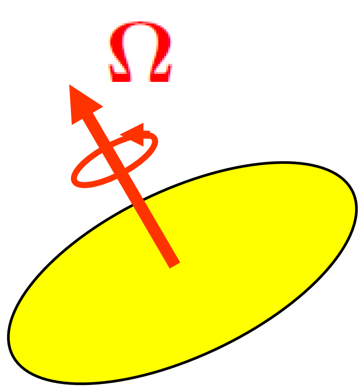
$$\mathcal{M} = \mathcal{M}_0\left[\mathbb{1} + \mathcal{V}\mathcal{M}_0\right]^{-1}$$

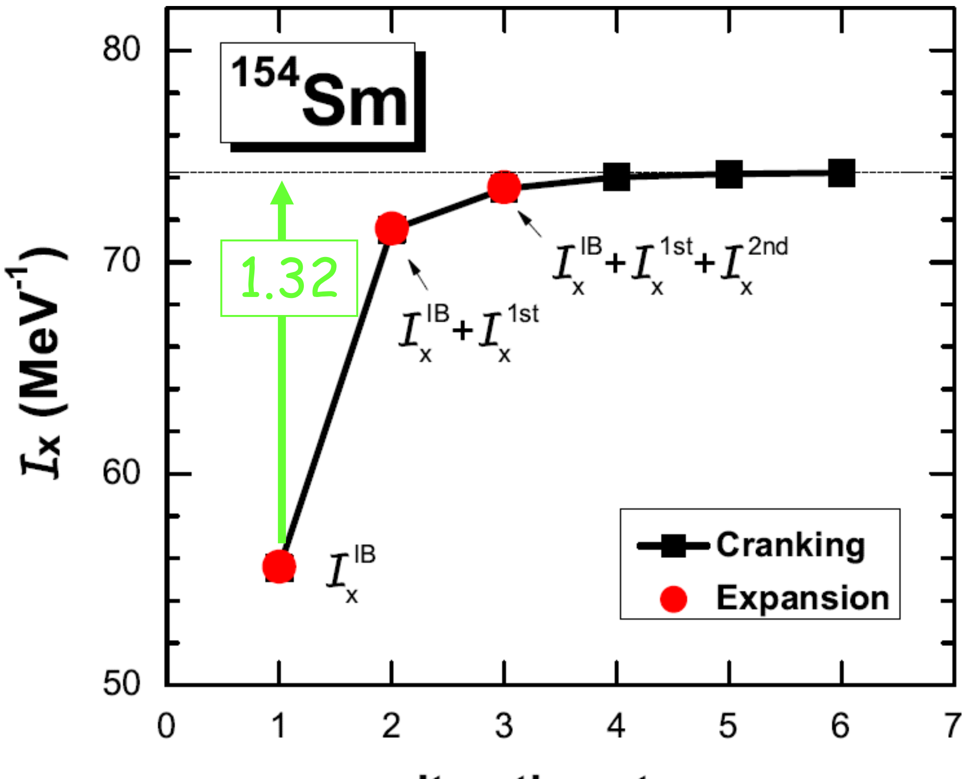
$$\boxed{\left(\mathcal{M}_0^{-1}\right)_{php'h'} = (\epsilon_p - \epsilon_h)\delta_{pp'}\delta_{hh'}}$$

$$\mathcal{M} = \mathcal{M}_0 - \mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \mathcal{M}_0\mathcal{V}\mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \cdots .$$

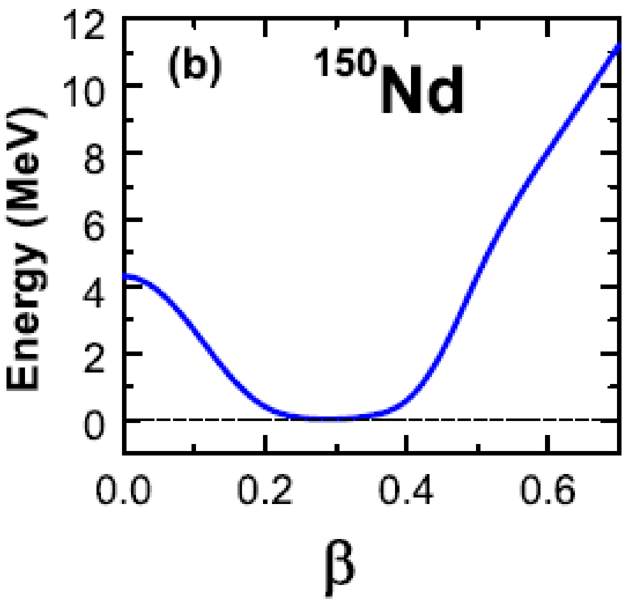
Zhipan Li et al PRC 86 (2012)

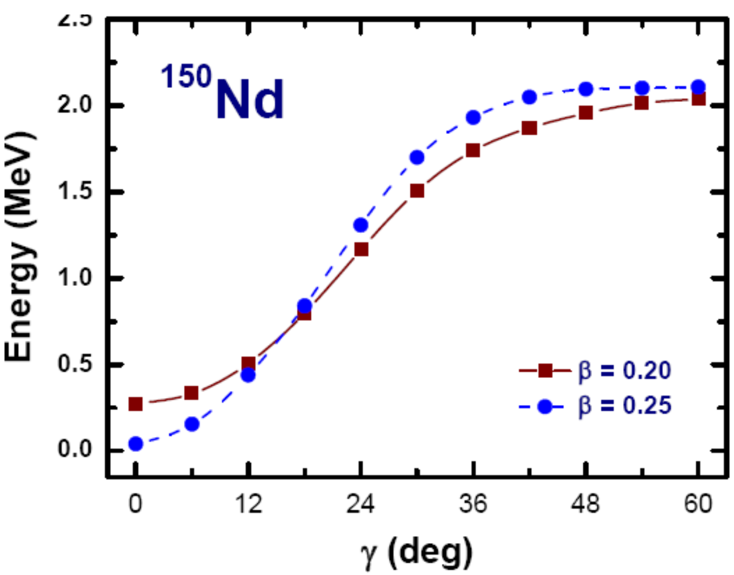
Moment of inertia

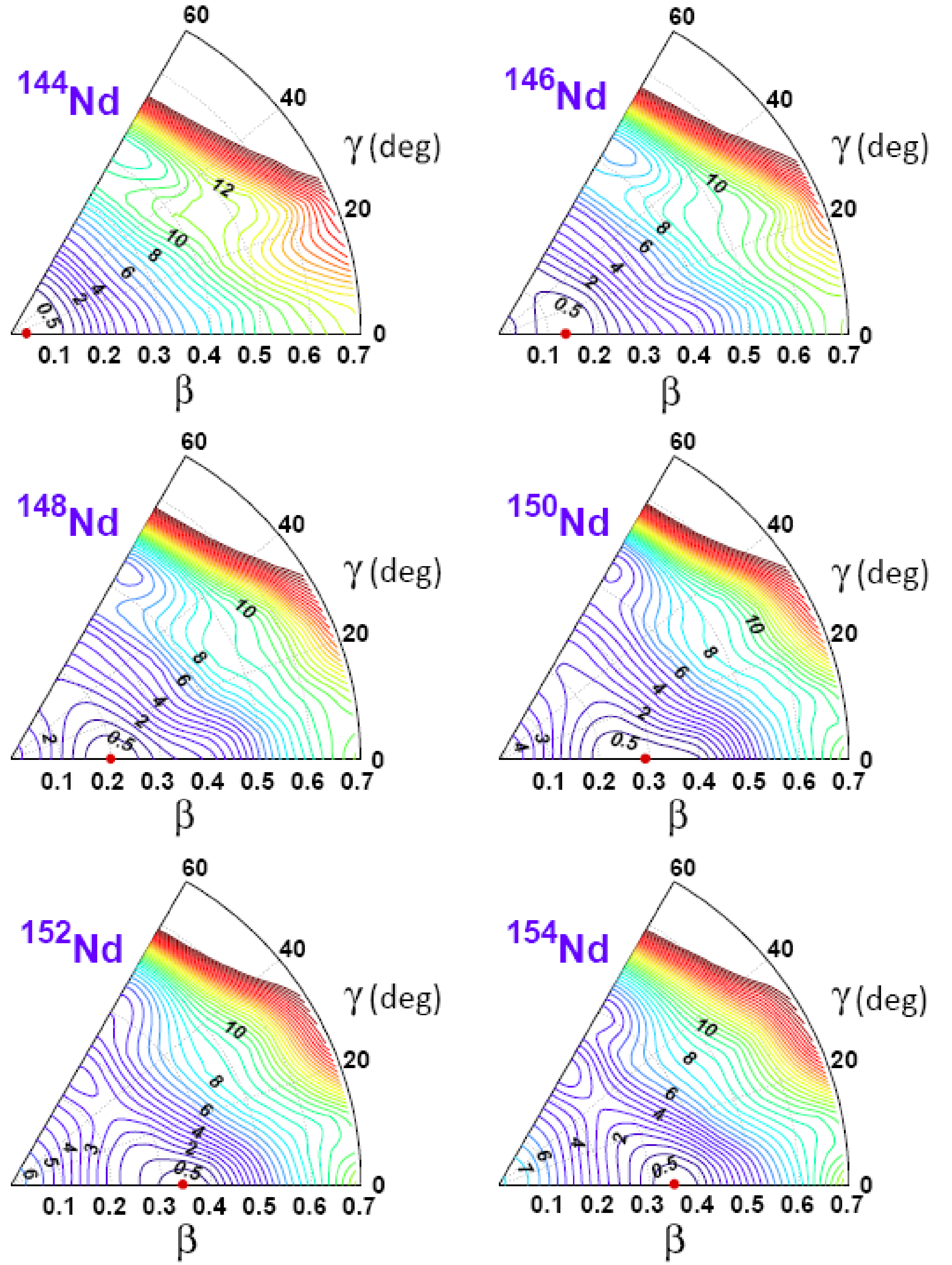




Potential energy surfaces:

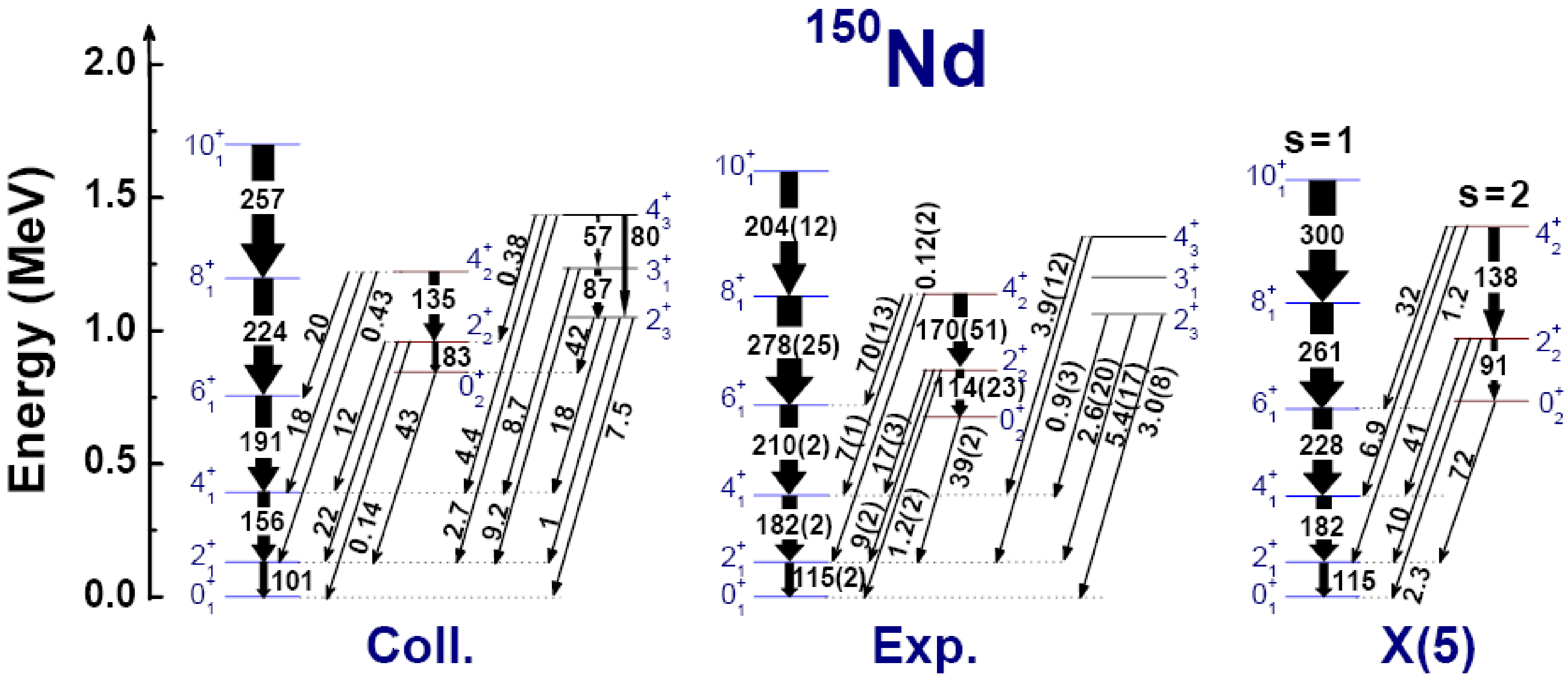






Microscopic analysis of nuclear QPT:

- **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

Content:

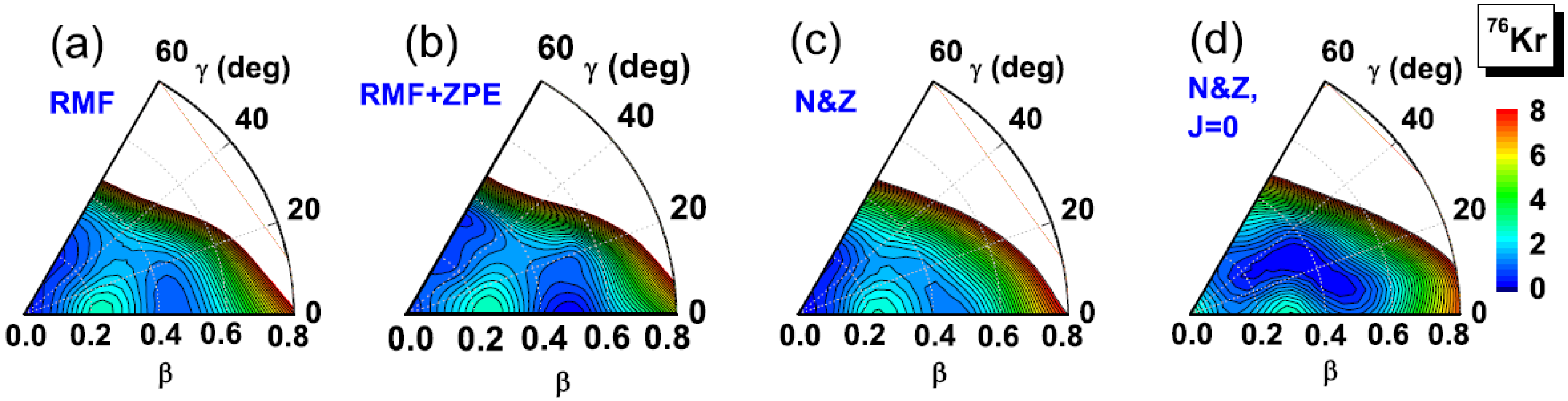
- Generator-Coordinate Method (GCM)
- Applications:

  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure N=28 isotones

  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- **Benchmark calculations (full GCM ↔ 5DCH): ^{76}Kr**
- Nuclear matrix elements for 0ν-ßß decay
- Outlook

Transitional nuclei: DFT beyond mean field:



Generator-Coordinates: q = (β,γ)
Projection on J and N: (5 angles)

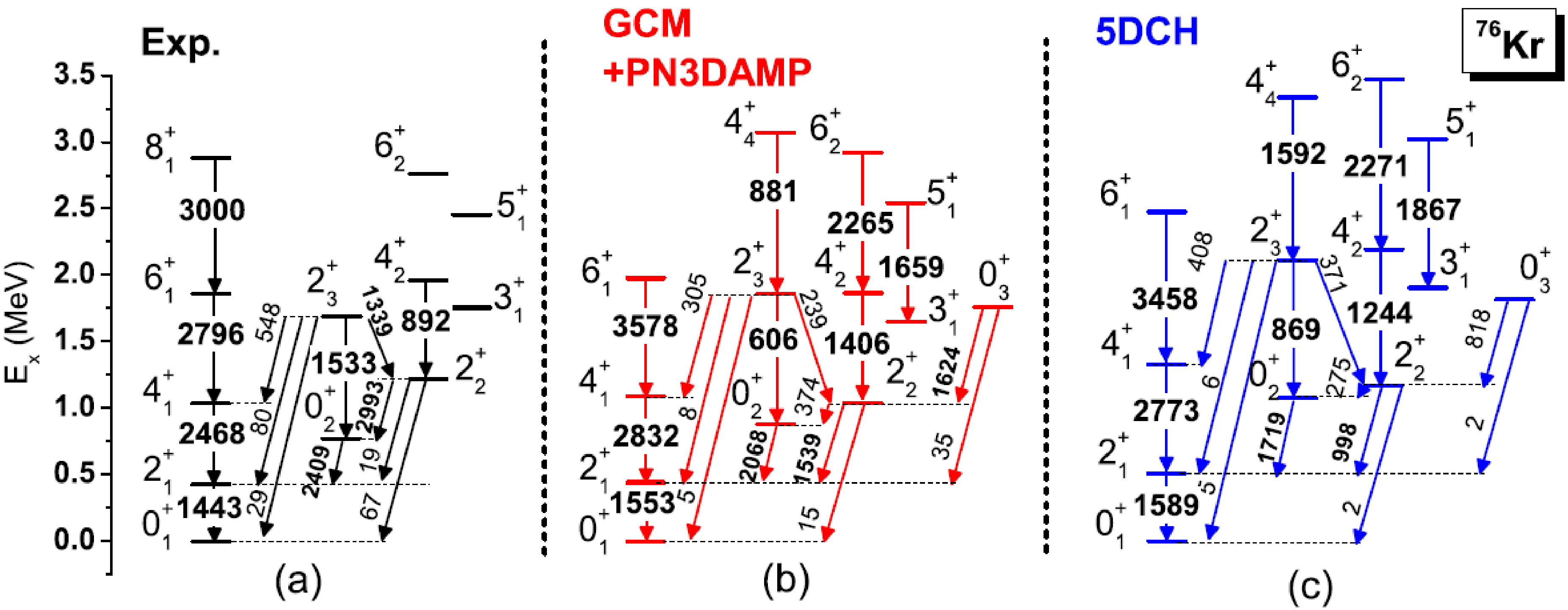
$$|J\,N\,Z;\alpha\rangle = \sum_{q,K} f_\alpha^{JK}(q)\,\hat{P}^J_{MK}\,\hat{P}^N\,\hat{P}^Z|q\rangle,$$

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

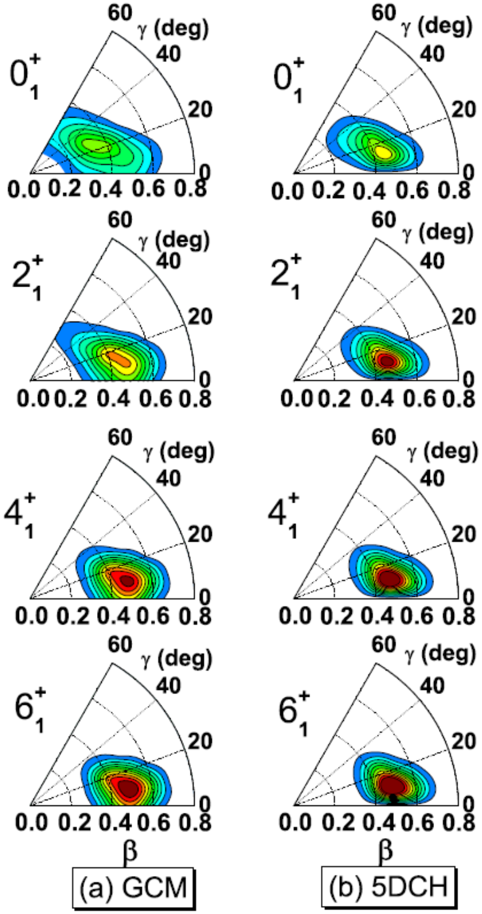
J.M. Yao, K. Hagino, Z.P. Li, P.R. , J. Meng PRC (2014)

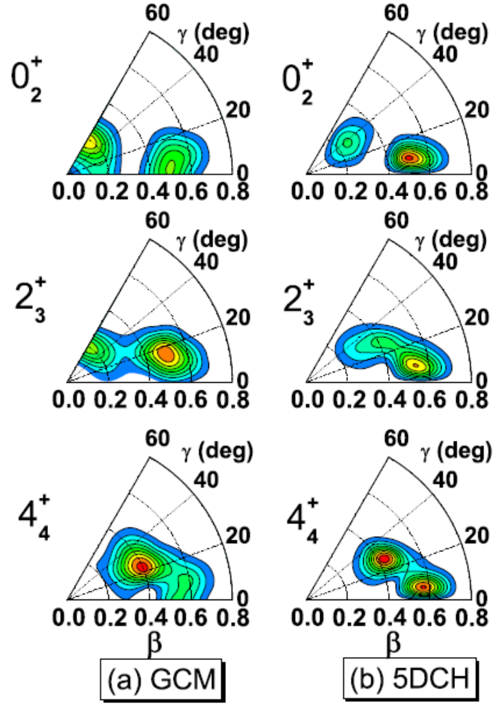
Spectra: GCM (7D)
Bohr Hamiltonian (5DCH)

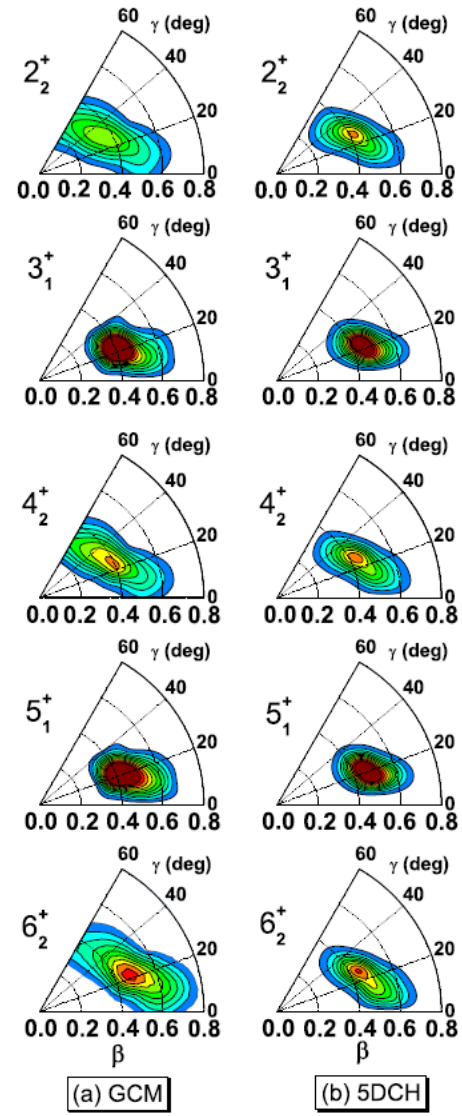
PC-PK1



J.M. Yao et al, PRC (2014)







quasi-β band

ground state band

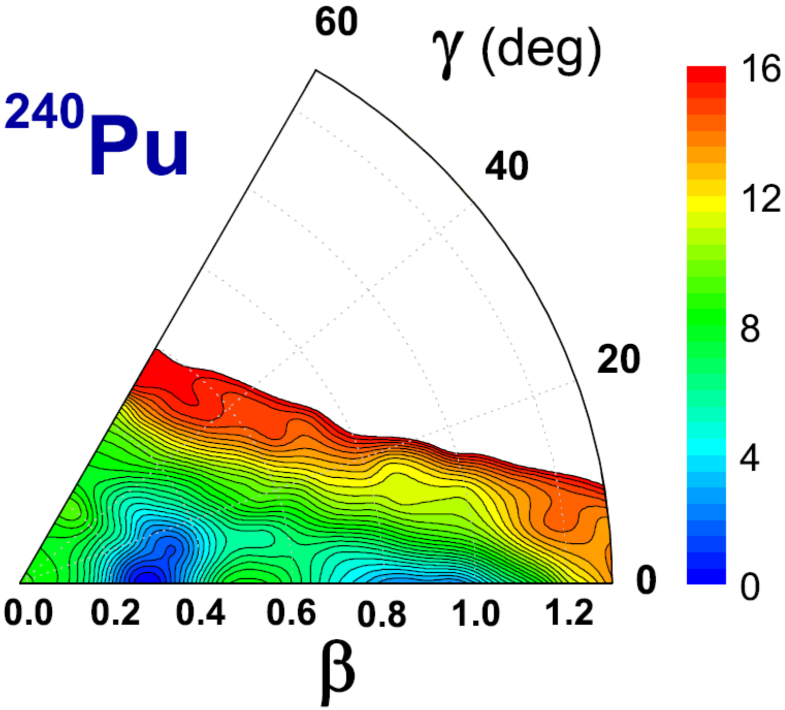
wave functions

quasi-γ band

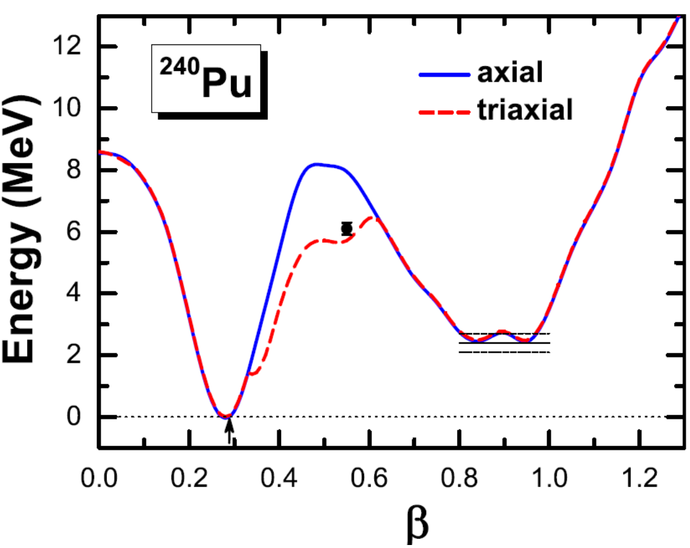
J.M. Yao et al, PRC (2014)

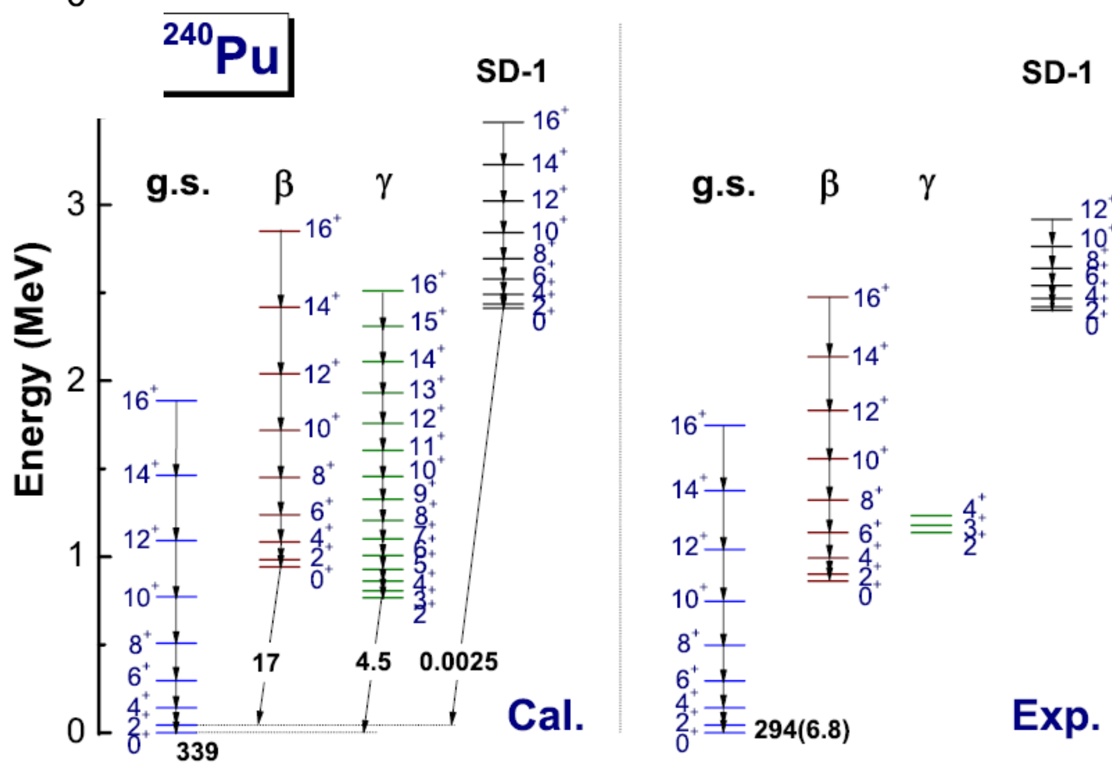
Fission barrier and super-deformed bands in ^{240}Pu

Zhipan Li et al, PRC (2010)



DD-PC1





Content:

- Generator-Coordinate Method (GCM)
- Applications:

  Quantum Phase Transitions in finite systems (QPT)

  Importance of single particle structure N=28 isotones

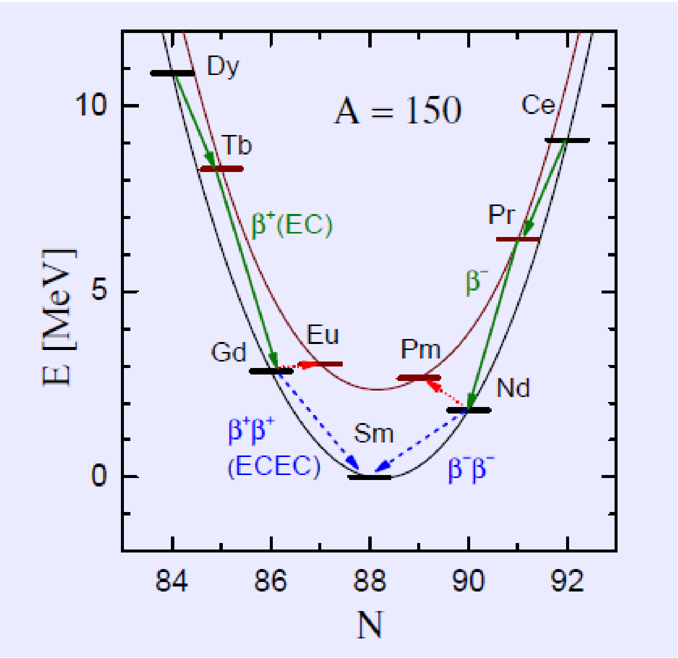
  α-clustering in light nuclei
- Derivation of a Collective Hamiltonian (5DCH)
- Benchmark calculations (full GCM ↔ 5DCH)
- **Nuclear matrix elements for 0ν-ßß decay**
- Outlook

Introduction

In ββ-decay the nucleus (A,Z) decays:

(A , Z) → (A , Z ± 2) + 2e$^{\mp}$ + light particles

emitting 2 electrons (positrons) and, usually, additional light particles.



It can be observed in some even–even nuclei, where single beta-decay is energetically forbidden, as for instance in the nucleus ^{150}Nd.

for β$^-$β$^-$ we have:

2v-ββ: (A,Z) → (A,Z+2) + 2e$^-$ + 2v

0v-ββ: (A,Z) → (A,Z+2) + 2e$^-$

others exotic modes

Neutrino-less double beta-decay is not observed yet in experiment

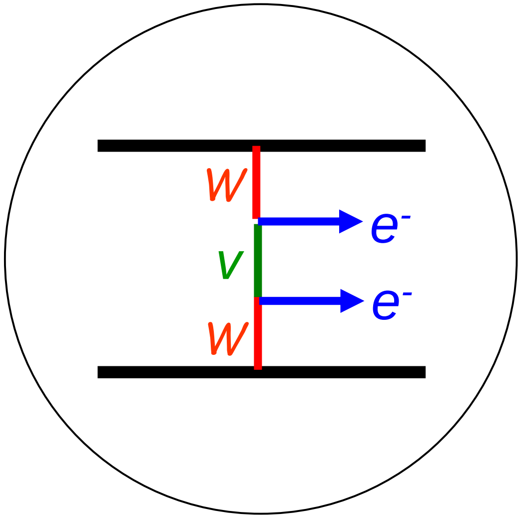
Lepton number is violated.

Its observation would prove that the neutrino is a Majorana particle

Half live of 0νββ decay

Assuming the light neutrino decay mechanism, we find the decay rate:

$$\left[T^{0\nu}_{1/2}\right]^{-1} = G_{0\nu}\, g_A^4 \frac{\langle m_\nu \rangle^2}{m_e^2} |M^{0\nu}|^2$$



g_A : axial vector coupling constant

m_e : electron mass

$G_{0\nu}$: kinematic phase space factor

$\langle m_\nu \rangle$: effective neutrino mass: $\langle m_\nu \rangle = \sum_k U_{ek}^2 m_k \xi_k$

$M^{0\nu}$: nuclear matrix element (NME)

Kotila 2012: PRC 85, 034016

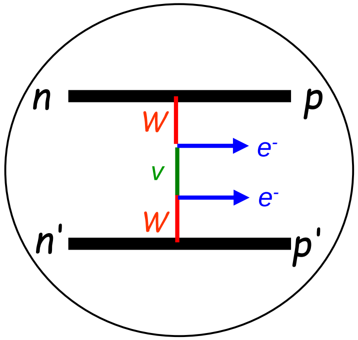
Bilenky 1987: RMP 59, 671

The observation of 0νββ-decay

would teach us the nature of the neutrino.

and the neutrino mass (provided that the NME is known)

Nuclear matrix element NME:



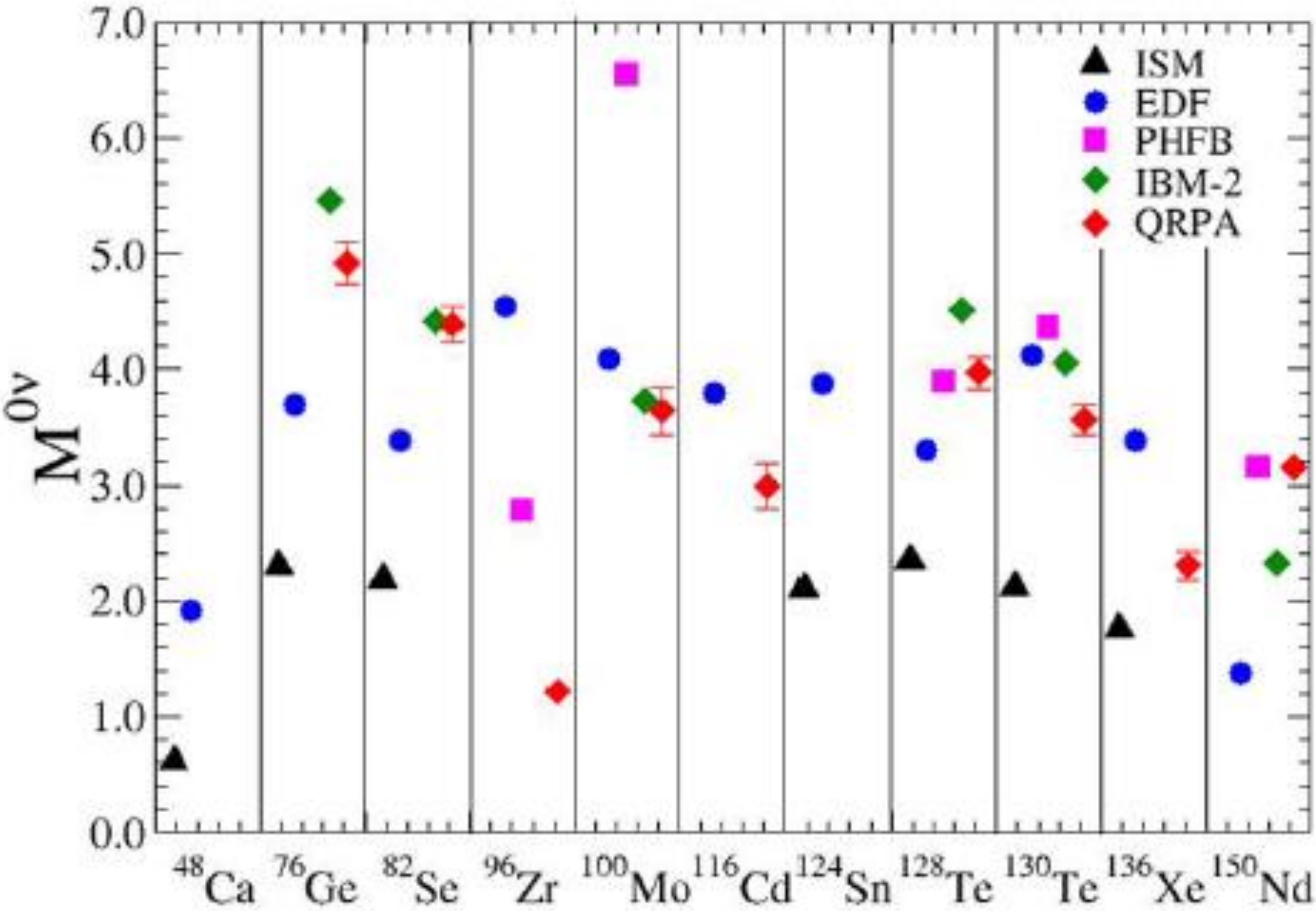
$$M^{0\nu} = \langle \Psi_F(Z+2) | \mathcal{O}^{0\nu} | \Psi_I(Z) \rangle$$

depends on the nuclear wave functions $|\Psi_I\rangle$ and $|\Psi_F\rangle$ and $\mathcal{O}^{0\nu}$ is an effective 2-body transition operator

Various non-relativistic models have been used in the literature:

- ✓ Quasiparticle random phase approximation (QRPA)
  Simkovic 1999, PRC 60, 055502; Simkovic 2008, PRC 77, 045503; Fang 2011, PRC 83, 034320; Kortelainen 2007, PRC 75, 051303(R); Mustonen 2013, PRC 87, 064302; ...
- ✓ Interacting shell model (ISM)
  Caurier 2008, PRL 100, 052503; Menéndez 2009, NPA 818, 139; Neacsu 2012, PRC 86, 067304; ...
- ✓ Interacting boson model (IBM)
  Barea 2009, PRC 79, 044301; Barea 2013, PRC 87, 014315
- ✓ Projected Hartree-Fock-Bogoliubov (PHFB)
  Rath 2010, PRC 82, 064310; Rath 2013, PRC 88, 064322; ...
- ✓ Energy density functional theory (EDF)
  Rodrígez 2010, PRL 105, 252503; Rodrígez 2011, PPNP 66, 436; Rodrígez 2013, PLB 719, 174; Vaquero 2013, PRL 111, 142501; ...

Present status for the Nuclear matrix element NME:



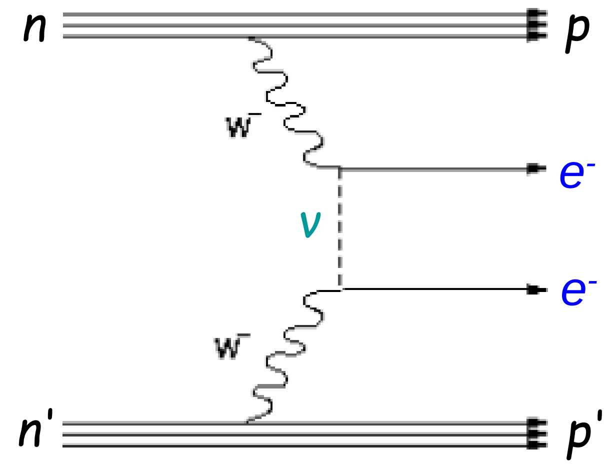
Present work:

- We use:

  Beyond mean field covariant density functional theory

- It is based on a unified density functional
  - no parameters,
  - full space
- Correlations are taken into account
  - by deformed and superfluid intrinsic wave functions,
  - by superposition of deformed wave functions (GCM),
  - by projection and the restoration of the broken symmetries
- Systematic investigations over a large number of nuclei
- We study:
  - Influence of relativistic effects
  - Influence of deformations
  - Influence of pairing correlations

0νßß - matrix elements:



weak interaction:

$$\mathcal{H}_{\text{weak}}(x) = \frac{G_F \cos\theta_C}{\sqrt{2}} j^\mu(x) J_\mu^\dagger(x) + h.c.$$

leptonic current (V-A):

$$j^\mu(x) = \bar{e}(x)\gamma^\mu(1-\gamma_5)\nu_e(x)$$

hadronic current:

$$J_\mu^\dagger(x) = \bar{\psi}_p(x)\left[g_V(q^2)\gamma_\mu - i g_M(q^2)\frac{\sigma_{\mu\nu}}{2m_p}q^\nu - g_A(q^2)\gamma_\mu\gamma_5 + g_P(q^2)\gamma_5 q_\mu\right]\tau_-\psi_n(x)$$

Second order perturbation theory and integration over leptonic sector:

$$\mathcal{O}^{0\nu} = \frac{4\pi R}{g_A^2}\int \frac{d^3q}{(2\pi)^2}\frac{e^{i\mathbf{q}(\mathbf{x}_1-\mathbf{x}_2)}}{q}\sum_m \frac{J_\mu^\dagger(\mathbf{x}_1)|m\rangle\langle m|J^{\mu\dagger}(\mathbf{x}_2)}{q+E_m-E_0-Q_{\beta\beta}/2}$$

$E_m - E_0 - Q_{\beta\beta}/2 \rightarrow E_d$ and closure approximation: $\sum_m |m\rangle\langle m| \rightarrow 1$

Decay operator in Fermion space:

The operator is decomposed into five terms with different coupling properties:

$$\mathcal{O}^{0\nu} = \sum_i \mathcal{O}_i \quad (i = VV, AA, AP, PP, MM)$$

with

$$\mathcal{O}_i = \frac{4\pi R}{g_A^2} \int \frac{d^3q}{(2\pi)^2} \frac{e^{i\mathbf{q}(\mathbf{x}_1 - \mathbf{x}_2)}}{|\mathbf{q}|} \frac{[J_\mu^\dagger J^{\mu\dagger}]_i}{|\mathbf{q}| + E_d}$$

and

$$[J_\mu^\dagger J^{\mu\dagger}]_{VV} = g_V^2(q^2)(\bar{\psi}\gamma_\mu \tau_- \psi)^{(1)}(\bar{\psi}\gamma^\mu \tau_- \psi)^{(2)}$$

$$[J_\mu^\dagger J^{\mu\dagger}]_{AA} = g_A^2(q^2)(\bar{\psi}\gamma_\mu \gamma_5 \tau_- \psi)^{(1)}(\bar{\psi}\gamma^\mu \gamma_5 \tau_- \psi)^{(2)}$$

$$[J_\mu^\dagger J^{\mu\dagger}]_{AP} = g_A(q^2) g_P(q^2)(\bar{\psi}\gamma_\mu \gamma_5 \tau_- \psi)^{(1)}(\bar{\psi} q^\mu \gamma_5 \tau_- \psi)^{(2)}$$

$$[J_\mu^\dagger J^{\mu\dagger}]_{PP} = -g_P^2(q^2)(\bar{\psi}\gamma_5 \tau_- \psi)^{(1)}(\bar{\psi}\gamma_5 \tau_- \psi)^{(2)}$$

$$[J_\mu^\dagger J^{\mu\dagger}]_{MM} = g_M^2(q^2)(\bar{\psi}\frac{\sigma_{\mu\nu} q^\nu}{2m_p} \tau_- \psi)^{(1)}(\bar{\psi}\frac{\sigma^{\mu\rho} q_\rho}{2m_p} \tau_- \psi)^{(2)}$$

Basic assumptions:

- Closure approximation
- Higher order currents are fully incorporated
- The tensorial part is included automatically
- Finite nuclear size corrections are taken into accout by form factors $g(q^2)$ (from Simkovic et al, PRC 2008)
- Short range correlations are neglected
- $g_A(0) = 1.254$ (no renormalization)

Nuclear wave functions:

- Intrinsic state:
  self-consistent constained RMF+BCS calculations: $|\beta\rangle = |\Phi(\beta)\rangle$

- Projected state: $|JZN,\beta\rangle = \hat{P}^J \hat{P}^Z \hat{P}^N |\beta\rangle$

- Generator coordinate method (GCM): shape mixing

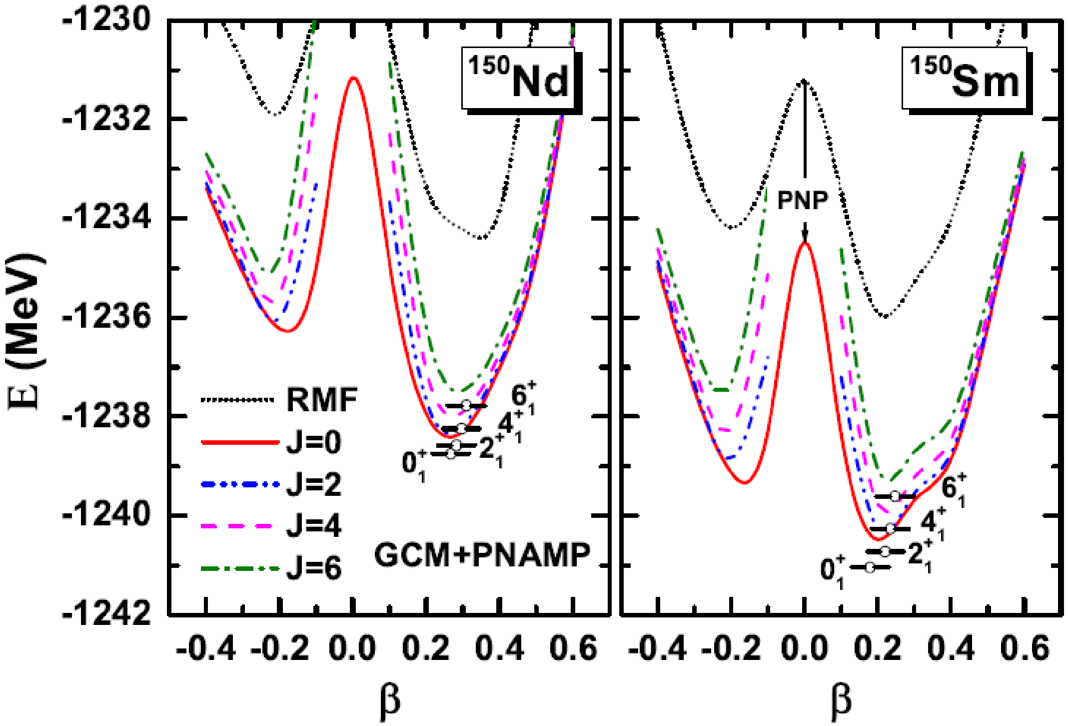
$$|\Psi^{JZN}\rangle = \int d\beta f(\beta)|JZN,\beta\rangle$$

- Transition matrix element:

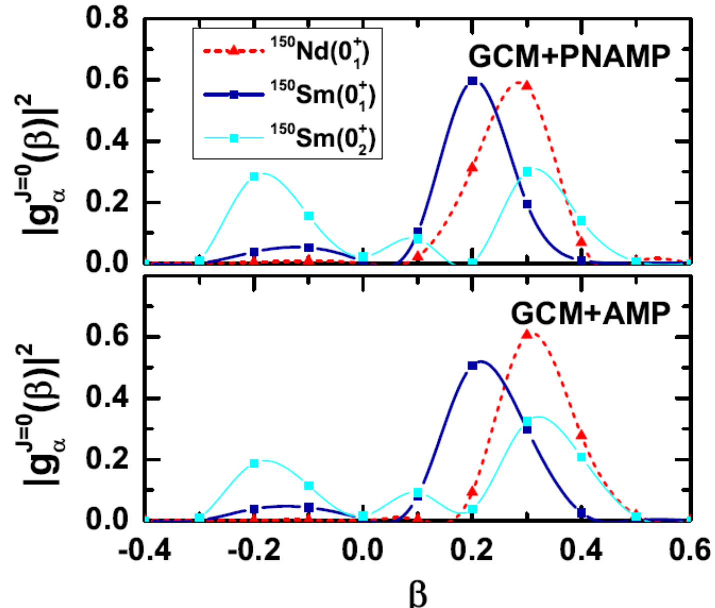
$$M^{0\nu} = \int\int d\beta_F d\beta_I\, f^*(\beta_F) f(\beta_I)\, M^{0\nu}(\beta_F,\beta_I)$$

$$M^{0\nu}(\beta_F,\beta_I) = \sum_{pp'nn'} \langle pp'|\mathcal{O}|nn'\rangle\langle\beta_F|c_p^\dagger c_p^\dagger c_n c_n|IZN,\beta_I\rangle$$

Results for the transition ^{150}Nd $\rightarrow$ ^{150}Sm:

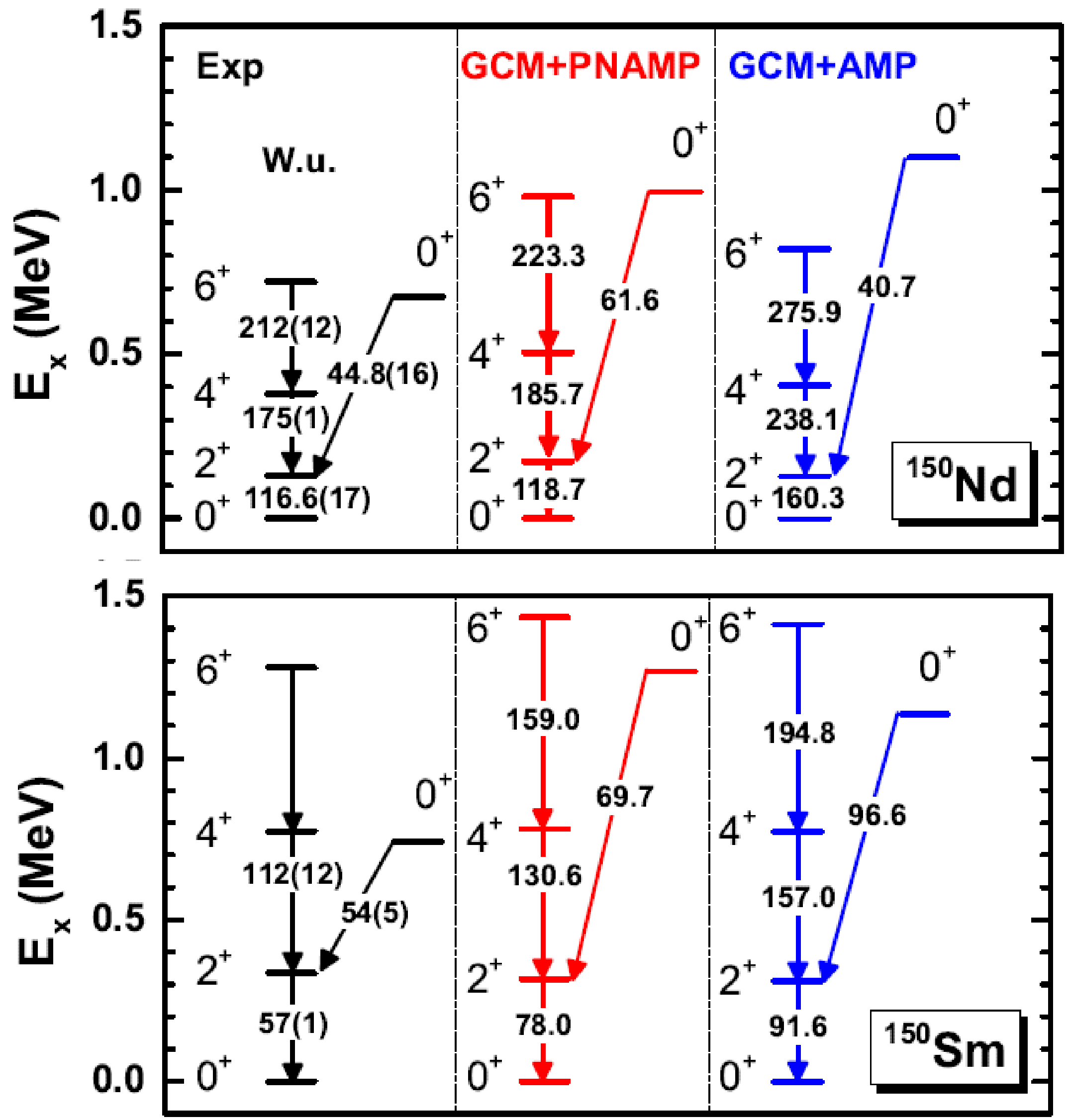


Energy surfaces

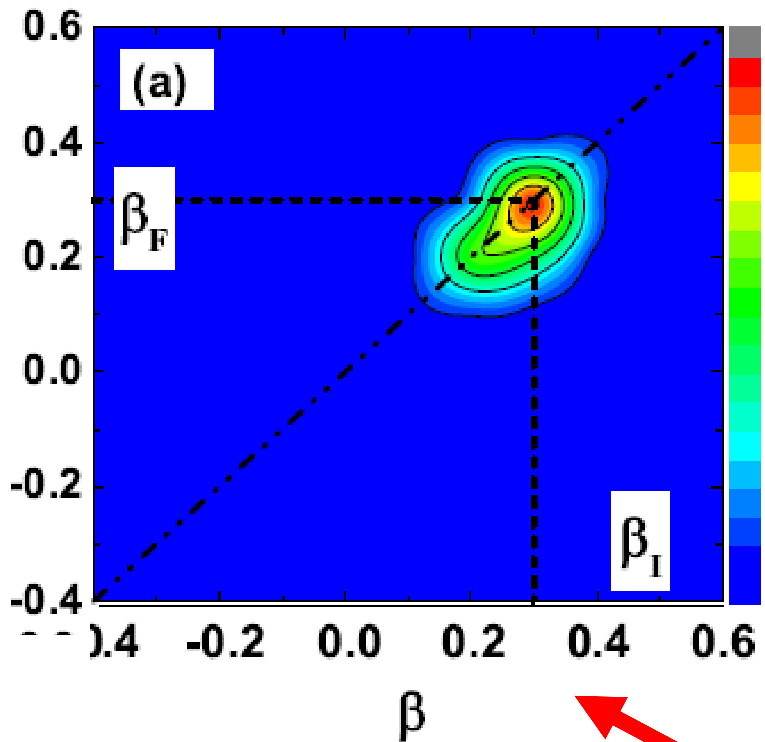


probabilities for deformation:

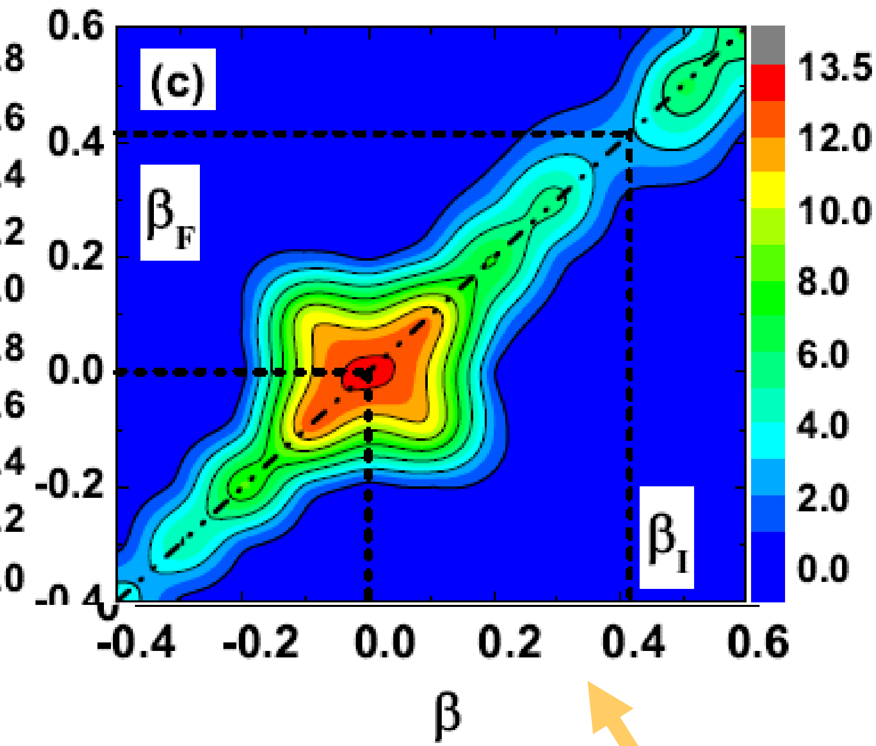
Low-lying spectra in ^{150}Nd and ^{150}Sm:



Contributions to NME



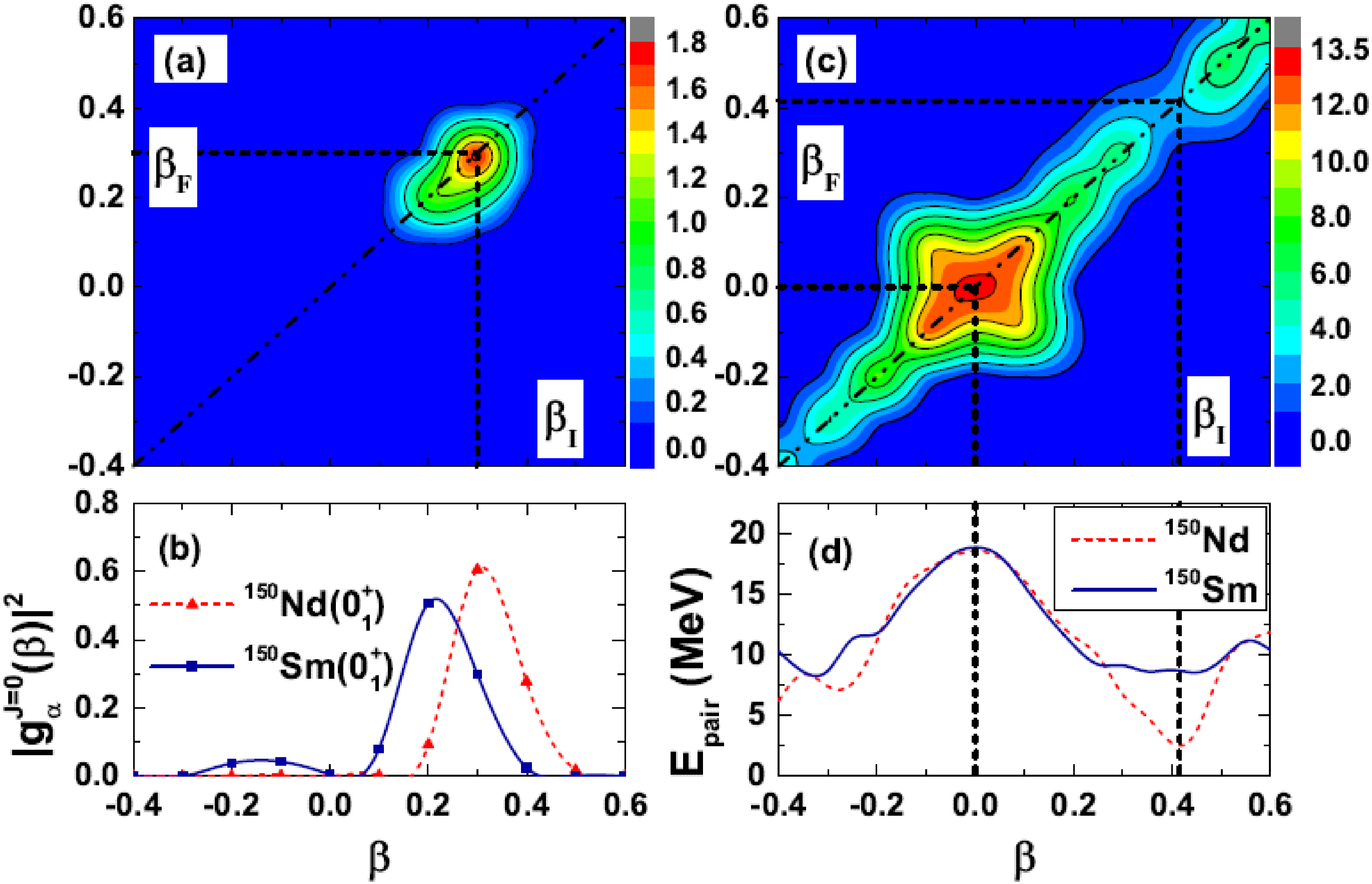
NME at fixed deformations



$$M^{0\nu} = \int\int d\beta_F d\beta_I \, f^*(\beta_F) f(\beta_I) \, \boxed{M^{0\nu}(\beta_F, \beta_I)}$$

Contributions to NME

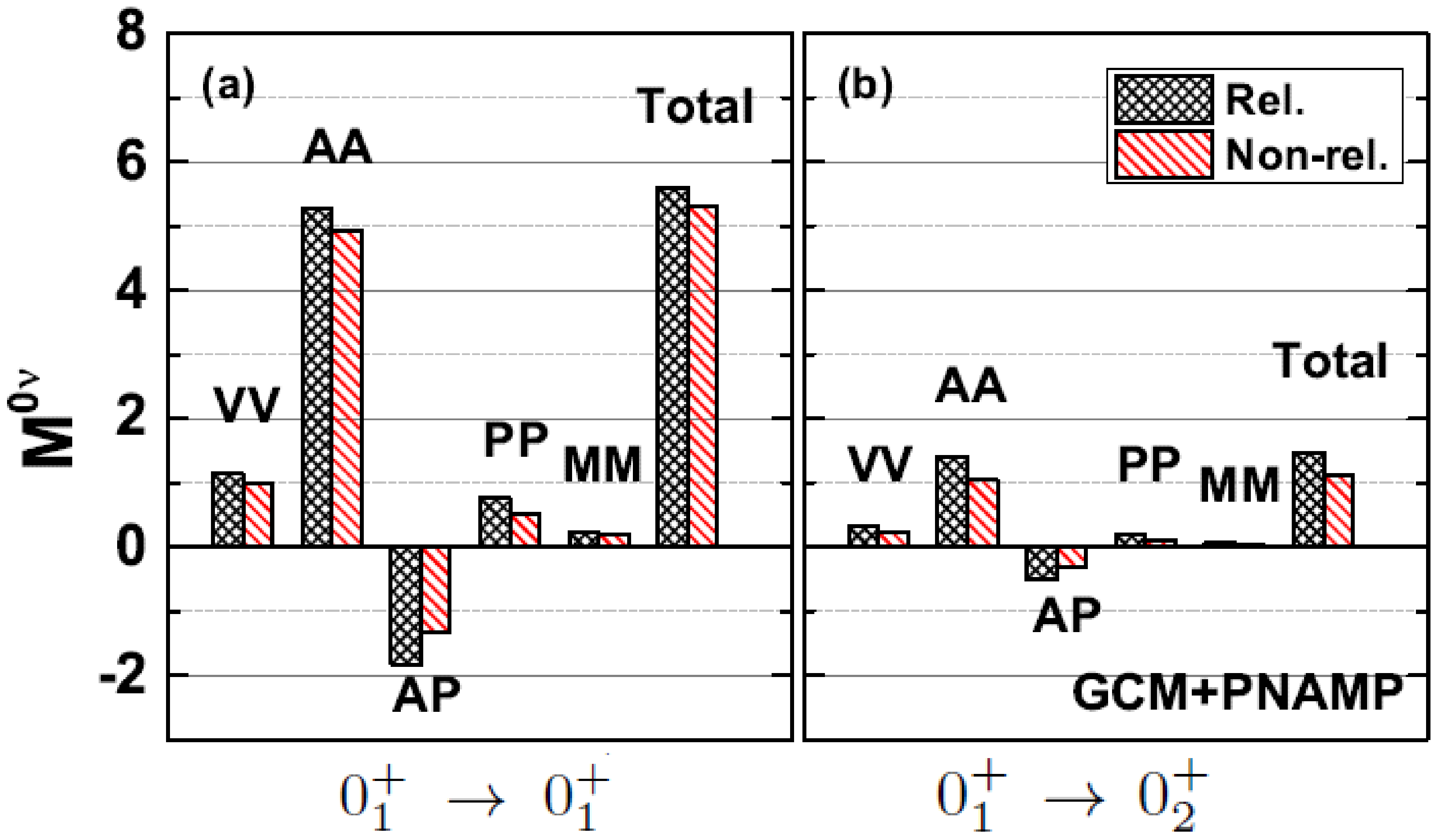
NME at fixed deformations



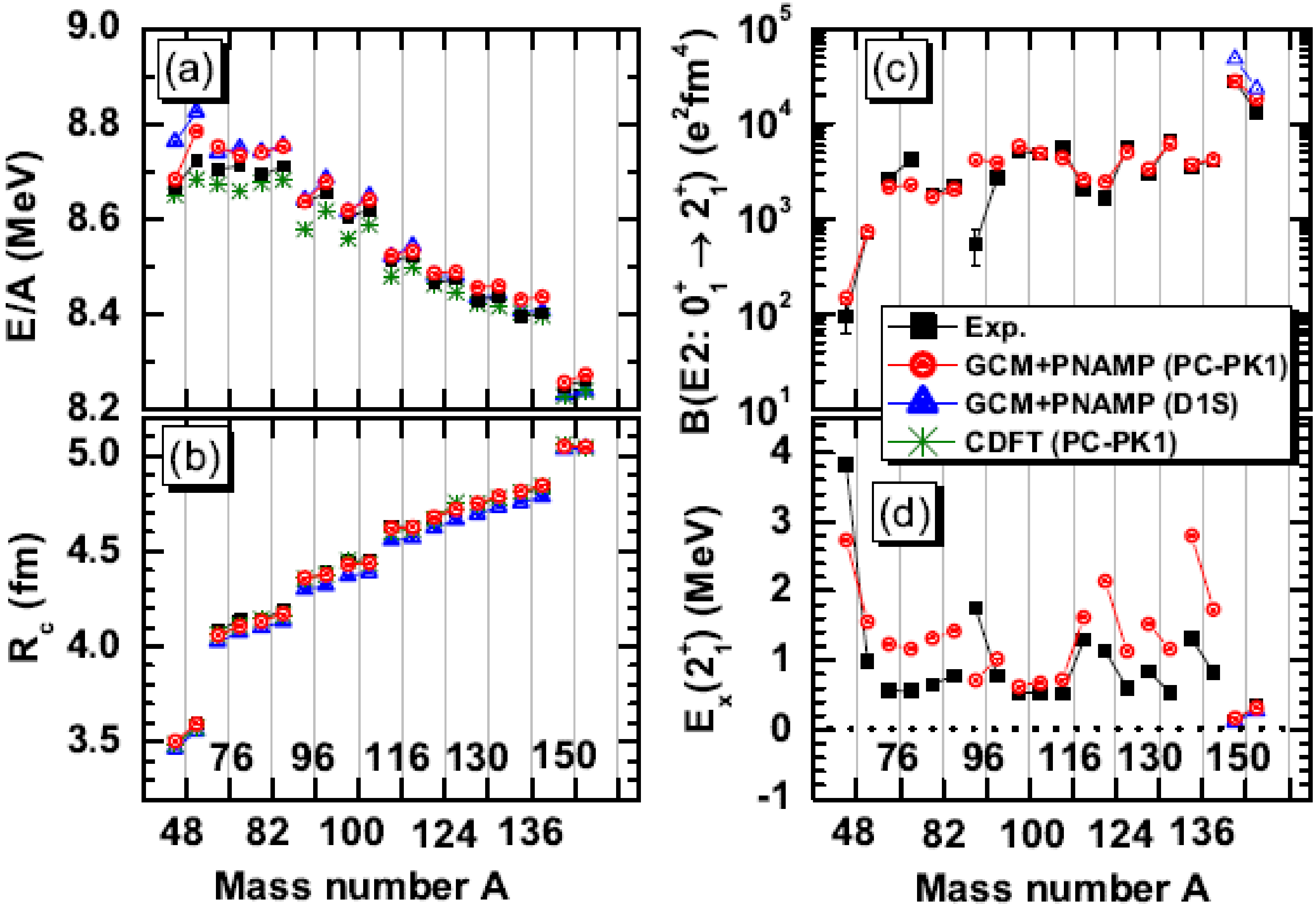
probability distributions

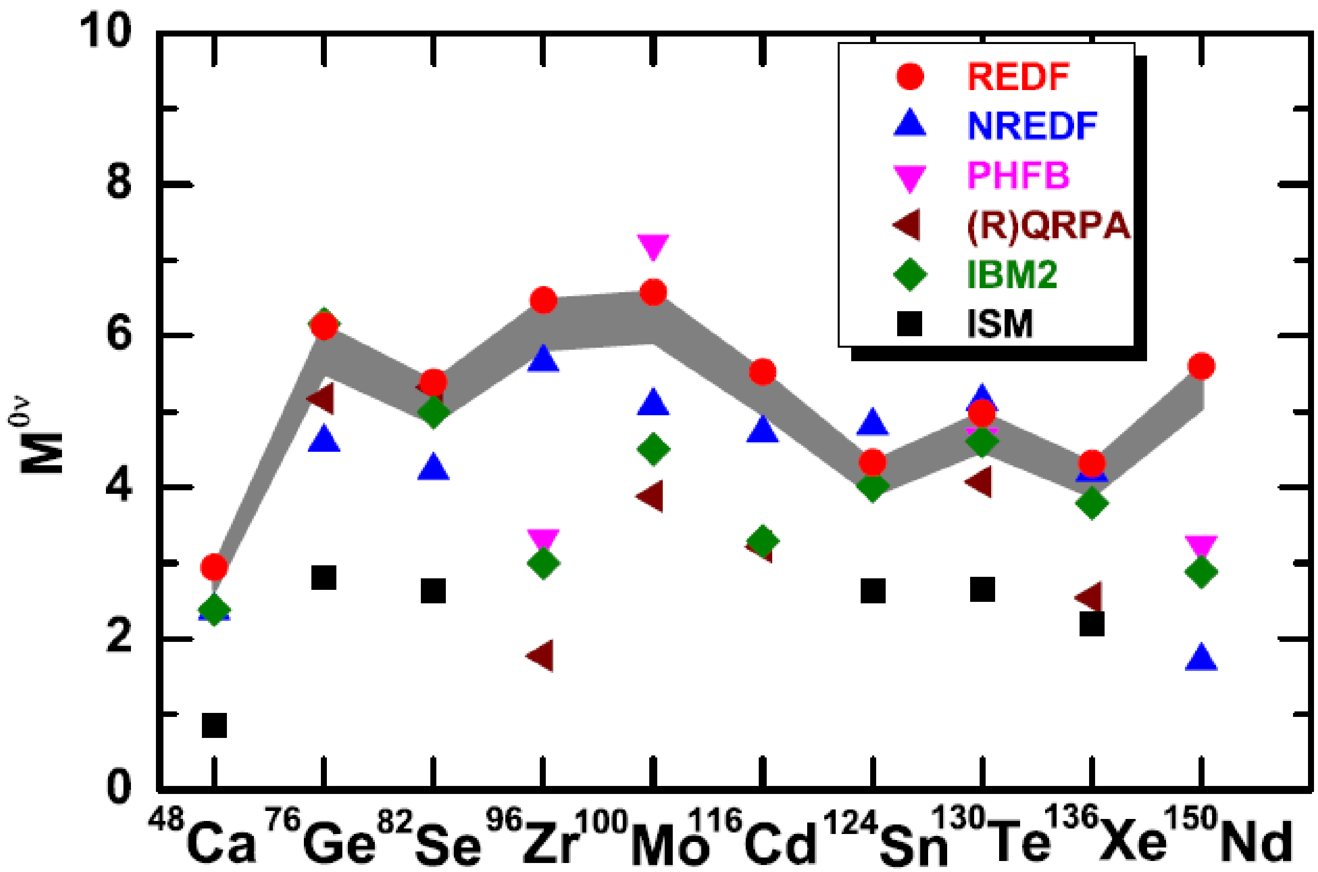
pairing energies

Transition ^{150}Nd $\rightarrow$ ^{150}Sm:
Matrix element of 0νββ decay and its contributions:



Systematic investigations: ground state properties





- The matrix elements differ by a factor 2 to 3
- Density functionals are at the upper end
- Not much sensitivity to the EDF (except for ^{150}Nd)
- Relativistic effects and tensor terms are with 10 %

J.M. Yao, L.S. Song, K.Hagino, P.R., J.Meng, PRC 91, 24316 (2015)

Upper limits for neutrino masses:

$$\left[T_{1/2}^{0\nu}\right]^{-1} = G_{0\nu}\, g_A^4 \frac{\langle m_\nu \rangle^2}{m_e^2} |M^{0\nu}|^2$$

Upper limits of the effective neutrino mass $\langle m_\nu \rangle$ (eV) based on:

a) the nuclear matrix elements $M^{0\nu}$ from this work

b) the lower limits of the half lives $T_{1/2}^{0\nu}(\times 10^{24}$yr) for the $0\nu\beta\beta$-decay from recent measurements

c) the phase space factors $G_{0\nu}(\times 10^{-15}$yr$^{-1})$

	^{48}Ca	^{76}Ge	^{82}Se	^{100}Mo	^{130}Te	^{136}Xe	^{150}Nd
$\langle m_{\beta\beta} \rangle$	$\leqslant 2.92$	$\leqslant 0.20$	$\leqslant 1.00$	$\leqslant 0.38$	$\leqslant 0.33$	$\leqslant 0.11$	$\leqslant 1.72$
$T_{1/2}^{0\nu}$	$\geqslant 0.058$	$\geqslant 30$	$\geqslant 0.36$	$\geqslant 1.1$	$\geqslant 2.8$	$\geqslant 34$	$\geqslant 0.018$
$G_{0\nu}$	24.81	2.363	10.16	15.92	14.22	14.58	63.03

Conclusions

- Static DFT in nuclei has is limits:

  no energy dependence in self energy (level density, width of GR)
  no good quantum numbers (spectroscopic data)
  no fluctuations (shape coexistens, transitions)

- Generator-Coordinate Method
  succesful, but complicated ,
  problem with moment of inertia

- Derivation of a collective Hamiltian (from GCM, from ATDHF)
  benchmark calculations show excellent agreement

- Application for Quantum Phase Transitions (QPT)
  parameterfree, microscopic description
- Application to α-clustering in light nuclei
  dissolution of the $\alpha+^{16}O$ molecular structure with increasing spin

- Application for neutrinoless double-beta decay
  Influence of relativistic effects, pairing, deformation

General remarks to DFT beyond mean field:

- Present methods of DFT beyond MF are very successful
  but there exists no clear derivation (**Intelligent Cooking**)
  completely different concepts are mixed
- For small amplitudes: energy dependent self-energy in PVC
  mixes the DFT self-energy with perturbation theory
  - problems of **overcounting**
  - problems of **divergencies** (non-renormalizable)
- For large amplitudes: GCM is based on DFT-Slater-determinats
  mixes the concept of „local density“ with global wave functions picture
  - **extremely complicated:** derivation of a Bohr-Hamiltonian may help
  - **Egido-poles**: maybe technical
  - limitation to **very few collective coordinates** (intelligent guess)

Problems for the future:

- **Improved (more universal)** density functionals
- **Ab initio derivation** of the density functional
  may help to determine the relevant terms (e.g. tensor)
  and to reduce the number of free parameters essentially
  only fine-tuning with very few parameters has to be done
- **The Projected Shell model**
  will allow a general configuration-mixing for heavy nuclei
- Search for methods of a **consistent treatment** of DFT and beyond MF

Thanks to my collaborators:

Jiangming Yao	(Chongqing)
Zhipan Li	(Chongqing)
En-Fu Zhou	(Chongqing)
Língshuang Song	(Beijing)
Jie Meng	(Beijing)
K. Hagino	(Sendai)
T. Niksic	(Zagreb)
D. Vretenar	(Zagreb)
L. Prochniak	(Lublin)
E. Litvinova	(WMU)
V. Tselyaev	(St. Petersburg)

Prediction of the half lives ($\left[T_{1/2}^{0\nu}\right]^{-1} = G_{0\nu} g_A^4 \left|\frac{\langle m_\nu \rangle}{m_e}\right|^2 |M^{0\nu}|^2$)

Neutrino mass $\langle m_\nu \rangle = 50$ meV; Phase space factors $G_{0\nu}$ from Kotila 2012, Phys. Rev. C 85, 034316.

	Rel. full	only AMP	NR-Gogny
$M^{0\nu}(0_1^+ \to 0_1^+)$	5.60	4.68	1.71, 2.19
$T_{1/2}^{0\nu}(0_1^+ \to 0_1^+)$ $[10^{25}$ yr$]$	2.1	3.1	22.9, 14.0
$M^{0\nu}(0_1^+ \to 0_2^+)$	1.48	2.42	2.81,
$T_{1/2}^{0\nu}(0_1^+ \to 0_2^+)$ $[10^{25}$ yr$]$	70.7	26.4	19.6, –

Rodriguez et al

	QRPA	IBM-2	PHFB
$M^{0\nu}(0_1^+ \to 0_1^+)$	3.16, 2.71	2.321	2.83
$T_{1/2}^{0\nu}(0_1^+ \to 0_1^+)$ $[10^{25}$ yr$]$	6.7 , 9.1	12.4	8.4
$M^{0\nu}(0_1^+ \to 0_2^+)$	–	0.395	–
$T_{1/2}^{0\nu}(0_1^+ \to 0_2^+)$ $[10^{25}$ yr$]$	–	992.7	–

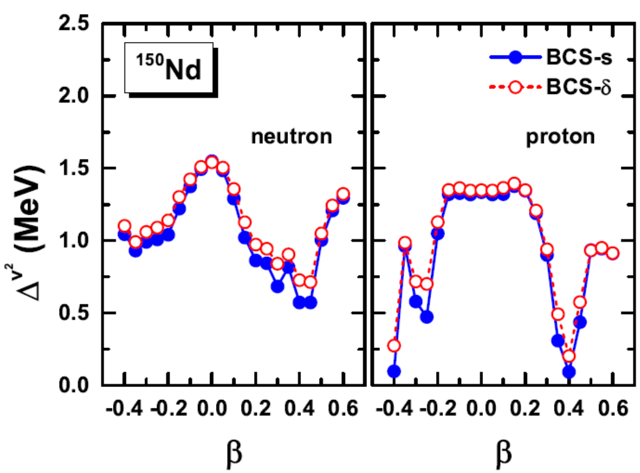
Tübingen, Engel | Iachello | Rath

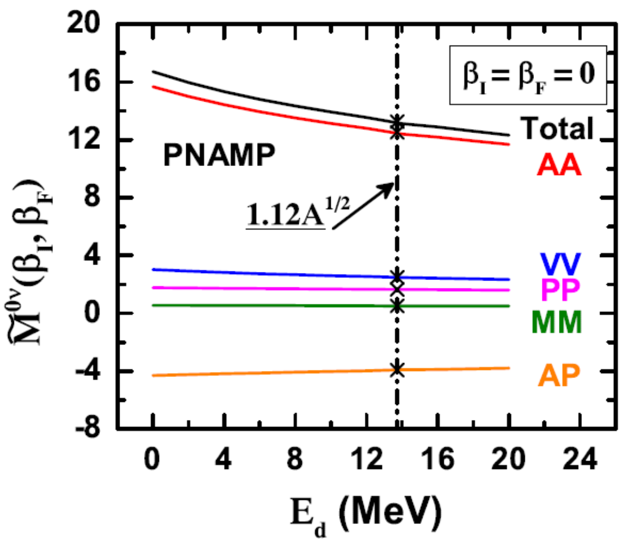
GT-part, relativistic effects, and tensor contributions:

Sph+PNP (PC-PK1)	$M^{0\nu}$	R_{AA}	$M^{0\nu}_{\mathrm{NR}}$	$\Delta_{\mathrm{Rel.}}$	R_T
$^{48}Ca \rightarrow {}^{48}Ti$	3.66	81%	3.74	−2.1%	−2.4%
$^{76}Ge \rightarrow {}^{76}Se$	7.59	94%	7.71	−1.6%	3.5%
$^{82}Se \rightarrow {}^{82}Kr$	7.58	93%	7.68	−1.4%	2.9%
$^{96}Zr \rightarrow {}^{96}Mo$	5.64	95%	5.63	0.2%	3.6%
$^{100}Mo \rightarrow {}^{100}Ru$	10.92	95%	10.91	0.1%	3.5%
$^{116}Cd \rightarrow {}^{116}Sn$	6.18	94%	6.13	0.7%	1.9%
$^{124}Sn \rightarrow {}^{124}Te$	6.66	94%	6.78	−1.8%	4.9%
$^{130}Te \rightarrow {}^{130}Xe$	9.50	94%	9.64	−1.4%	4.3%
$^{136}Xe \rightarrow {}^{136}Ba$	6.59	94%	6.70	−1.7%	4.1%
$^{150}Nd \rightarrow {}^{150}Sm$	13.25	95%	13.08	1.3%	2.5%

Numerical details:

- axially symmetric calculation: |q> = |β>
- interaction: density dependent point coupling PC-PK1
- pairing: zero range interaction (adjusted to Gogny):
- number of oscillator shells: $N = 12$
- number of meshpoints in Euler angle (1DAMP): n = 14
- mesh points in q-space: $-0.4 \leq \beta \leq 0.6$, $\Delta\beta = 0.05$
- energy denominator: $E_d = 1.12\ A^{1/2}$ (Haxton PPNP 1984)





Derivation of a collective Hamiltonian from GCM:

$$\int dq' \, \langle q|H|q'\rangle \, f(q') = E \int dq' \, \langle q|q'\rangle f(q'),$$

$$|q+s\rangle = e^{is\hat{P}}|q\rangle \quad \text{with} \quad \hat{P} = \frac{1}{i}\frac{\partial}{\partial q}$$

$$\langle q|q+s\rangle = \langle q|e^{is\hat{P}}|q\rangle \approx \prod_{i=1}^{A} \langle \varphi_i^*(q)\varphi_i(q+s)\rangle$$

Gaussian overlap approach:

$$\approx (1-\varepsilon s^2)^A \approx \boxed{\exp(-\gamma s^2)}$$

$$\gamma(q) = \langle q|\hat{P}^2|q\rangle \quad \text{grows with } A$$

$$\langle q|H|q'\rangle = h(q,q')\langle q|q'\rangle$$

$$\approx \left((h_0(q) - \frac{\partial}{\partial q} h_2(q) \frac{\partial}{\partial q} \right) \langle q|q'\rangle$$

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

$$\int dq' \; \left(h(q,q') - E\,\right) \langle q|q'\rangle f(q') = 0,$$

$$\left(-\frac{\partial}{\partial q} h_2(q) \frac{\partial}{\partial q} + h_0(q) - E\right) \int dq' \langle q|q'\rangle f(q') = 0$$

$$\boxed{\left(-\frac{\partial}{\partial q}\frac{1}{2B_{\mathrm{Y}}(q)}\frac{\partial}{\partial q} + V(q) - \varepsilon_0(q) - E\right) g(q) = 0}$$

$$V(q) = \left\langle q \left| \hat{H} \right| q \right\rangle \qquad B_{\mathrm{Y}}(q) \approx \frac{\left\langle q \left| \left[\hat{P}, \left[\hat{H}, \hat{P}\right]_+\right]_+ \right| q \right\rangle}{4\left\langle q \left| \hat{P}^2 \right| q \right\rangle}$$

Yoccoz-inertia:

Adiabatic TDHF:

Baranger+Veneroni (1978)

$$i\dot\rho(t) = [h(\rho(t)), \rho(t)]$$

time-odd

$$\rho(t) = e^{i\chi(t)}\rho_0(t)e^{-i\chi(t)}$$

time-even

fixed path in deformation space $= q(t)$ $\qquad \rho(q) = e^{i\chi}\rho_0(q)e^{-i\chi}$

$$|\Phi_0(q+s)\rangle = e^{is\hat P}|\Phi_0(q)\rangle \qquad |\Phi(q+s)\rangle = e^{-ip\hat Q}|\Phi_0(q+s)\rangle$$

$$\left\langle q \middle| [\hat P, \hat Q] \middle| q \right\rangle = \frac{1}{i}$$

$$\boxed{E = H(p,q) = p\frac{1}{B_{\mathsf{TV}}(q)}p + V(q)}$$

$$B_{\mathsf{TV}}^{-1}(q) = \left\langle q \middle| \left[\hat Q, \left[\hat H, \hat Q\right]\right] \middle| q \right\rangle \qquad B_{\mathsf{TV}}(q) = (P - P^*)\mathcal{M}\begin{pmatrix} P \\ -P^* \end{pmatrix}$$