Changes in the nuclear shapes in the N = 40, 60, 90 regions

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This work is dedicated to the memory of Adam Prášek

Outline

- Historical overview
- Experimental signatures of structural change
- Shell model interpretation
- Microscopic self-consistent calculations
- Algebraic Collective Model calculations

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Historical overview

- 1975-1979: A. Arima and F. Iachello introduce the Interacting Boson Model (IBM)
  F. Iachello and A. Arima, The Interacting Boson Model(Cambridge U. Press, 1987)
- 1977: Federman and Pittel mechanism
  P. Federman and S. Pittel, Phys. Lett. B 69, 385 (1977)
- 1980-1981: *Shape* phase transitions in the classical limit of the IBM
  A. E. L. Dieperink, O. Scholten and F. Iachello, Phys.Rev. Lett. 44, 1747 (1980)
  D. H. Feng, R. Gilmore and S. R. Deans, Phys. Rev. C 23, 1254 (1981)
- 2000-2001: E(5), X(5) critical point symmetries
  F. Iachello, Phys. Rev. Lett. 85, 3580 (2000)
  F. Iachello, Phys. Rev. Lett. 87, 052502 (2001)

Collective shape variables (β,γ)

$$R(\theta,\varphi) = R_0\left[1 + \sum_{\mu=-2}^{2} \alpha_\mu Y^*_{2,\mu}(\theta,\varphi)\right]$$

Transformation to principal axes

$$a_\nu = \sum_{\mu=-2}^{2} \alpha_\mu D^*_{\mu,\nu}(\theta_i) \Rightarrow \begin{cases} a_2 = a_{-2} \\ a_1 = a_{-1} = 0 \end{cases}$$

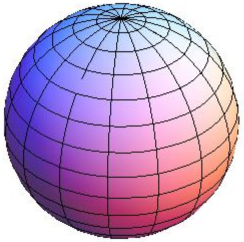
$$a_0 = \beta\cos\gamma$$

$$a_2 = \beta\sin\gamma\big/\sqrt{2}$$

β,γ Intrinsic (shape)

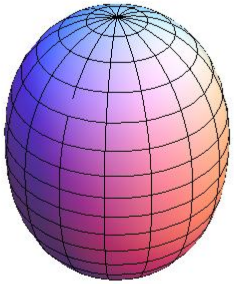
$\theta_i, (i = 1,2,3)$ orientation

Spherical



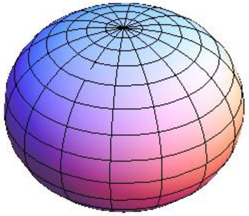
$\beta = 0$

Prolate



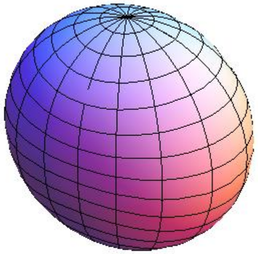
$\beta \neq 0, \gamma = 0^\circ$

Oblate



$\beta \neq 0, \gamma = 60^\circ$

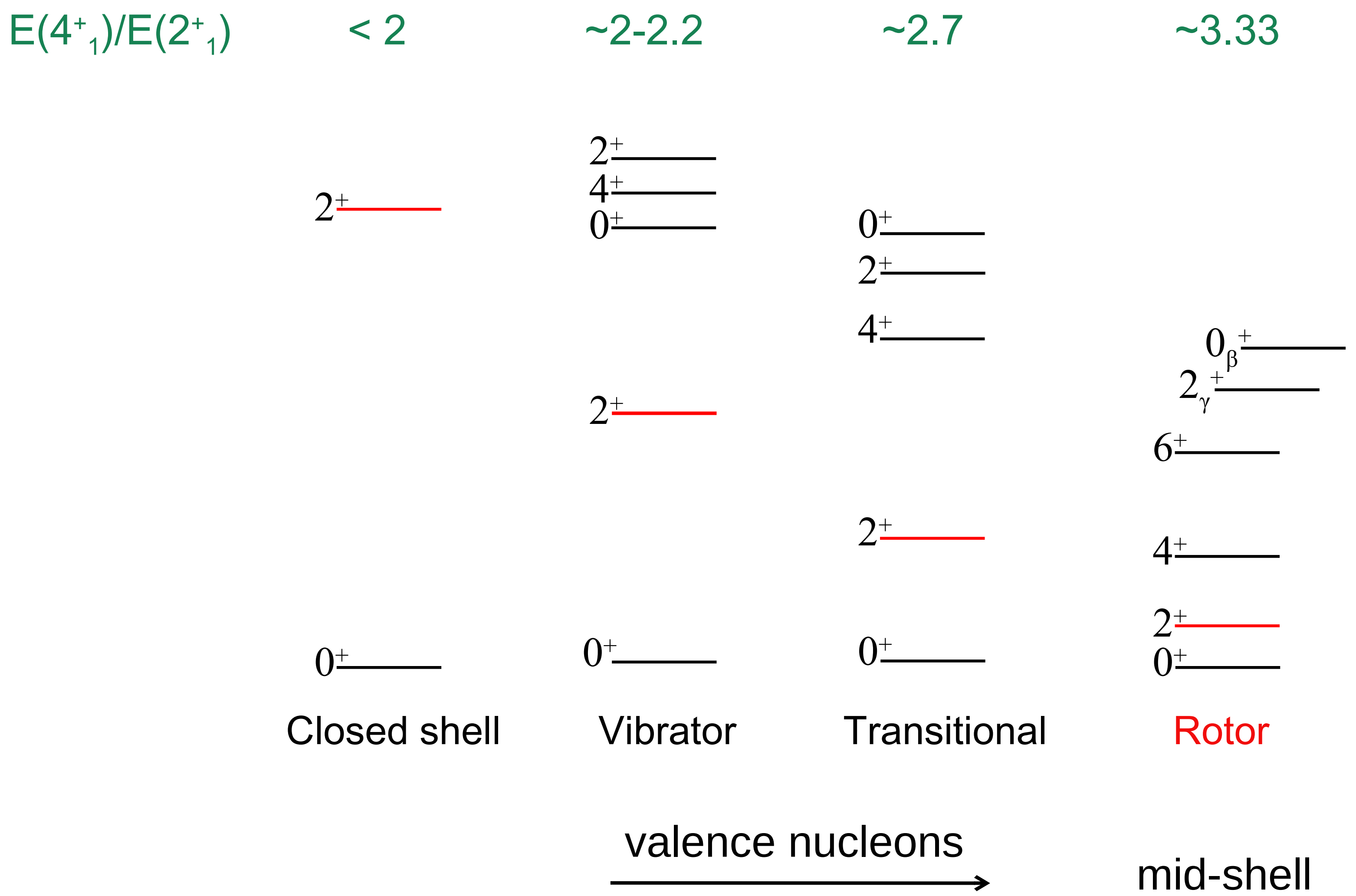
Triaxial



$\beta \neq 0, \gamma \neq 0^\circ, 60^\circ$

deformed

Schematic evolution of structure

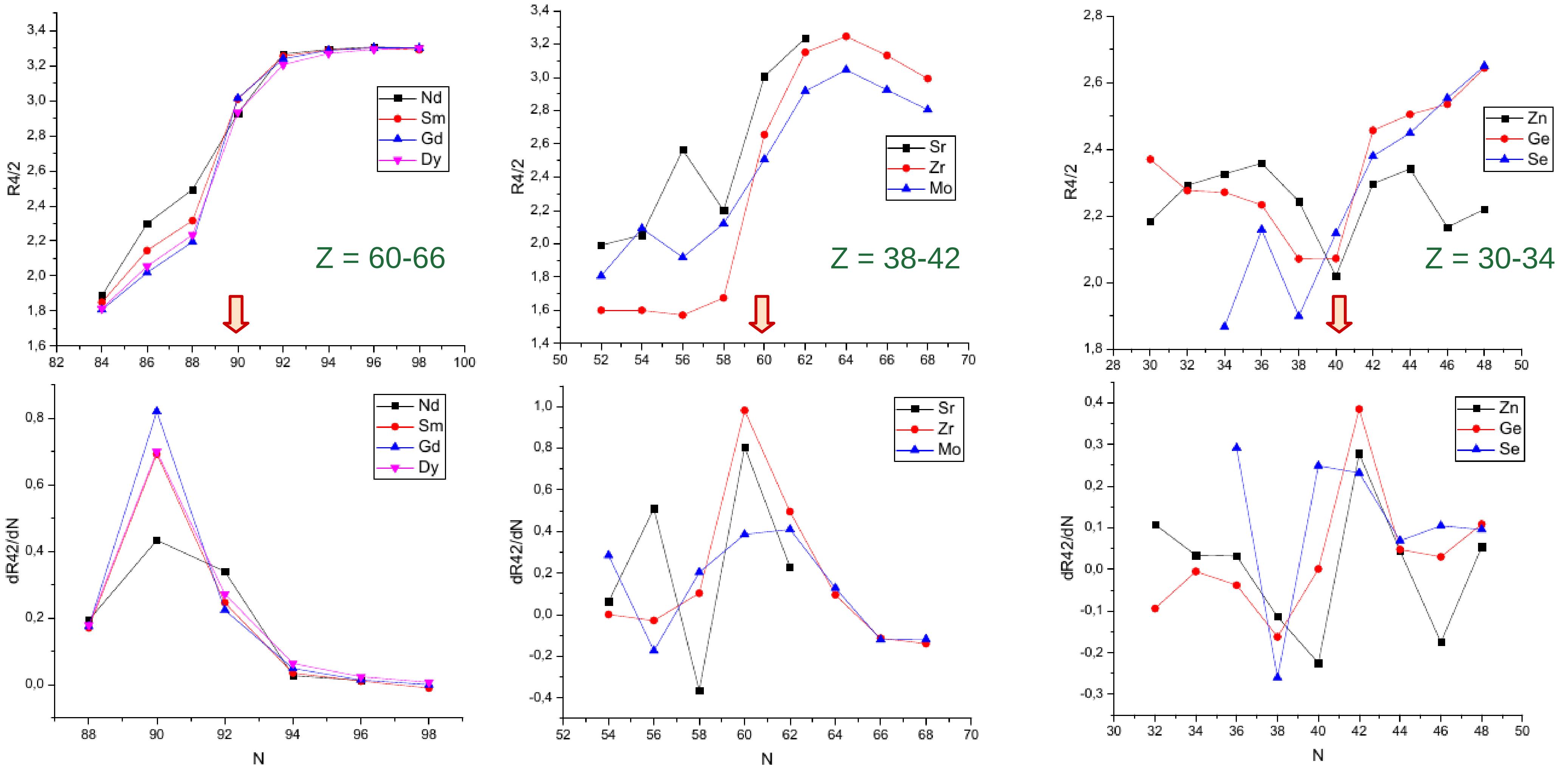


Adapted from:
R. F. Casten, Nuclear Structure from a Simple Perspective (2nd ed., Oxford University Press, Oxford, 2000)

Energy ratios $R_{4/2}(N)$

$$R_{4/2} = \frac{E(4_1^+)}{E(2_1^+)}$$

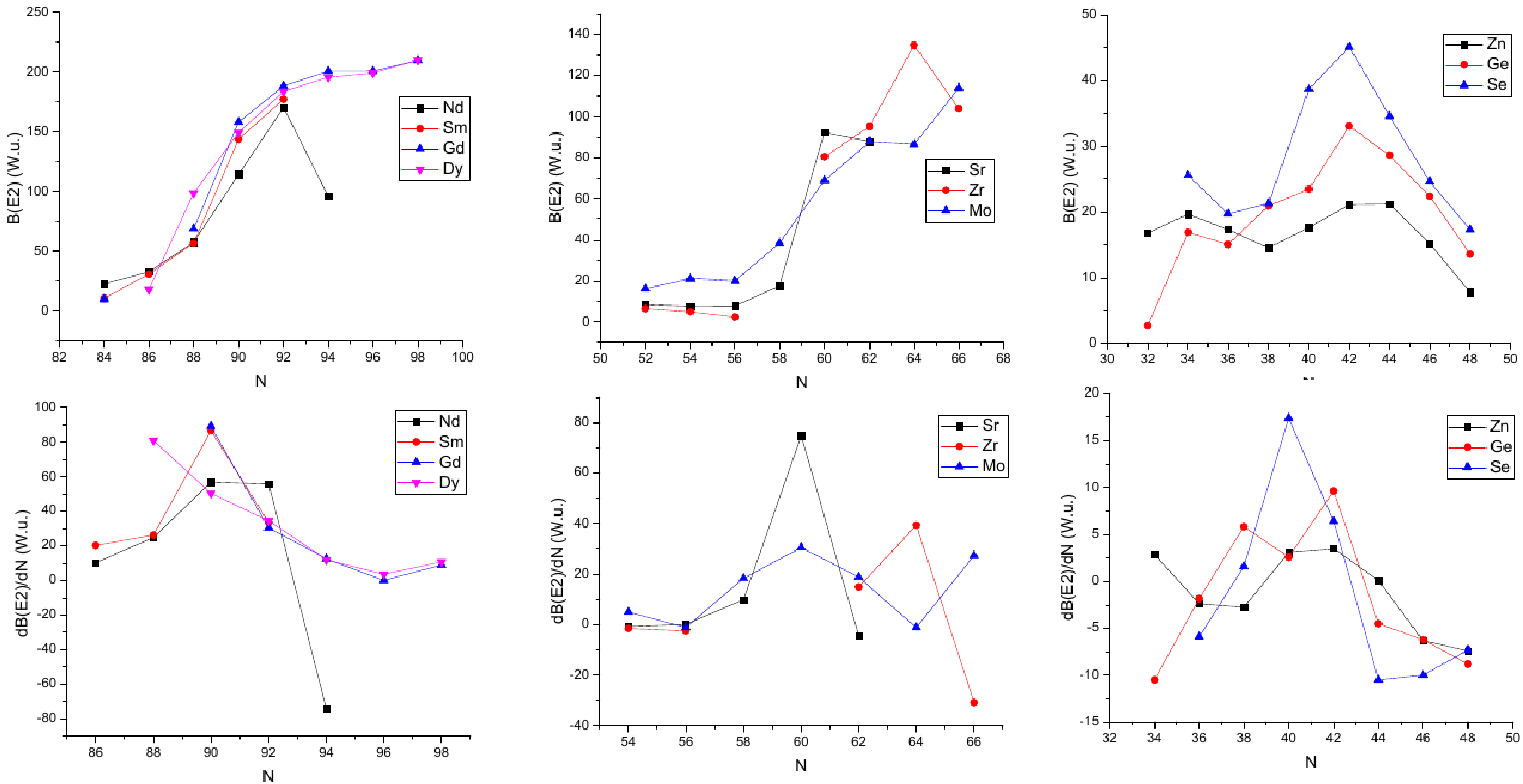
$$\frac{dR_{4/2}}{dN}(N) = R_{4/2}(N) - R_{4/2}(N-2)$$



B(E2) transition rates

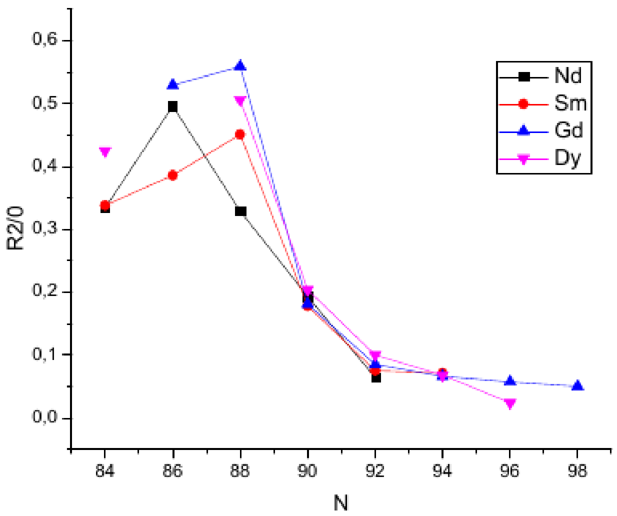
$$B(E2; 2_1^+ \rightarrow 0_1^+)$$

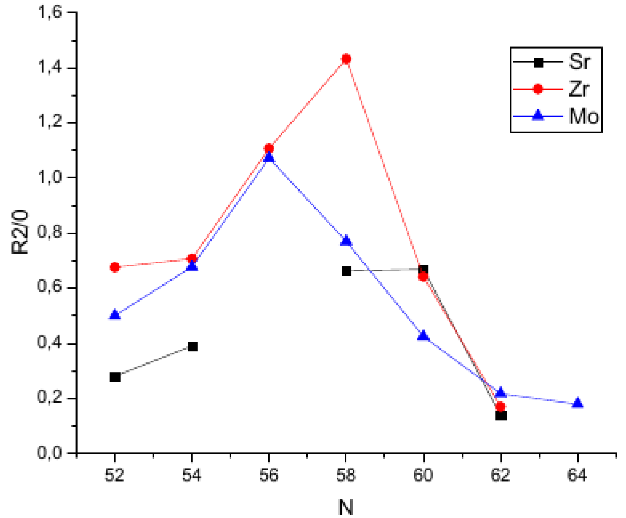
$$\frac{dB(E2; 2_1^+ \rightarrow 0_1^+)}{dN}(N) = B(E2; 2_1^+ \rightarrow 0_1^+)(N) - B(E2; 2_1^+ \rightarrow 0_1^+)(N-2)$$

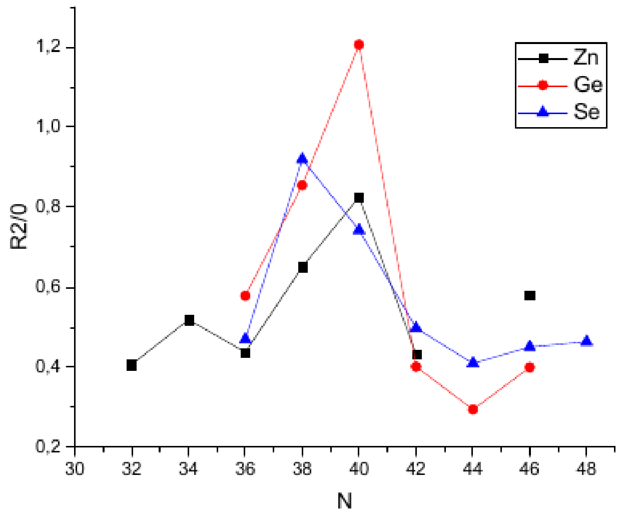


Energy ratios $R_{2/0}$

$$R_{2/0} = \frac{E(2_1^+)}{E(0_2^+)}$$



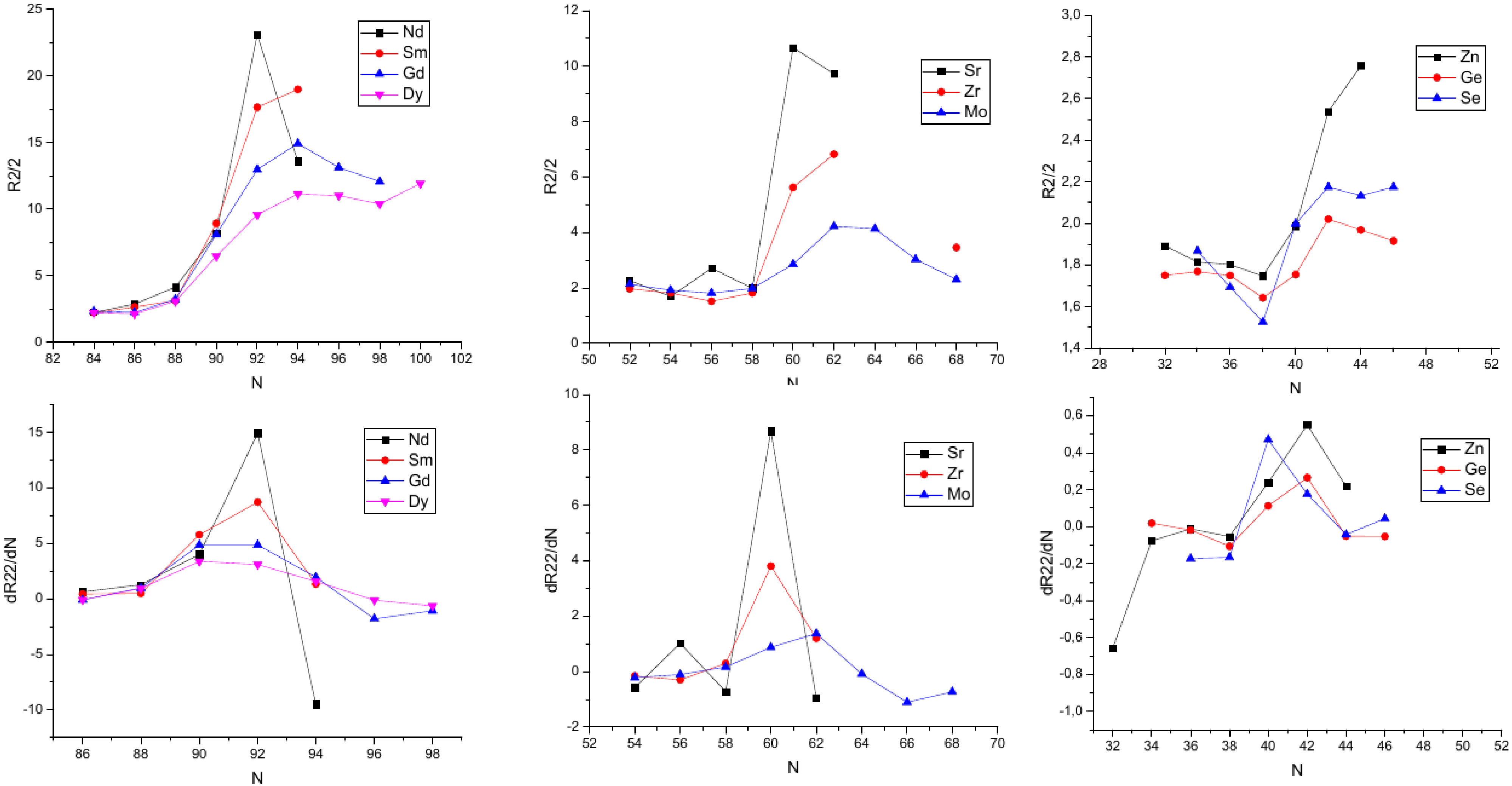




Energy ratios $R_{2/2}$

$$R_{2/2} = \frac{E(2^+_\gamma)}{E(2^+_1)}$$

$$\frac{dR_{2/2}}{dN}(N) = R_{2/2}(N) - R_{2/2}(N-2)$$



A mechanism for the onset of deformation

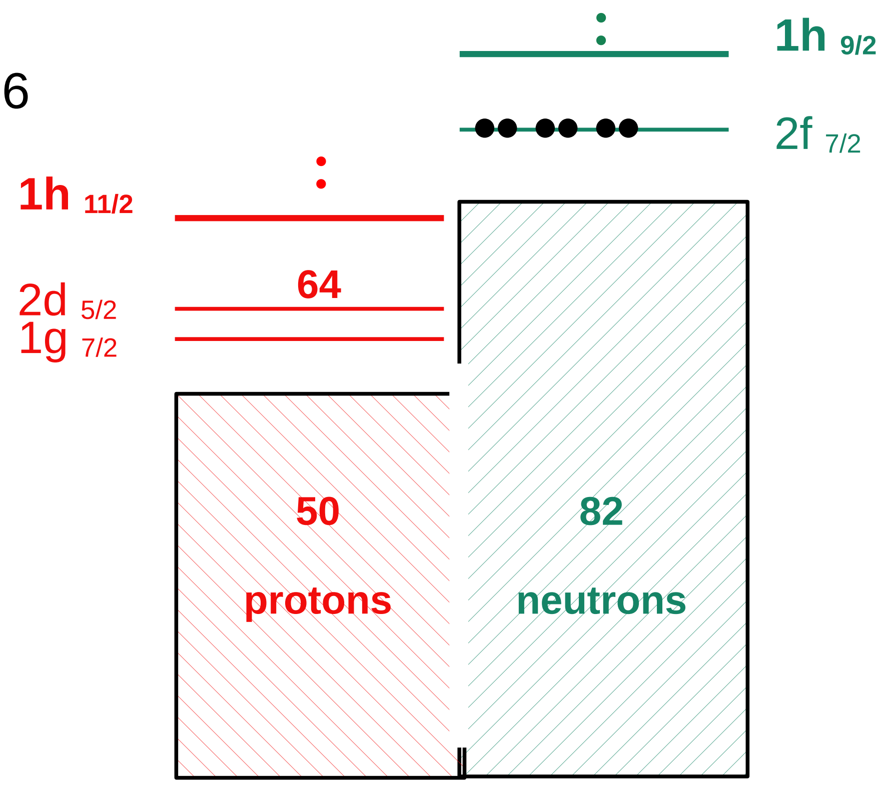
Shell model magic numbers: 2, 8, 20, 28, 50, 82, 126
=> major shells

subshell structure (gaps) depends on the number of protons and neutrons present
=> *effective* shells

e.g. for Z ≈ 60, N ≈ 90
when N < 90 *effective* proton shell: Z = 50 - 64

=> midshell at Z ≈ 56

=> but, as the neutron **$h_{9/2}$** begins to fill



monopole p-n interaction between spin-orbit partner orbitals **$h_{11/2}$** proton and **$h_{9/2}$** neutron lowers the **$h_{11/2}$** proton level, eliminating the Z = 64 gap

P. Federman and S. Pittel, Phys. Lett. B 69, 385 (1977)
R. F. Casten, Nuclear Structure from a Simple Perspective (2nd ed., Oxford University Press, Oxford, 2000)
T. Otsuka, Physics 4, 258 (2022)

A mechanism for the onset of deformation

when N ≥ 90 *effective* proton shell: Z = 50 - 76

=> new midshell position at Z ≈ 62

=> new position for the lowest-lying 2^+_1

=> affects nuclei with Z = 60-66 (Nd, Sm, Gd, Dy)

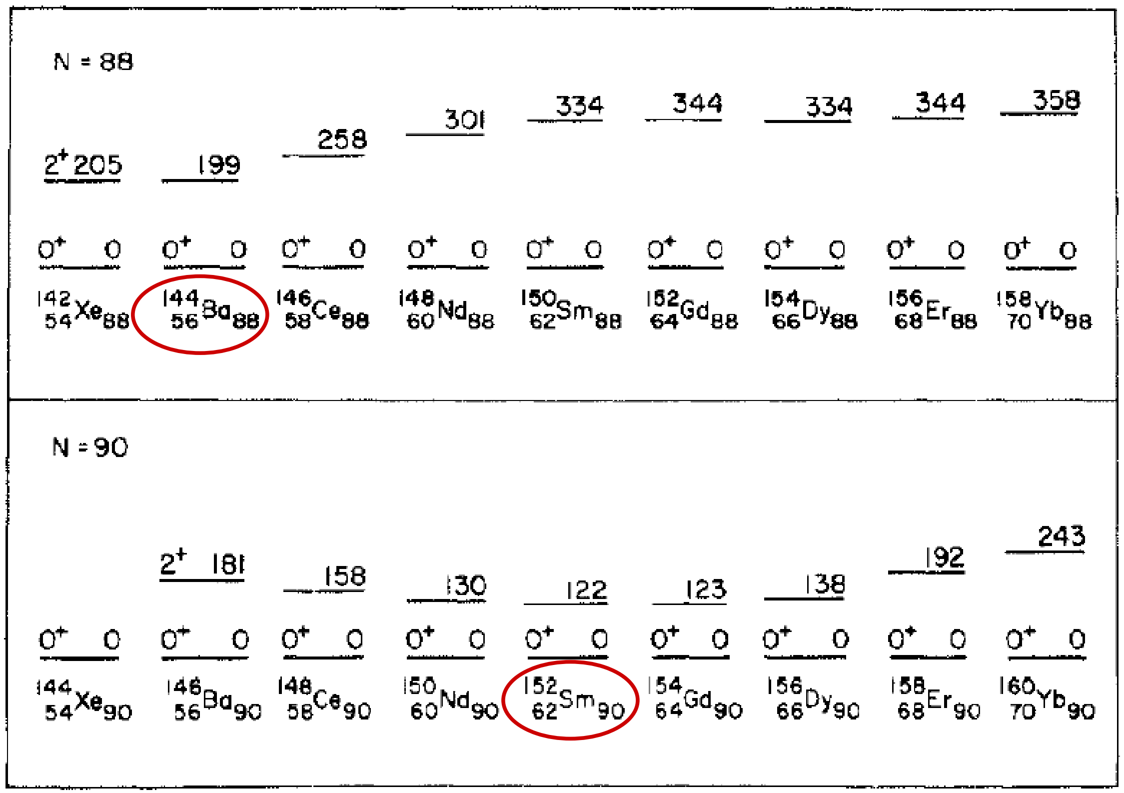
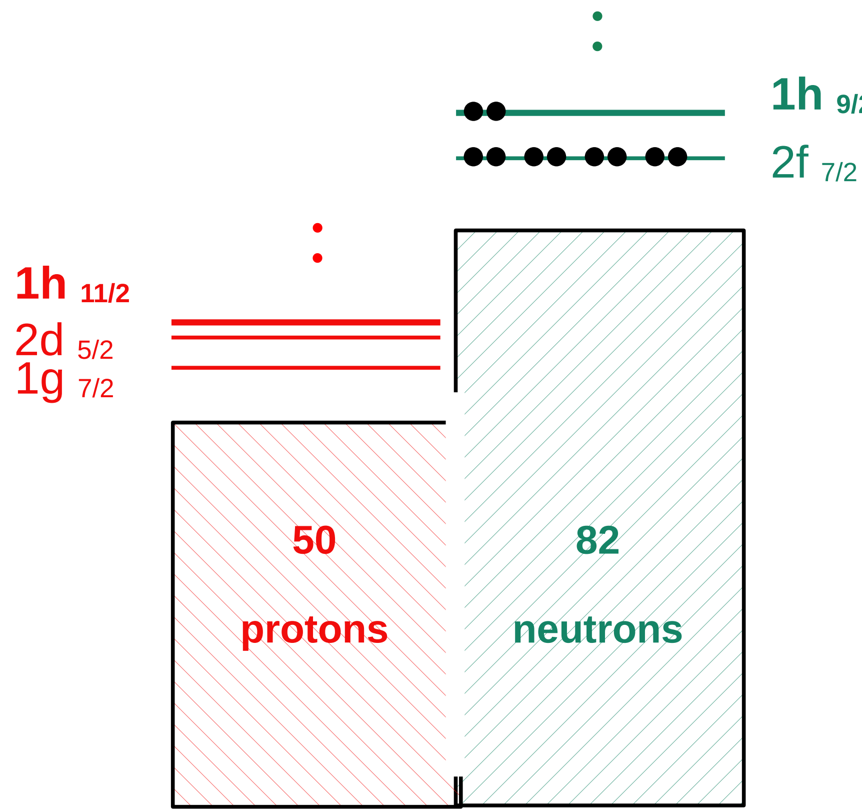


fig. from R. F. Casten *op.cit.*



in the A = 100 region:
proton $1g_{7/2}$, neutron $1g_{7/2}$

Microscopic calculations: SHF + BCS

Hartree-Fock equation

+

Skyrme effective interaction

→

mean-field

$$\hat{h}\psi_\alpha = \varepsilon_\alpha \psi_\alpha$$

+

BCS

$$(\varepsilon_\alpha - \epsilon_{F,q_\alpha})(u_\alpha^2 - v_\alpha^2) = \Delta w_\alpha u_\alpha v_\alpha$$

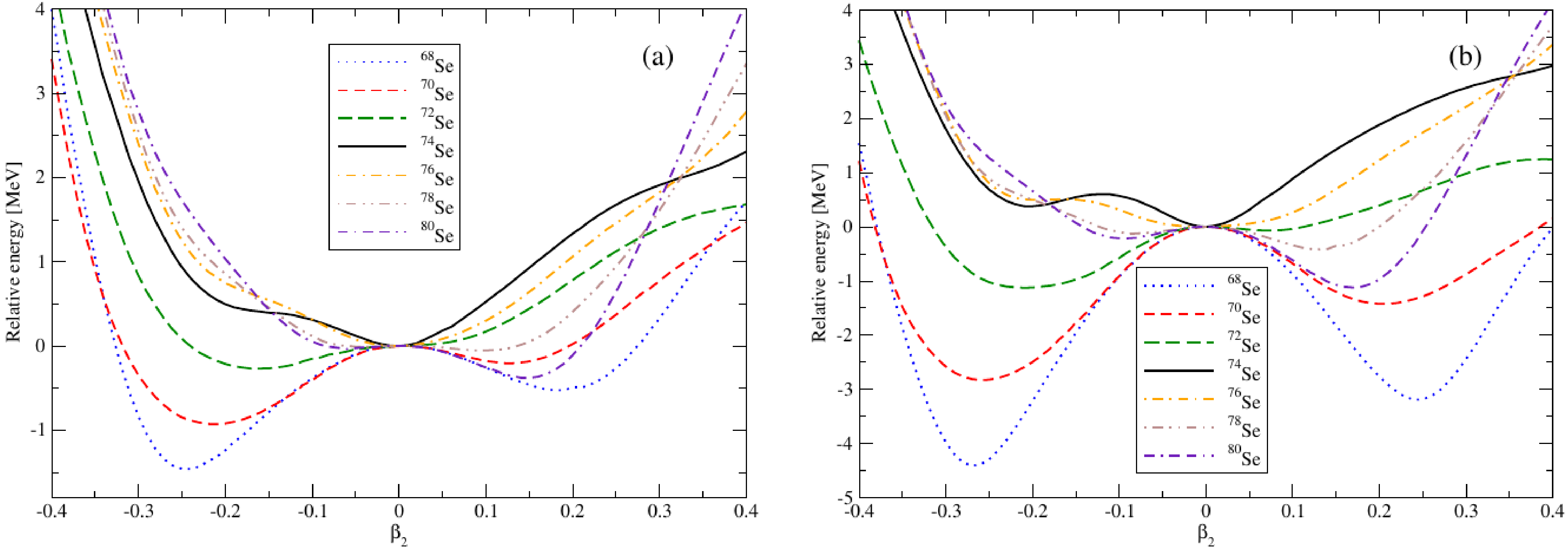
SkyAx code:
initial single particle states = **Nilsson** orbitals → $\boldsymbol{\beta}$ > 0: prolate, $\boldsymbol{\beta}$ < 0: oblate

P.-G. Reinhard, B. Schuetrumpf, and J. A. Maruhn, Comp. Phys. Comm. 258, 107603 (2021).

15 Skyrme parametrizations: {SV-bas, SV-tls, SV-mas07,... }

constrained calculations: (quadrupole) moment is fixed => Potential Energy Curves (PEC)

PEC for $_{34}$Se isotopes (N=34-46)

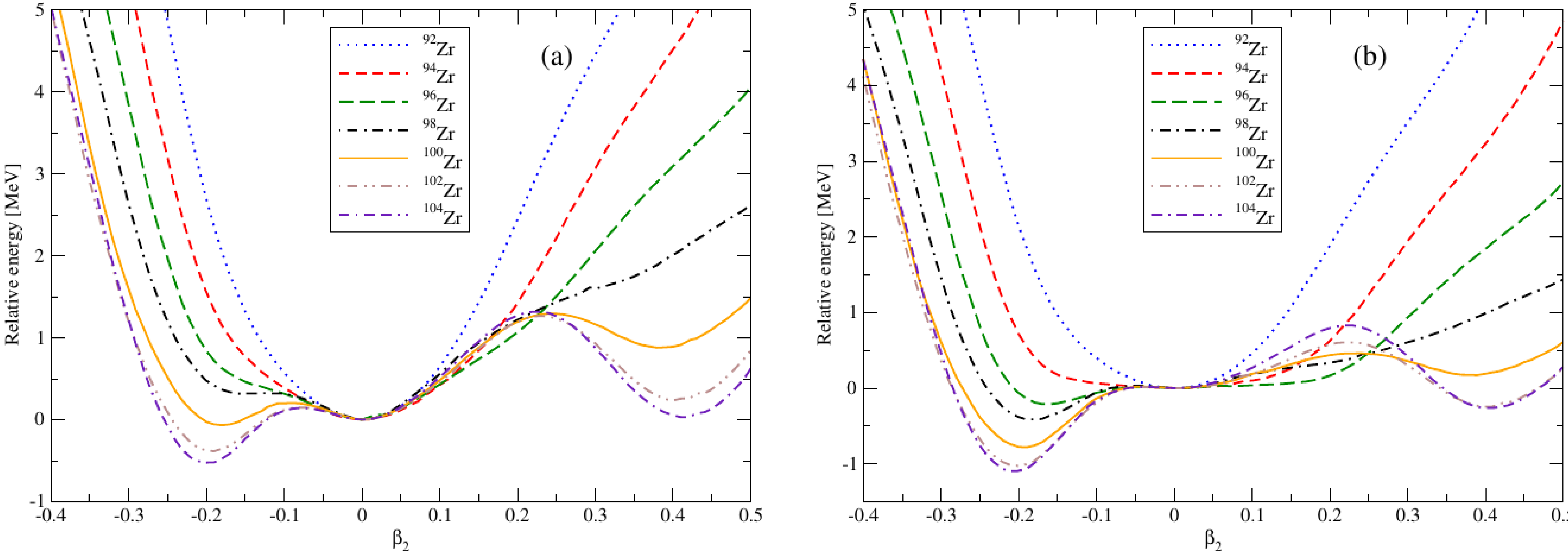


SV-bas

N = 40 → ^{74}Se

SV-mas07

PEC for $_{40}$Zr isotopes (N=52-64)

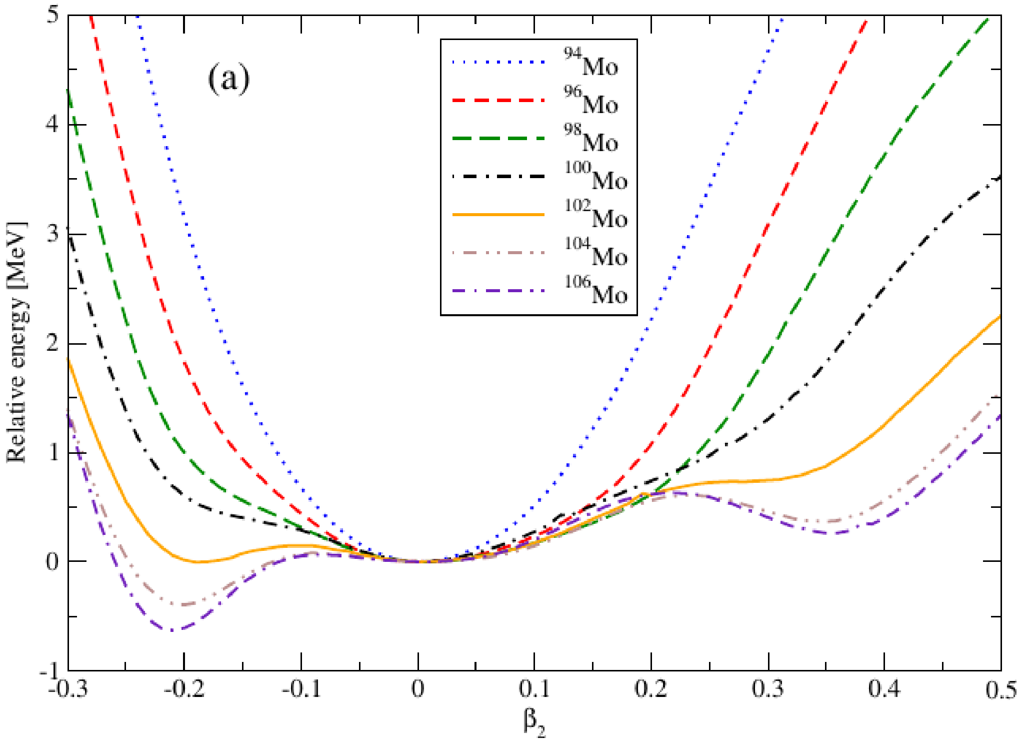


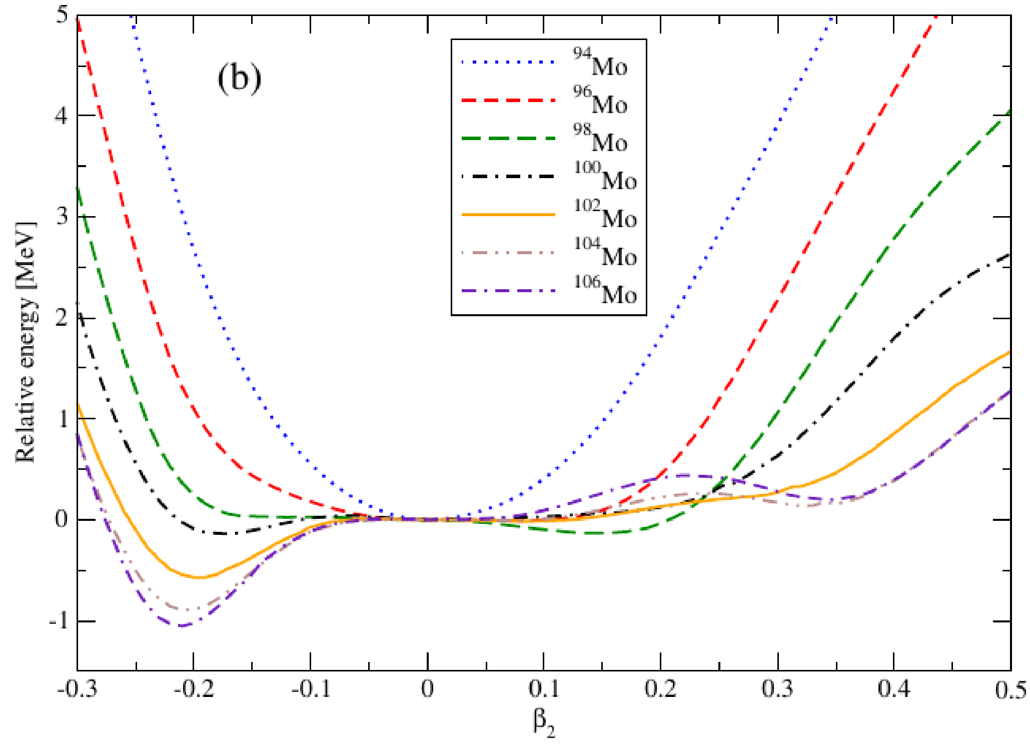
SV-bas

N = 60 → ^{100}Zr

SV-mas07

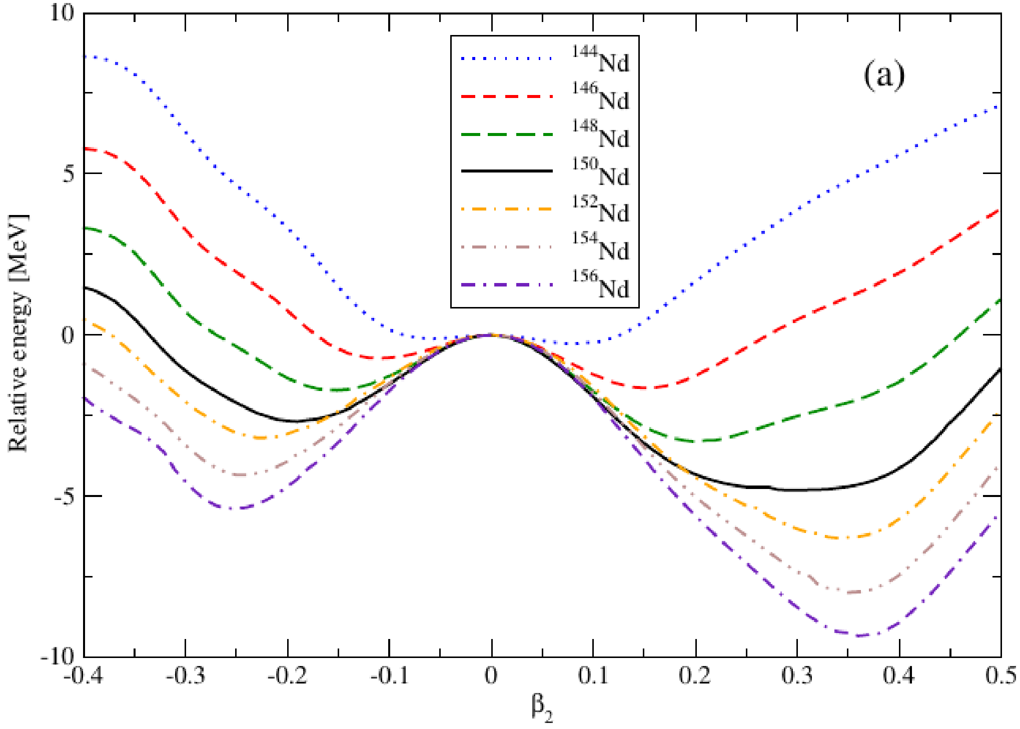
PECs for $_{42}$Mo isotopes (N=52-64)

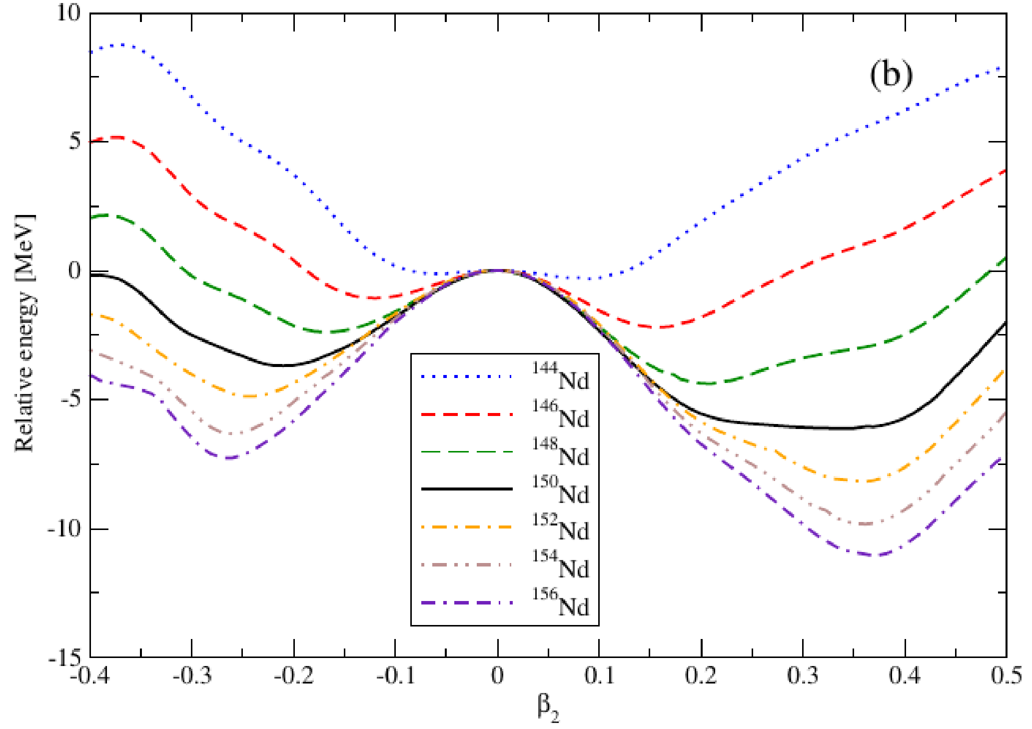




SV-bas N = 60 → ^{102}Mo SV-mas07

PECs for $_{60}$Nd isotopes (N=84-96)





SV-bas

N = 90 → ^{150}Nd

SV-mas07

Algebraic Collective Model (ACM)

A computationally tractable version of the collective model of **Bohr** and **Mottelson**

$$\hat{H} = x_1 \nabla^2 + x_2 + x_3 \beta^2 + x_4 \beta^4 + \frac{x_5}{\beta^2} + x_6 \beta \cos 3\gamma + x_7 \beta^3 \cos 3\gamma + x_8 \beta^5 \cos 3\gamma + \frac{x_9}{\beta} \cos 3\gamma + x_{10} \cos^2 3\gamma + x_{11} \beta^2 \cos^2 3\gamma + x_{12} \beta^4 \cos^2 3\gamma + \frac{x_{13}}{\beta^2} \cos^2 3\gamma + \frac{x_{14}}{\hbar^2} [\hat{\pi} \otimes \hat{q} \otimes \hat{\pi}]_0$$

$$\nabla^2 = \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \frac{1}{\beta^2} \hat{\Lambda}$$

x_1-x_{14} parameters: fitted to data

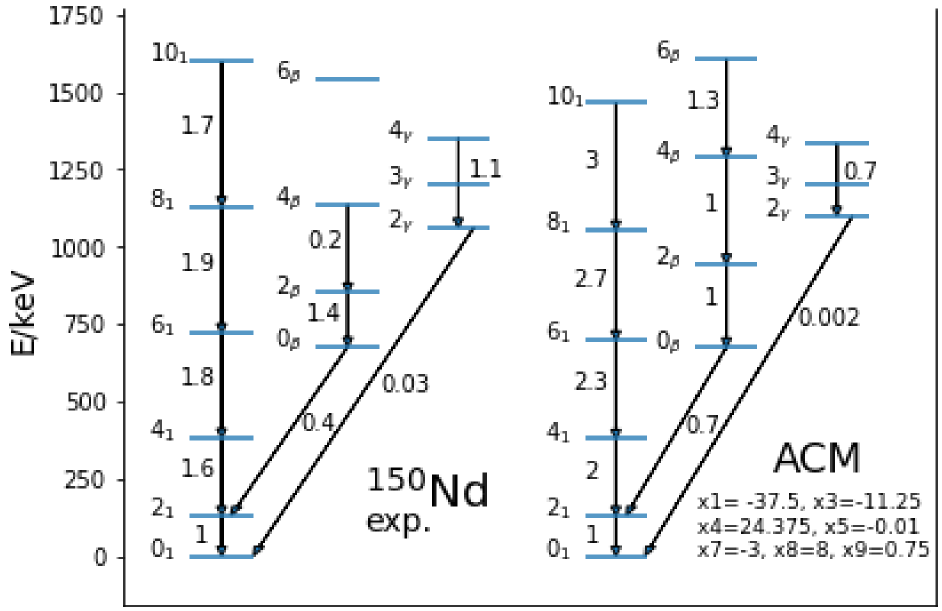
basis w.f.: $\mathrm{SU}(1,1) \times \mathrm{SO}(5) \supset \mathrm{U}(1) \times \mathrm{SO}(3) \supset \mathrm{SO}(2)$

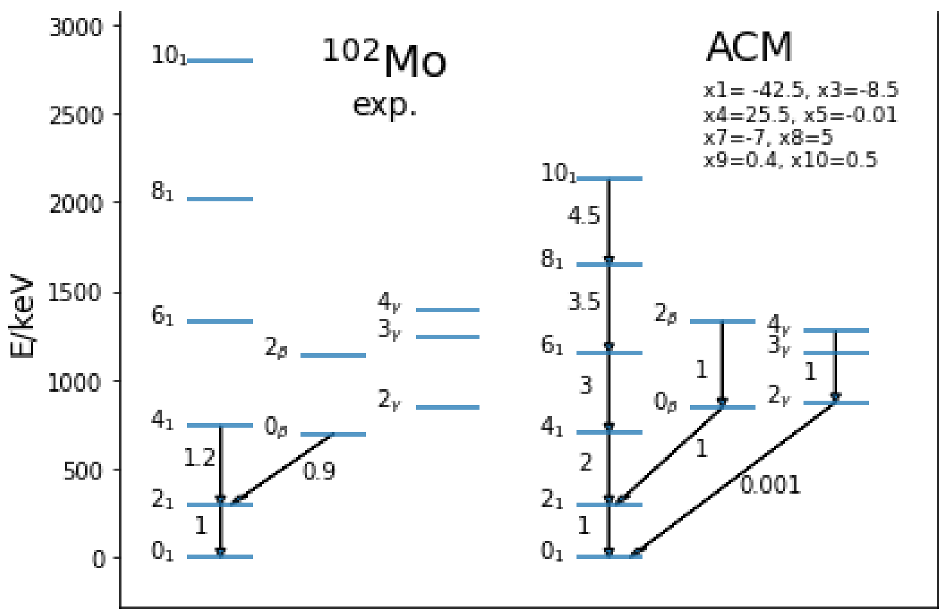
- $\mathrm{SU}(1,1)$ ↑ radial β-w.f.
- $\mathrm{SO}(5)$ ↑ angular 5-dim sph. har.

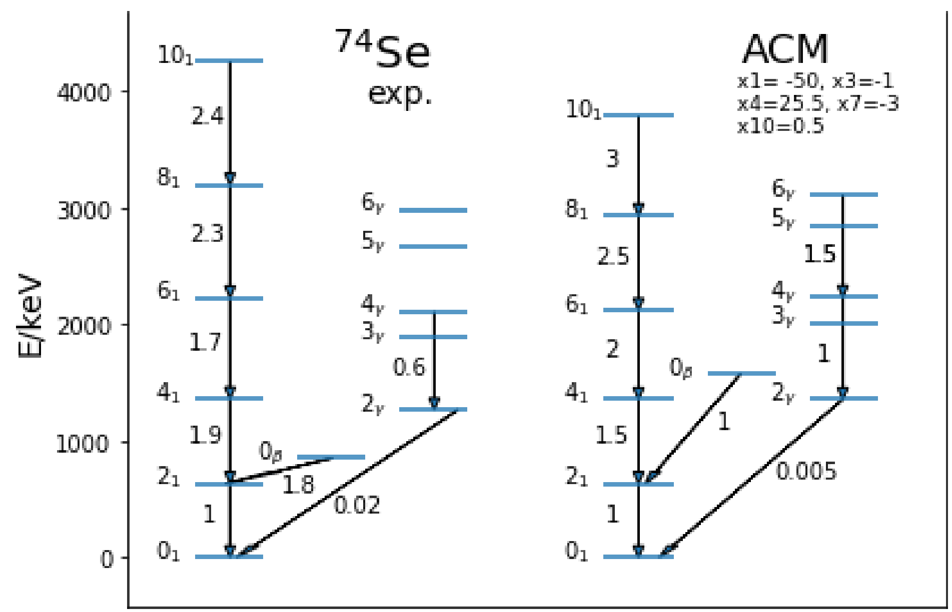
=> matrix elements computed analytically

D. J. Rowe, T. A. Welsh, and M. A. Caprio, Phys. Rev. C 79, 054304 (2009).
D. J. Rowe and J. L. Wood, Fundamentals of nuclear models (World Scientific, Singapore, 2010)
T. A. Welsh and D. J. Rowe, Comput. Phys. Commun. 200, 220 (2016)

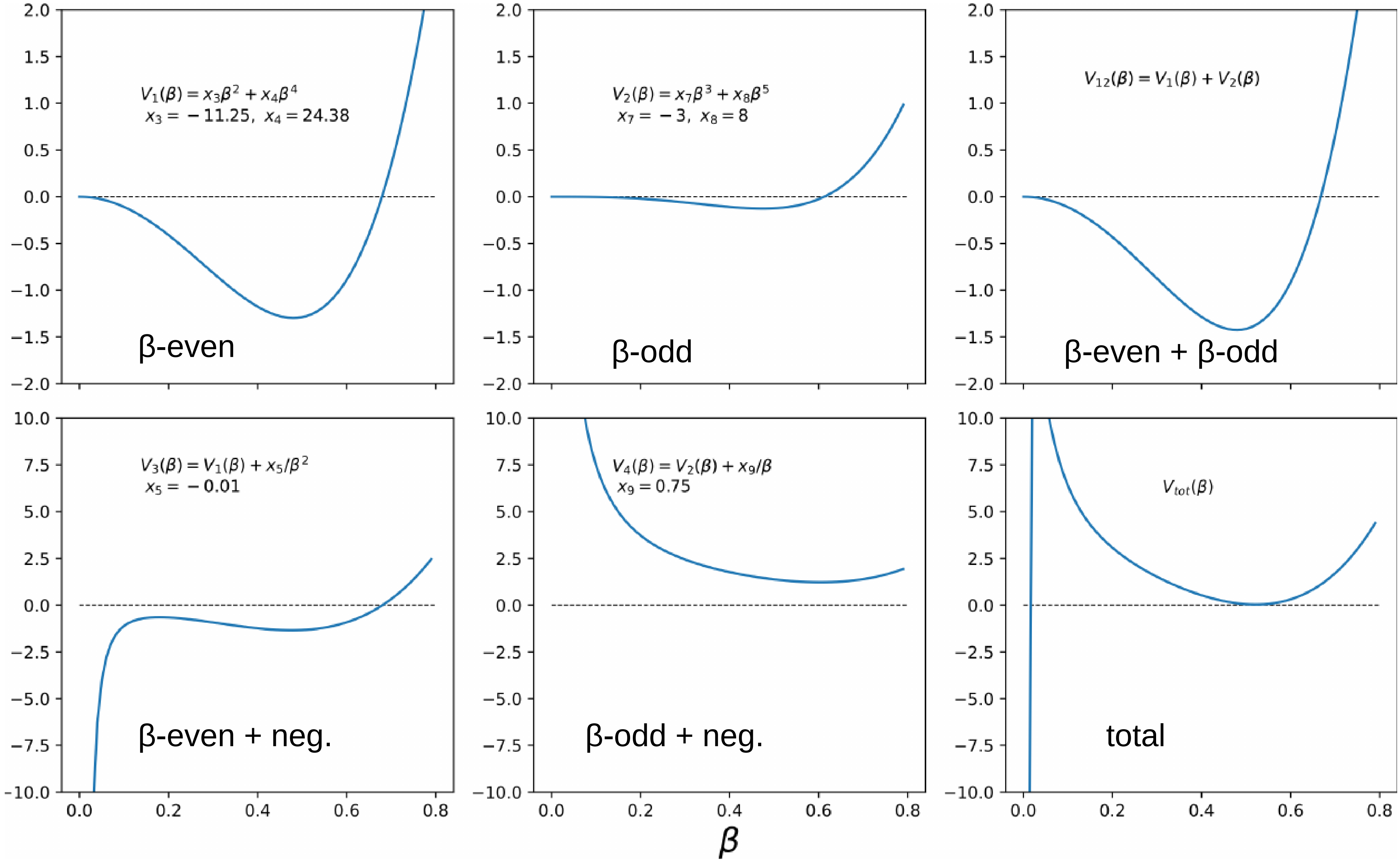
ACM calculations: spectra and B(E2)s





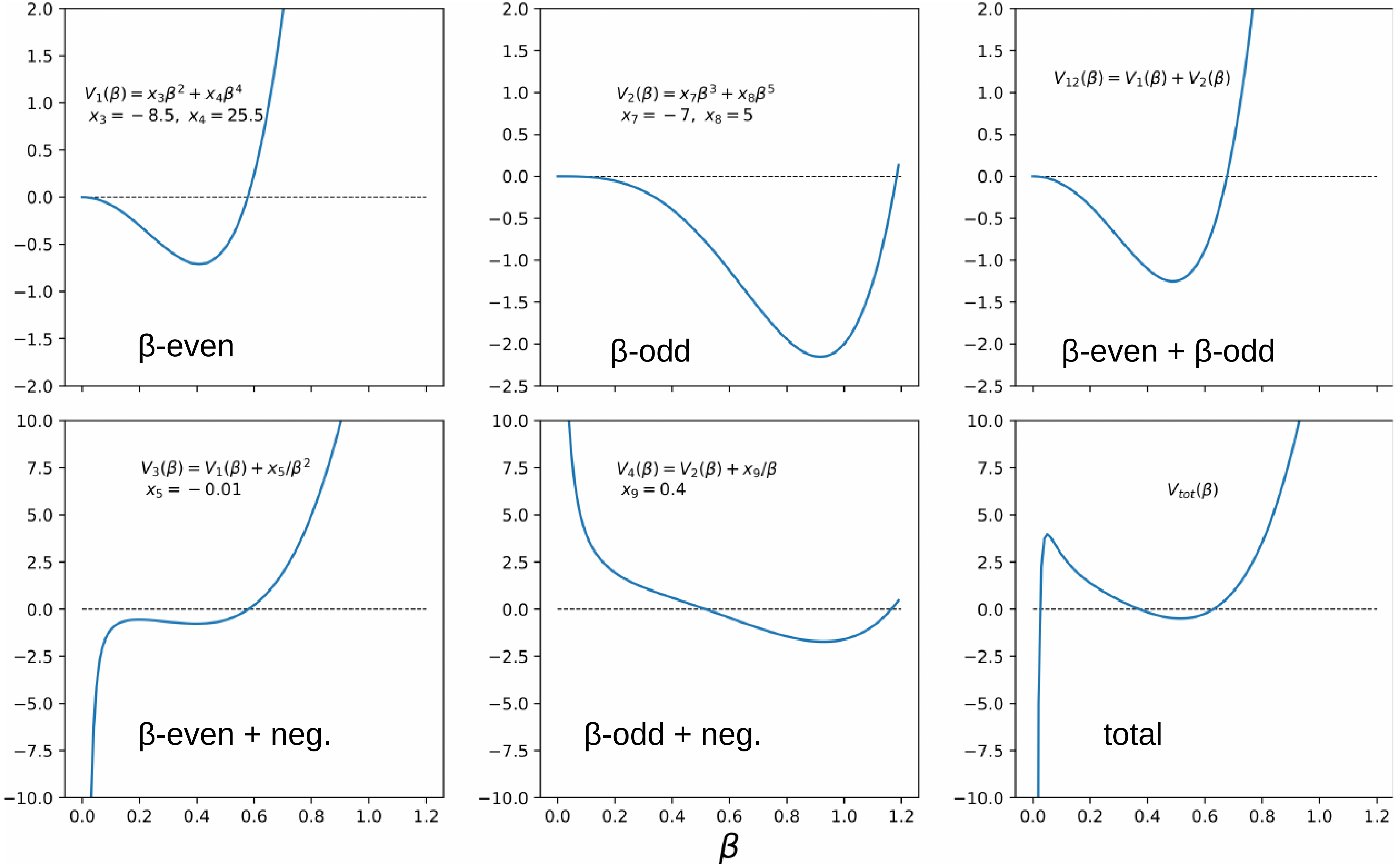


ACM Potential Energy Curves



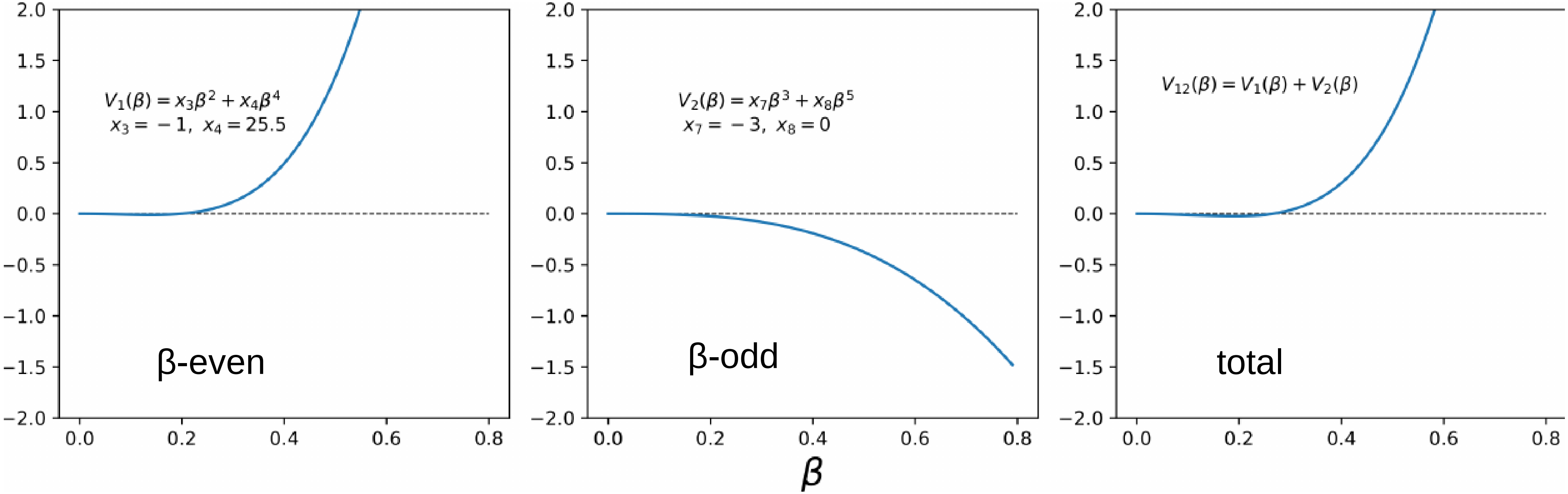
^{150}Nd

ACM Potential Energy Curves



^{102}Mo

ACM Potential Energy Curves



^{74}Se

In general, potentials resulting from ACM calculations show similarities with ones used in the Bohr Hamiltonian in the context of critical point symmetries, e.g.

- displaced infinite square well,
- infinite square well with a sloped wall,
- Davidson

Summary

- Certain experimental quantities, such as energy ratios: R4/2,… and B(E2) transition rates serve as benchmarks for nuclear structure
- Valence **p-n** interactions are the driving force for structural change
- Microscopic calculations in the N = 40, 60, 90 regions show signs of a *first*-order phase transition with coexisting minima in the PECs
- Potentials resulting from the ACM calculations show similarities with ones used in the context of the Bohr Hamiltonian (critical point symmetries)

IOP PUBLISHING JOURNAL OF PHYSICS G: NUCLEAR AND PARTICLE PHYSICS

J. Phys. G: Nucl. Part. Phys. **34** (2007) R285–R320 doi:10.1088/0954-3899/34/7/R01

TOPICAL REVIEW

Quantum phase transitions and structural evolution in nuclei

R F Casten and E A McCutchan

Wright Nuclear Structure Laboratory, Yale University, New Haven, CT 06520, USA

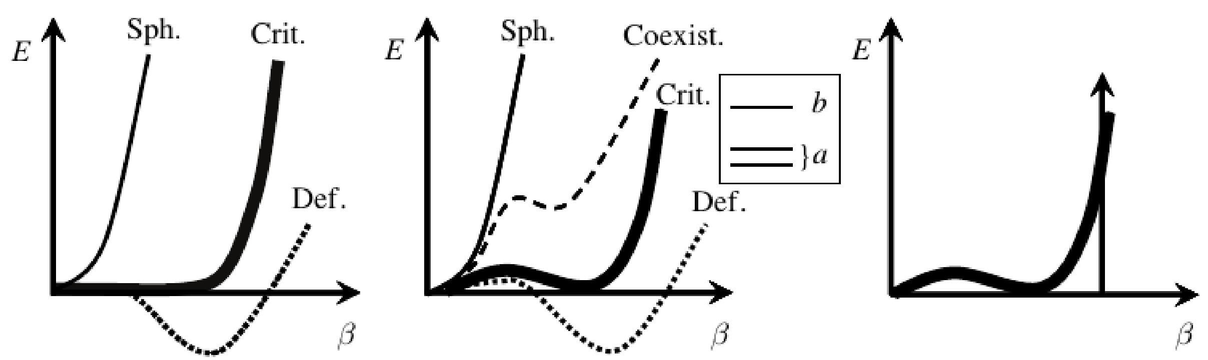


Figure 7. Energy surfaces for nuclei with successively larger numbers of valence nucleons plotted against the quadrupole deformation β (left) for a second-order phase transition and (middle) for a first-order phase transition. Right: the curve 'Crit.' repeated along with the square well ansatz that embodies the essential features of X(5) and E(5). The inset to the middle figure represents a set of shell model orbits a and b.

Bohr-Motelson collective model - Shapes

$$R(\theta,\varphi) = R_0\left[1 + \sum_{\mu=-2}^{2} \alpha_\mu Y^*_{2,\mu}(\theta,\varphi)\right]$$

Shape coordinates

Transformation to principal axes

$$a_\nu = \sum_{\mu=-2}^{2} \alpha_\mu D^*_{\mu,\nu}(\theta_i) \Rightarrow \begin{cases} a_2 = a_{-2} \\ a_1 = a_{-1} = 0 \end{cases}$$

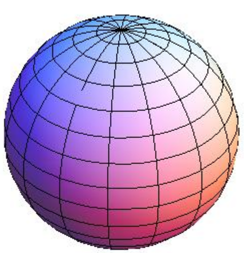
$$a_0 = \beta\cos\gamma$$

$$a_2 = \beta\sin\gamma/\sqrt{2}$$

β,γ Intrinsic (shape) β 0, 60° γ 0°

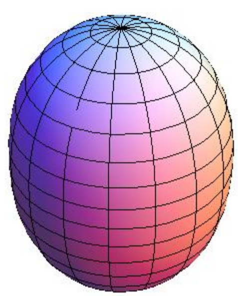
$\theta_i, (i = 1,2,3)$ Collective (orientation)

Spherical



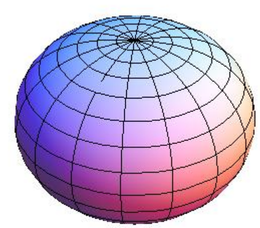
$\beta = 0$

Prolate



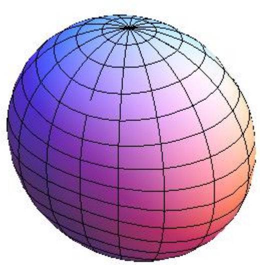
$\beta \neq 0, \gamma = 0^\circ$

Oblate



$\beta \neq 0, \gamma = 60^\circ$

Triaxial

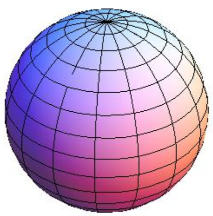


$\beta \neq 0, \gamma \neq 0^\circ, 60^\circ$

Vibrations and Rotations

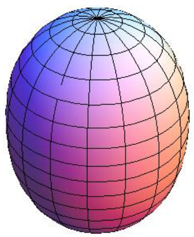
Equilibrium shape

Spherical



$\beta_0 = 0$

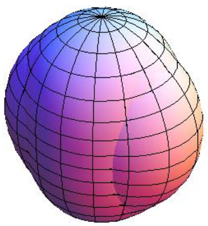
Axially deformed



$\beta_0 \neq 0$

$\gamma_0 = 0$

γ- unstable

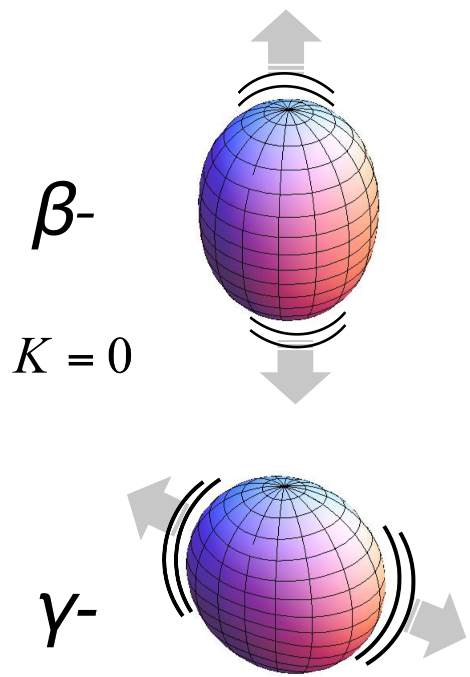


$\beta_0 \neq 0$

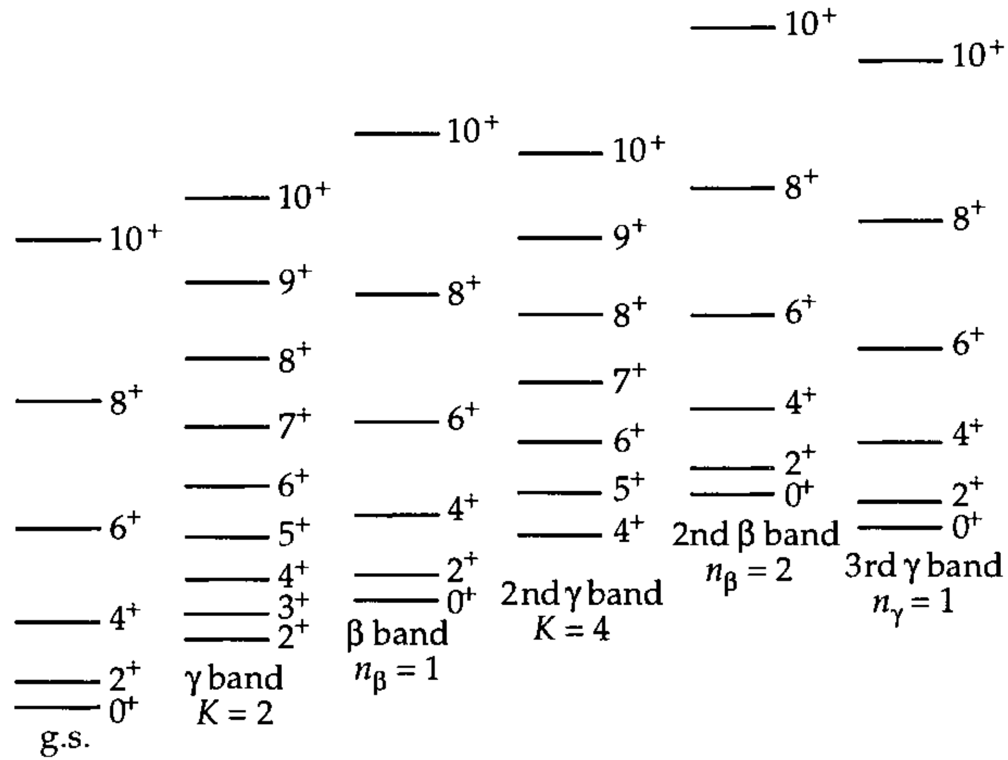
$V(\beta)$

Energy minima at

Spectrum of axially deformed nucleus



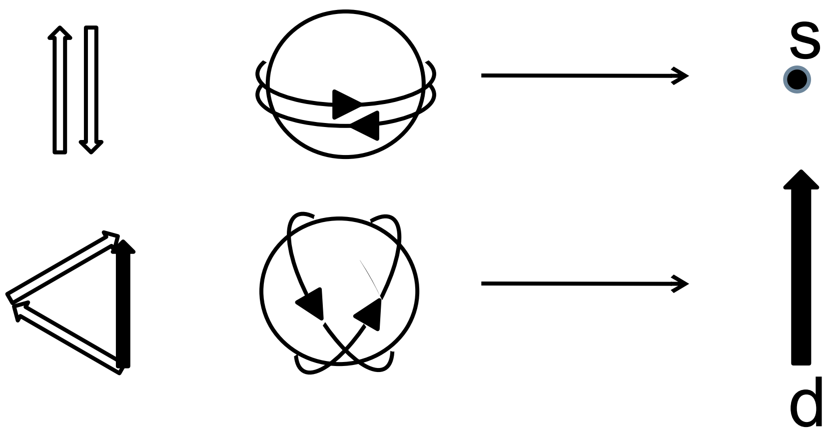
Typical rotation-vibrational spectrum



from Greiner and Maruhn (1995)

IBM- the building blocks

Fermion Pairs | **Bosons**



$J^\pi = 0^+$

$J^\pi = 2^+$

$$\mapsto \begin{cases} s^\dagger, d_m^\dagger \\ s \;\;, d_m \end{cases} \qquad m = 0, \pm 1, \pm 2$$

$$\tilde{d}_m = (-1)^m d_m$$

Unitary tranformations

$$\text{6-dim} \begin{cases} s^\dagger|0\rangle \\ d_m^\dagger|0\rangle \end{cases} \longrightarrow \text{U(6)}$$

Closed shell

36 generators

$$G_{\alpha\beta} = b_\alpha^\dagger \tilde{b}_\beta\,,$$
$$(\alpha, \beta = 1, \ldots, 6)$$

Tensor products

$$G_\kappa^{(k)}(l, l') = [b_l^\dagger \times \tilde{b}_{l'}]_\kappa^{(k)},$$
$$(l, l' = 0, 2)$$

IBM-Algebraic structure

$$U(6) \supset \begin{cases} U(5) \supset SO(5) \supset SO(3) \\ |\, n_d \quad \tau \quad \nu_\Delta \quad L \;> \\ SU(3) \supset SO(3) \\ |(\lambda,\mu) \quad K_L \quad L \;> \\ SO(6) \supset SO(5) \supset SO(3) \\ |\, \sigma \quad \tau \quad \nu_\Delta \quad L \;> \end{cases}$$

[N]

Labeling the basis states

O(3) ⊃ O(2)

$| J \quad M >$

Casimir operators C of algebra g

$$[C, X] = 0, \forall X \in g$$

$$H = \kappa_1 C_1[U(5)] + \kappa'_1 C_2[U(5)] + \kappa_2 C_2[SU(3)] + \kappa_3 C_2[SO(6)] + \kappa_4 C_2[SO(5)] + \kappa_5 C_2[SO(3)]$$

Multipole expansion

$$H = E'_0 + \varepsilon_d \hat{n}_d + c_1(\hat{L}\cdot\hat{L}) + c_2(\hat{Q}^\chi \cdot \hat{Q}^\chi) + c_3(\hat{T}^{(3)} \cdot \hat{T}^{(3)}) + c_4(\hat{T}^{(4)} \cdot \hat{T}^{(4)})$$

Operators:

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

$$\hat{L} = \sqrt{10}[d^\dagger \times \tilde{d}]^{(1)} \qquad \hat{T}^{(k)} = [d^\dagger \times \tilde{d}]^{(k)}_m$$

The classical limit of IBM

Boson condensate

$$|N;\beta,\gamma\rangle = \frac{1}{\sqrt{N!}}\left[b^\dagger(\beta,\gamma)\right]^N|0\rangle$$

a_0 $a_{\pm 2}$

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

Energy surfaces

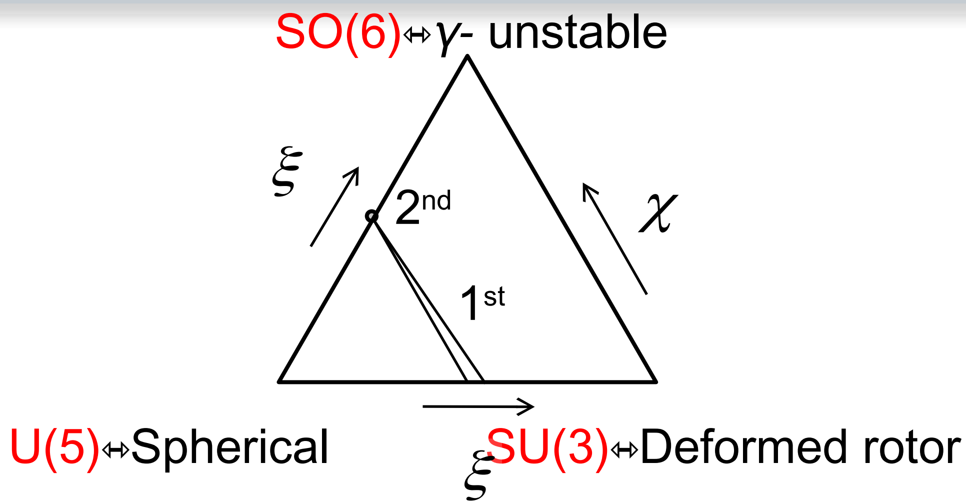
$$E(\beta,\gamma) = \lim_{N\to\infty}\langle N;\beta,\gamma|H|N;\beta,\gamma\rangle$$

…to be minimized

Shape phase transitions

Simplified Hamiltonian

$$H = \varepsilon_0 \left[(1-\xi)\hat{n}_d - \frac{\xi}{4N}\hat{Q}^{\chi}\cdot\hat{Q}^{\chi} \right]$$



ξ, χ: Control parameters

$\xi : 0 \rightarrow 1$

$U(5) \longrightarrow SU(3) : \chi = -\sqrt{7}/2$ 1st order

$U(5) \longrightarrow SO(6) : \chi = 0$ 2nd order

Signatures of phase transitions

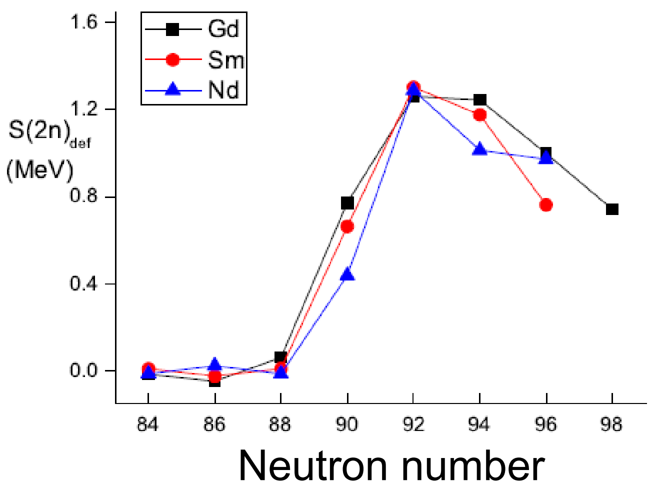
$$\hat{H}(\xi) = (1-\xi)\hat{H}_1 + \xi\hat{H}_2$$

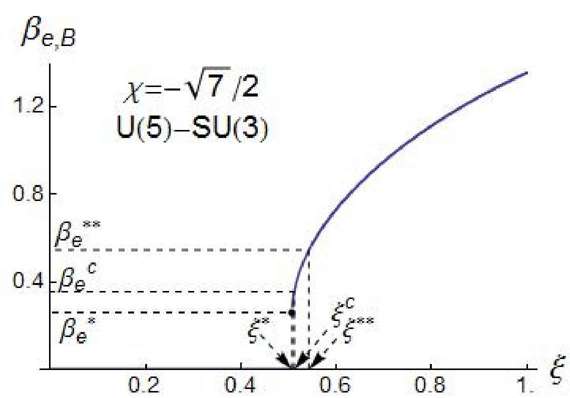
Ehrenfest:
Ground state energies
k-th order if discontinuity in $\dfrac{d^k E_0}{d\xi^k}$

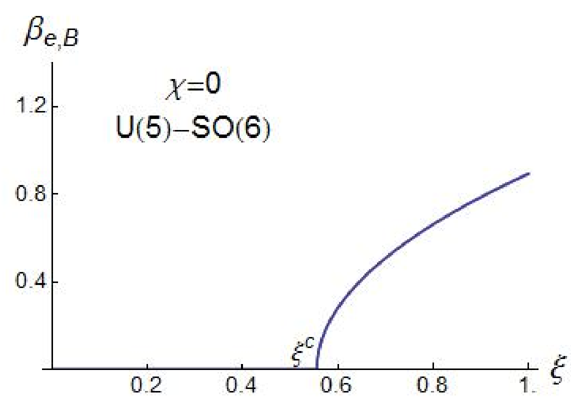
Landau:
Order parameters

Quantum: $\langle n_d \rangle_0$ Classical: $\beta_e, \quad \dfrac{d\beta_e}{d\xi}$

$$S_{2n} = E_0^{(N+1)} - E_0^{(N)} \propto \frac{dE_0}{d\xi}$$







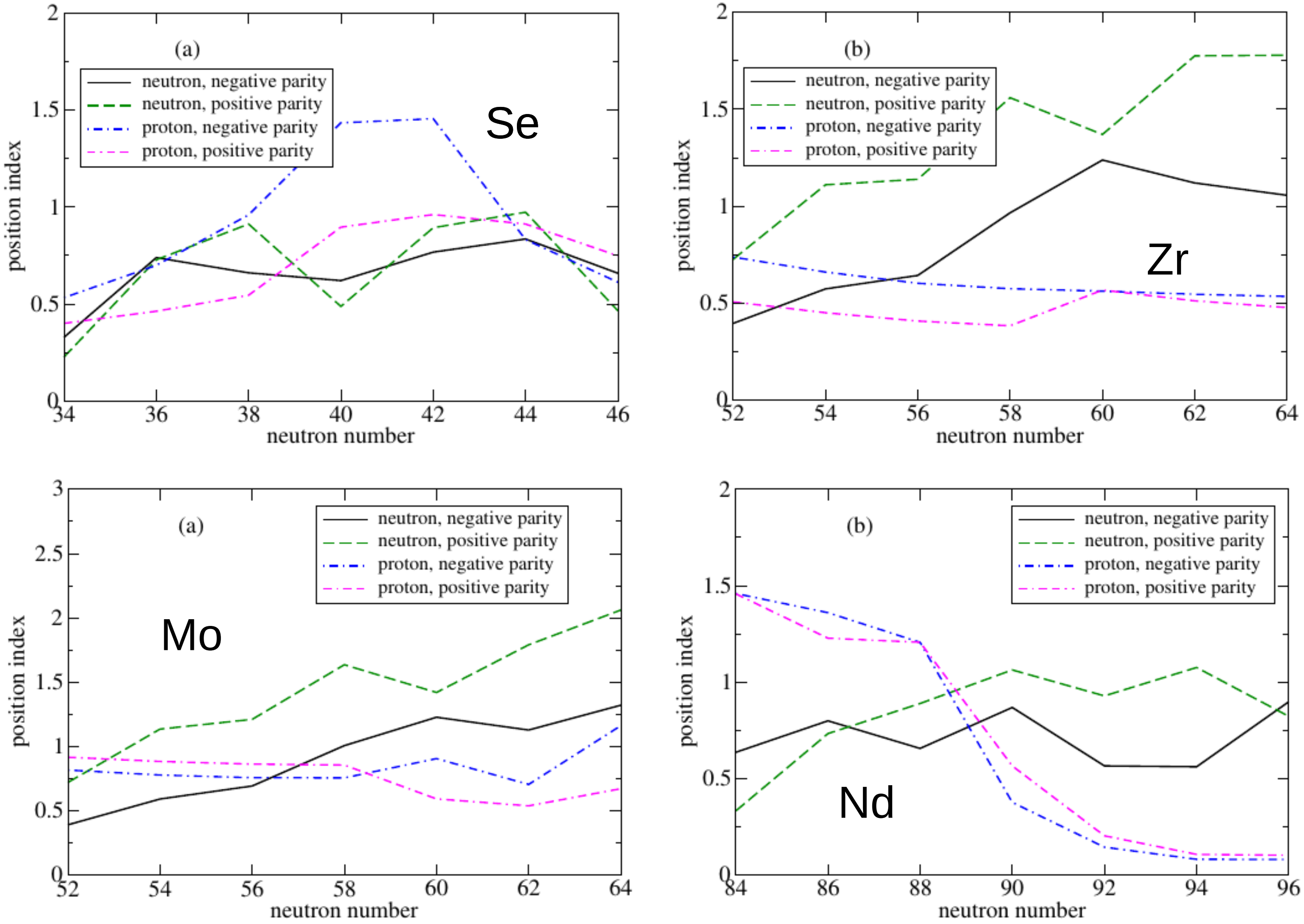
Position Index

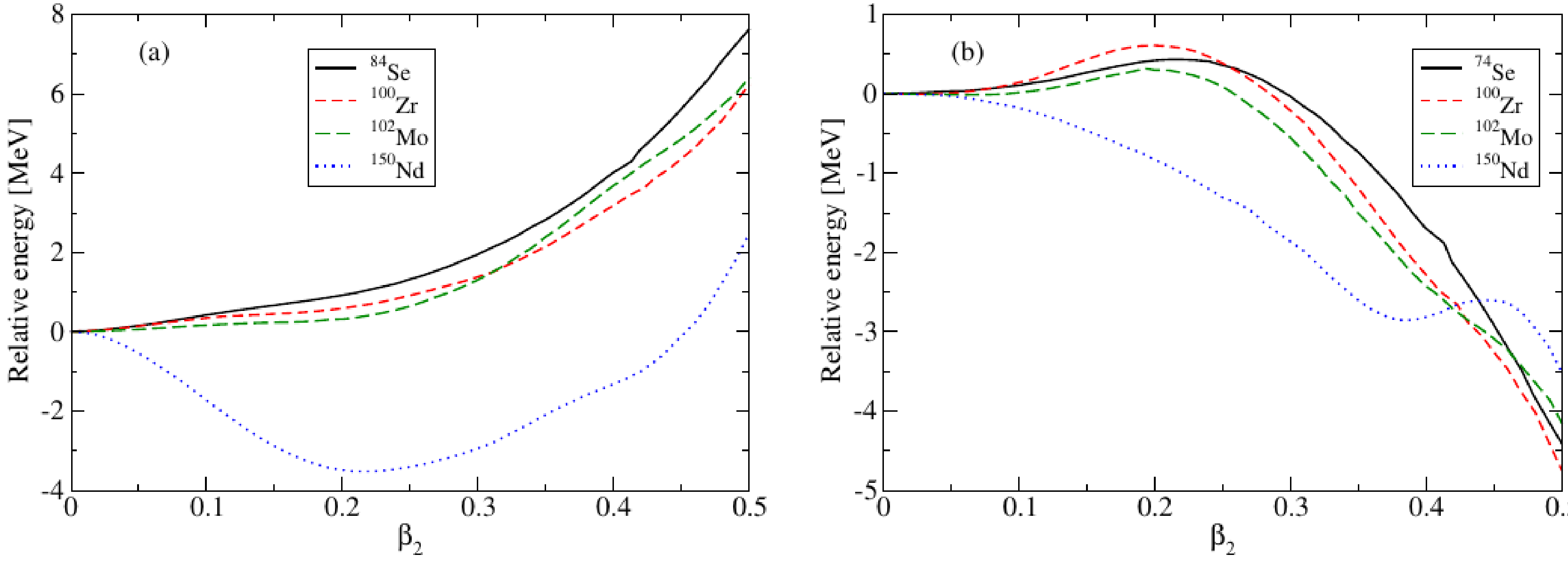
$$\mathrm{I}(\mathrm{q},\pi) = \sum_{i_{(q,\pi)}} \left(0.5 - \left|v_i^2 - 0.5\right|\right)$$

v_i^2: occupation probability of state i

$q = n, p$ and $\pi = \pm$

what kind of levels are closest to the Fermi surface




(a)
^{84}Se
^{100}Zr
^{102}Mo
^{150}Nd
Relative energy [MeV]
β_2
(b)
^{74}Se
^{100}Zr
^{102}Mo
^{150}Nd
Relative energy [MeV]
β_2