How well defined are phase transitions and critical points in the Interacting Boson Model

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Phase transitions in atomic nuclei.

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Macroscopic phase transitions

- Control parameter: variable that affect to the system, can be changed smoothly and "arbitrarily".

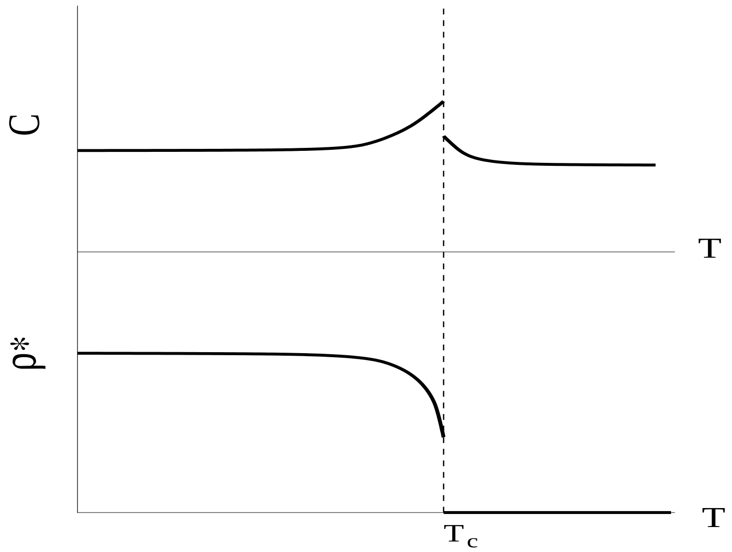
- Order paremeter: observable that change as a function of the control parameter.

- Ordered and disordered phases correspond to a value of the control parameter equal and different from zero, respectively.

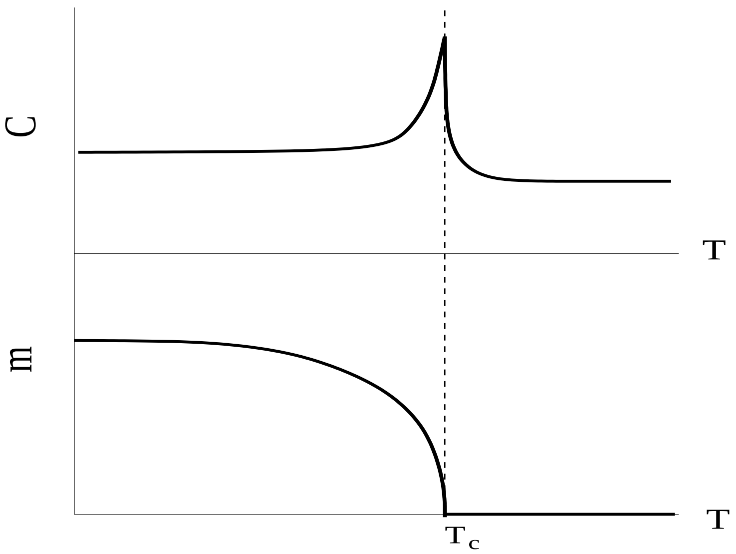
- Order of a phase transition: order of the first derivative of the Gibbs potential with respect to the control parameter that first experiences a discontinuity.

Examples of macroscopic phase transitions

- **First order phase transition: liquid-gas.**

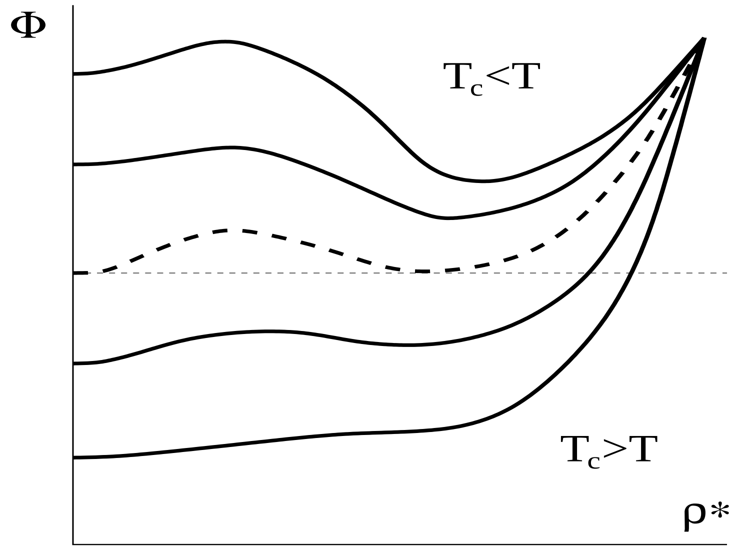


- **Second order phase transition: ferromagnetic material.**

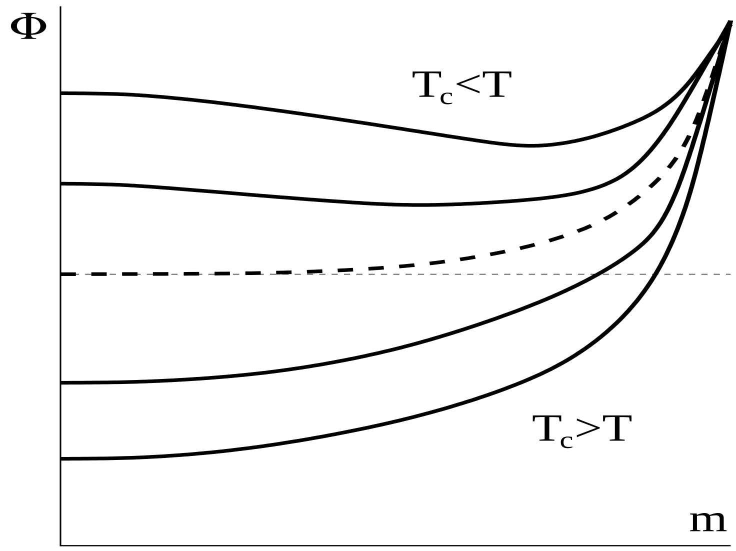


What is happening at the phase transition point

- **First order phase transition.**



- **Second order phase transition.**

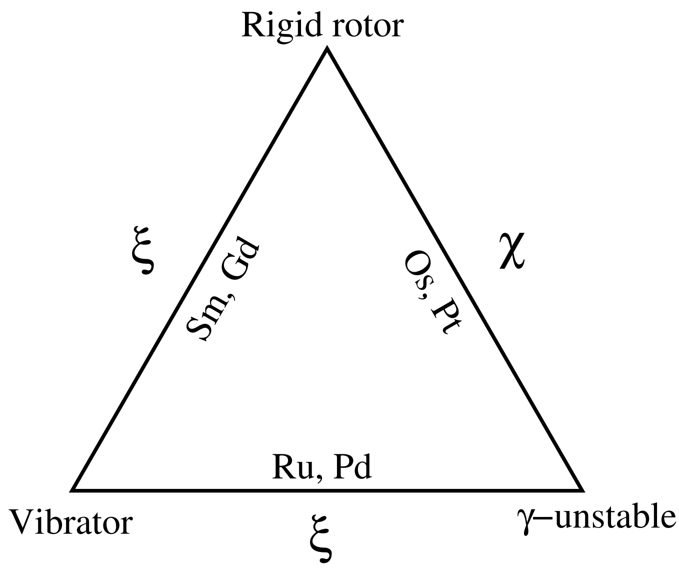


Phase transition in the atomic nuclei

$$\hat{H} = \kappa(N\frac{1-\xi}{\xi}\hat{n}_d - \hat{Q}\cdot\hat{Q})$$

$\hat{n}_d = d$ boson number operator

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



ξ or χ can be the control parameter

Order parameter in the atomic nuclei

- Variational procedure for finding the ground state energy.
- The trial wave function,

$$|c\rangle = \frac{1}{\sqrt{N!}}(\Gamma_c^\dagger)^N|0\rangle,$$

where

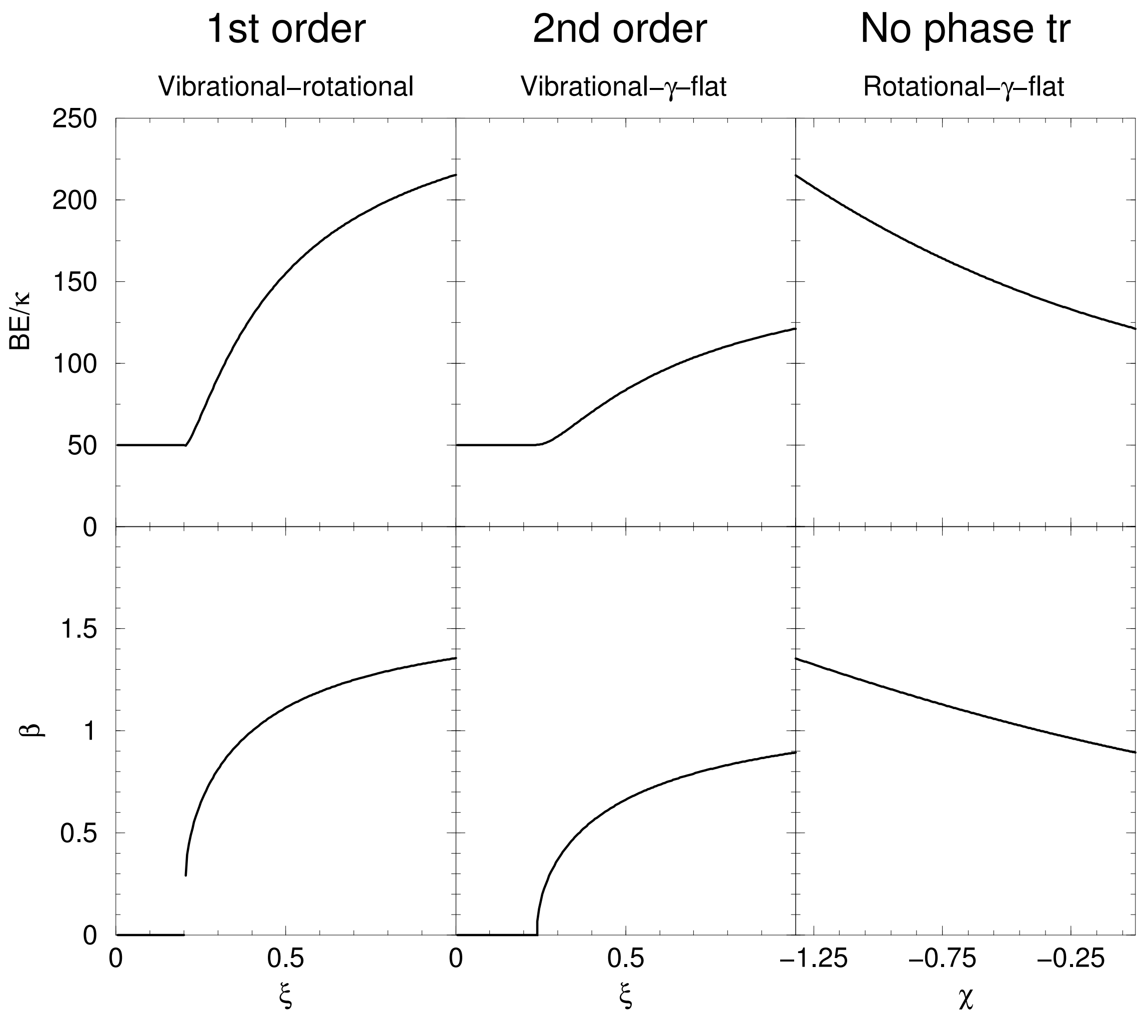
$$\Gamma_c^\dagger = \frac{1}{\sqrt{1+\beta^2}}\left(s^\dagger + \beta\cos\gamma\, d_0^\dagger + \frac{1}{\sqrt{2}}\beta\sin\gamma\,(d_2^\dagger + d_{-2}^\dagger)\right).$$

- The energy surface,

$$\begin{aligned}\langle c|H|c\rangle &= \frac{N\beta^2}{5(1+\beta^2)}(N\,\frac{1-\xi}{\xi} + 4 - \chi^2)\\ &+ \frac{N(N-1)}{(1+\beta^2)^2}(-4\beta^2 + \frac{4}{7}\sqrt{14}\chi\,\cos(3\gamma)\,\beta^3 - \frac{2}{7}\beta^4).\end{aligned}$$

- The values of β and γ that minimize the energy are the order parameters.
- Because $\gamma = 0, \pi/3$, **β is the only order parameter.**

The three transitional regions



Drawbacks

- ξ is not a true control parameter.
- ξ is fixed in every nucleus and cannot be changed *by hand.*
- ξ should be found fitting or reproducing as much observables as possible.

Two neutron separation energies (S_{2n})

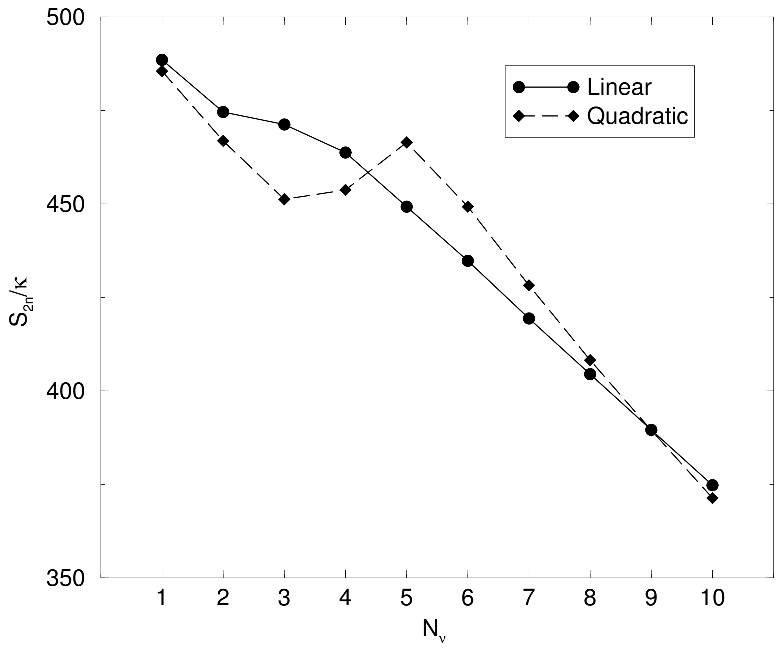
- Definition:

$$S_{2n}(N) = BE(N) - BE(N-1) + \mathcal{A} + \mathcal{B}N.$$

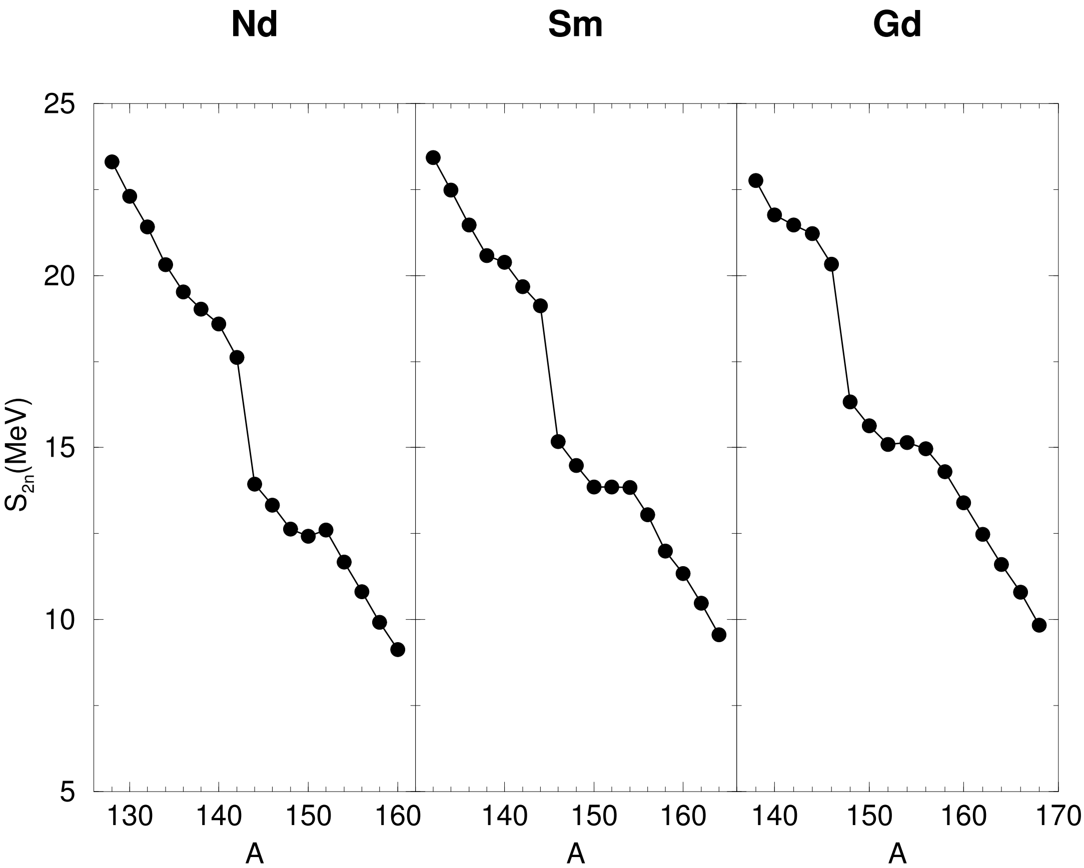
- Simulation of a first order phase transition: vibrational to rotational nuclei ($U(5) - SU(3)$).
- Relation between the control parameter and the number of bosons for fixed Z ($N_\pi = 5$).

$$\begin{aligned} \xi_{lin} &= 0.099N_\nu + 0.01, \\ \xi_{qua} &= 0.0099N_\nu^2 + 0.01. \end{aligned}$$

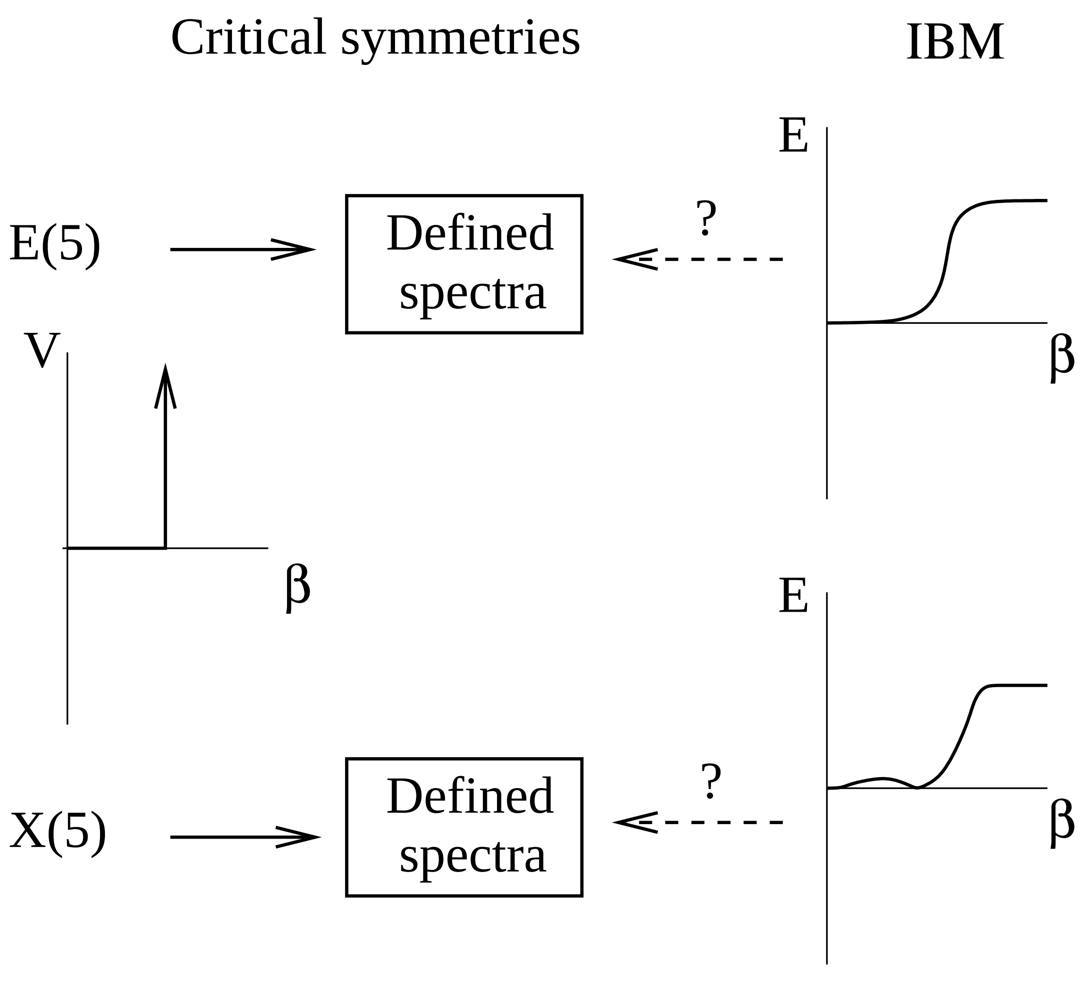
- Linear part for S_{2n}: $S_{2n}^{lin}/\kappa = 200 - 20N_\nu$.



Experimental S_{2n}



Spectra and energy surfaces



The IBM general case

- The Hamiltonian (up to two-body interactions)

$$\begin{aligned}\hat{H} &= \tilde{\mathcal{A}}\hat{N} + \tilde{\mathcal{B}}\frac{\hat{N}(\hat{N}-1)}{2} + \varepsilon_d \hat{n}_d + \kappa_0 \hat{P}^\dagger \hat{P} \\ &+ \kappa_1 \hat{L}\cdot\hat{L} + \kappa_2 \hat{Q}^\chi \cdot \hat{Q}^\chi + \kappa_3 \hat{T}_3 \cdot \hat{T}_3 + \kappa_4 \hat{T}_4 \cdot \hat{T}_4.\end{aligned}$$

- The energy surface

$$\begin{aligned}\langle c|\hat{H}|c\rangle &= \frac{N\tilde{\varepsilon}\beta^2}{(1+\beta^2)} + \frac{N(N-1)}{(1+\beta^2)^2}(a_1\beta^4 \\ &+ a_2\beta^3\cos(3\,\gamma) + a_3\beta^2 + \frac{u_0}{2}),\end{aligned}$$

where

$$\begin{aligned}\tilde{\varepsilon} &= \varepsilon_d + 6\,\kappa_1 - 4\,\kappa_2 + \chi^2\,\kappa_2 + \frac{7}{5}\,\kappa_3 + \frac{9}{5}\,\kappa_4, \\ a_1 &= \frac{1}{4}\,\kappa_0 + \frac{2}{7}\,\chi^2\,\kappa_2 + \frac{18}{35}\,\kappa_4, \\ a_2 &= -\frac{4}{7}\sqrt{14}\,\chi\,\kappa_2, \\ a_3 &= -\frac{1}{2}\,\kappa_0 + 4\,\kappa_2, \\ u_0 &= \frac{\kappa_0}{2}.\end{aligned}$$

Catastrophe theory for pedestrian I

- "*Catastrophe theory attempts to study how the qualitative nature of the solutions of equations depends on the parameters that appear in the equations*". (R. Gilmore, "Catastrophe theory for scientists and engineers", 1981).
- Equations: $\frac{\partial V(\phi_j; c_\alpha)}{\partial \phi_i} = 0.$
- $c_\alpha \longrightarrow \tilde{\varepsilon},\ \kappa_0,\ \kappa_1,\ \kappa_2, \chi,\ \kappa_3,\ \kappa_4.$
- $\phi_j \longrightarrow \beta,\ \gamma.$

Catastrophe theory for pedestrian II

- The goal is to find the equilibrium configurations through the construction of canonical forms of the potential.
- Steps
  1. Find the essential parameters of the system.
  2. Find all the critical points.
  3. Localize the critical point of maximum degeneracy.
  4. Find the locus in the parameter space where there exists two degenerated extrema: Maxwell set.
  5. Find the locus in the parameter space where the determinant of the Hessian matrix is zero: bifurcation set.
  6. Construct the separatrix of the system as the union of the Maxwell and bifurcation sets.
- **If one is able to arrive to the canonical form using an appropriated change of variables, the problem is finished and the solution is given!**

Catastrophe conventions

- They provide the means by which the canonical forms of Catastrophe theory are made available to physical applications.
- Delay convention: the system remains in a stable or metastable equilibrium state until that state disappears.
- Maxwell convention: the system state is one that globally minimize the potential.
- If the energy noise refered to the energy is very small the Delay convention is observed, however if both energies are comparable the Maxwell convention is observed.
- In Nuclear Physics both conventions should be used simultaneously.

Catastrophe theory and IBM

- The critical point of maximun degeneracy is $\beta = 0$; this point is always critical.
- If one makes an expanssion of E around $\beta = 0$;

$$\begin{aligned} E &= \frac{N(N-1)u_0}{2} + N(N-1)((a_3 - u_0 + \tilde{\varepsilon}/N)\beta^2 + \\ &+ a_2\beta^3 + (a_1 - 2a_3 + 3u_0/2 - \tilde{\varepsilon})\beta^4)) + \ldots \end{aligned}$$

- Impossing $\frac{\partial^2 E}{\partial \beta^2} = 0$ and $\frac{\partial^3 E}{\partial \beta^3} = 0$ at $\beta = 0$ one gets two equations for the parameters of the Hamiltonian.
- Impossing the extra condition $\frac{\partial^4 E}{\partial \beta^4} = 0$ at $\beta = 0$,

  * $a_1 - 2a_3 + 3u_0/2 - \tilde{\varepsilon} = 0$

  the energy becomes a constant; $E = \tilde{\varepsilon}N + a_1 N(N-1)$.
- **The number of essential parameter will be two**:

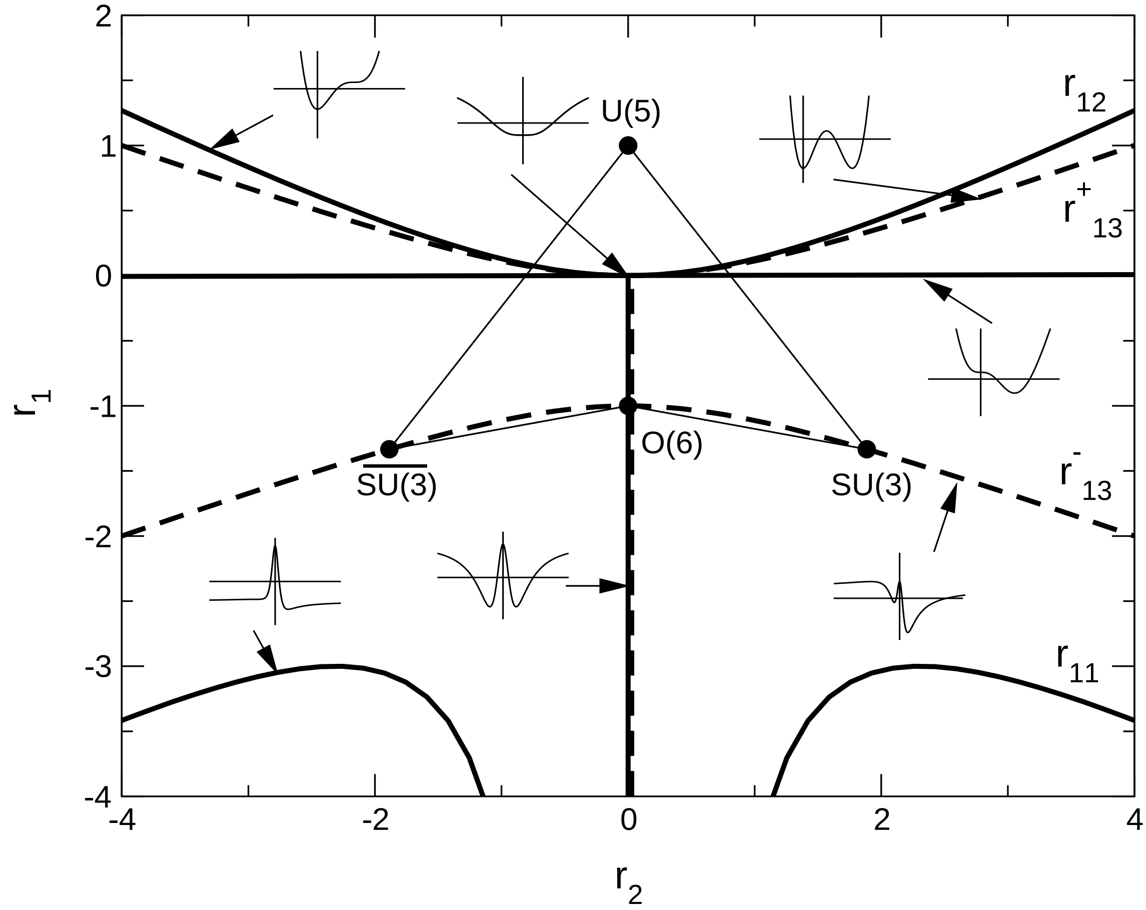
$$r_1 = \frac{a_3 - u_0 + \tilde{\varepsilon}/(N-1)}{2a_1 + \tilde{\varepsilon}/(N-1) - a_3},$$

$$r_2 = -\frac{2a_2}{2a_1 + \tilde{\varepsilon}/(N-1) - a_3}.$$

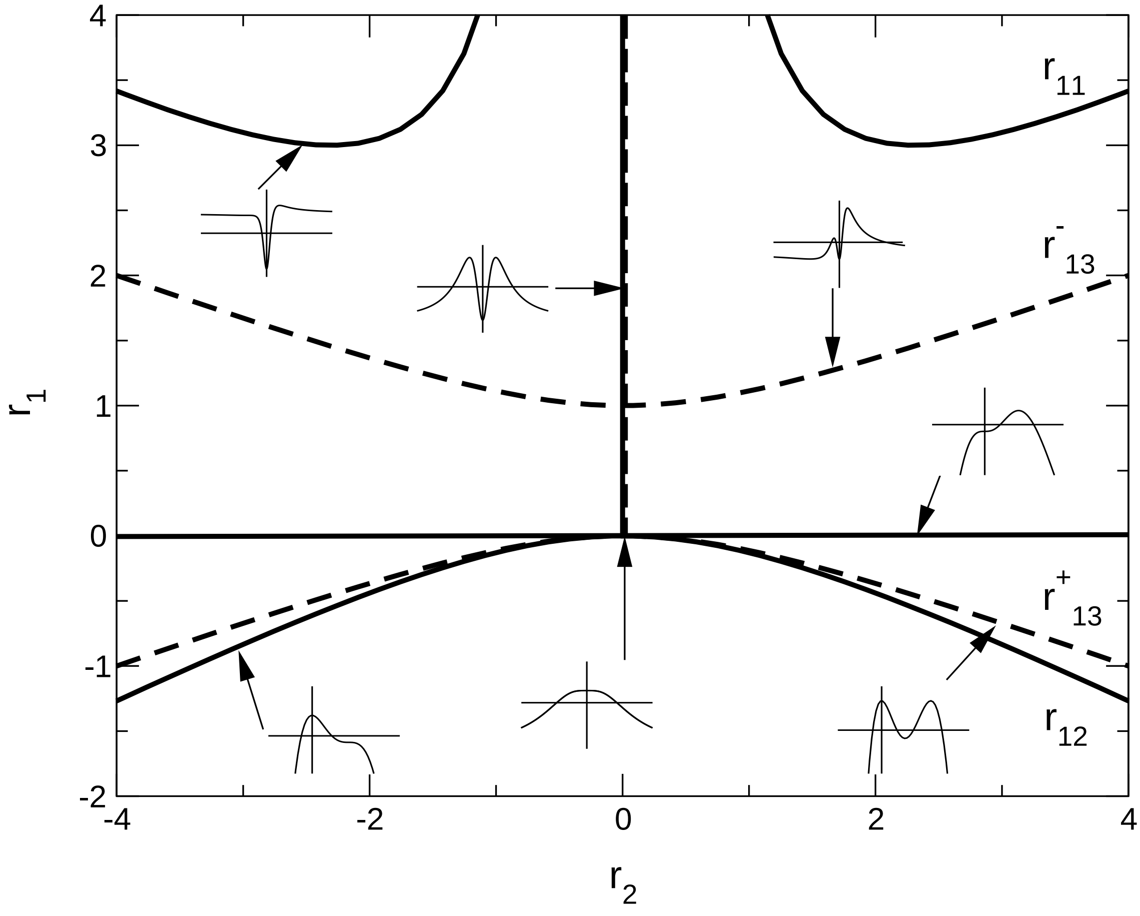
Catastrophe theory and IBM II

- The catastrophe of the IBM is β^4 ("germ") and is called A_{+3} or *cusp* although depending on the sign of the scale can become $-\beta^4$, called A_{-3} or *dual cusp*.

Separatrix of the IBM: positive energy scale



Separatrix of the IBM: negative energy scale



Application: Sm isotopes

- A single Hamiltonian, except for the single particle energy, is used.
- Parameter of the Hamiltonian in keV:

	Atomic mass							
	146	148	150	152	154	156	158	160
$_{62}$Sm	1427.3	1393.5	1289.3	1210.8	1158.6	1192.5	1312.2	1452.0

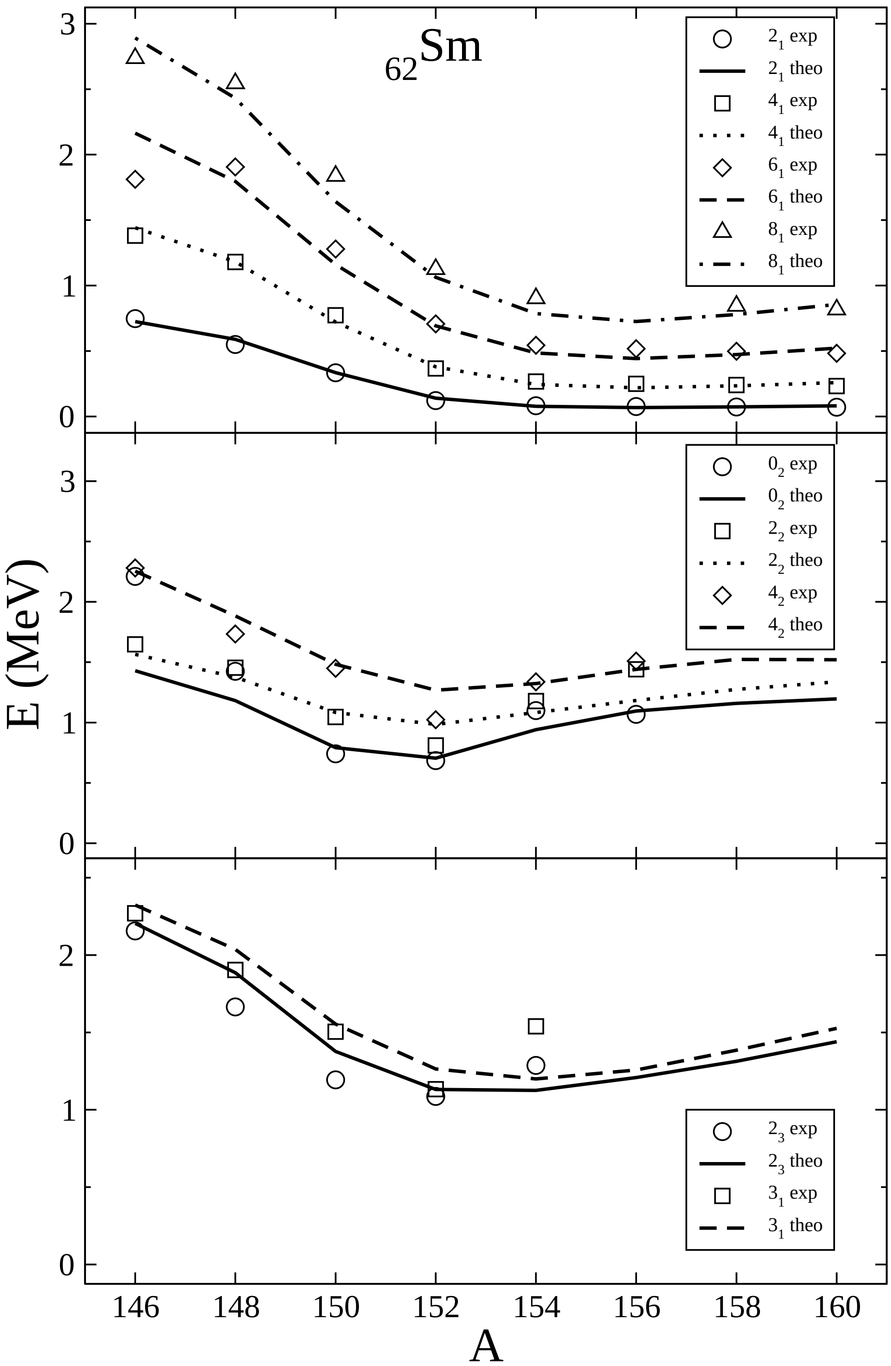
	κ_0	κ_1	κ_2	κ_3	κ_4	χ
$^{146-160}_{62}$Sm	53.209	-11.267	-14.674	-31.769	-131.24	$-\frac{\sqrt{7}}{2}$

	$\mathcal{A}$	$\mathcal{B}$
$^{146-160}_{62}$Sm	18.05	-0.46

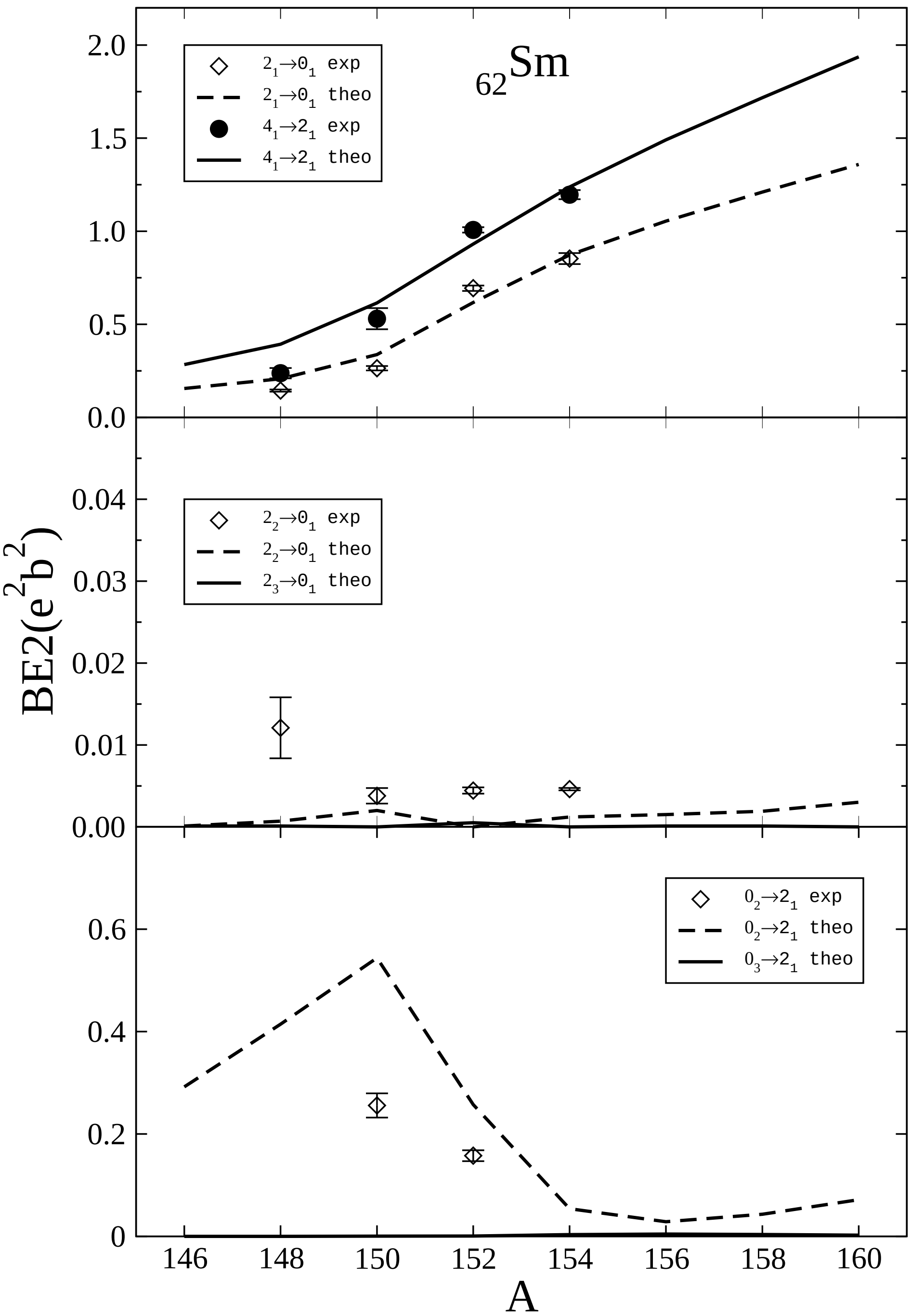
- Single $B(E2)$ transition operator:

$$\hat{T}^{E2}_M = 0.119 \left[(s^\dagger \tilde{d} + d^\dagger \tilde{s})^{(2)}_M - 1.69 (d^\dagger \times \tilde{d})^{(2)}_M \right] eb$$

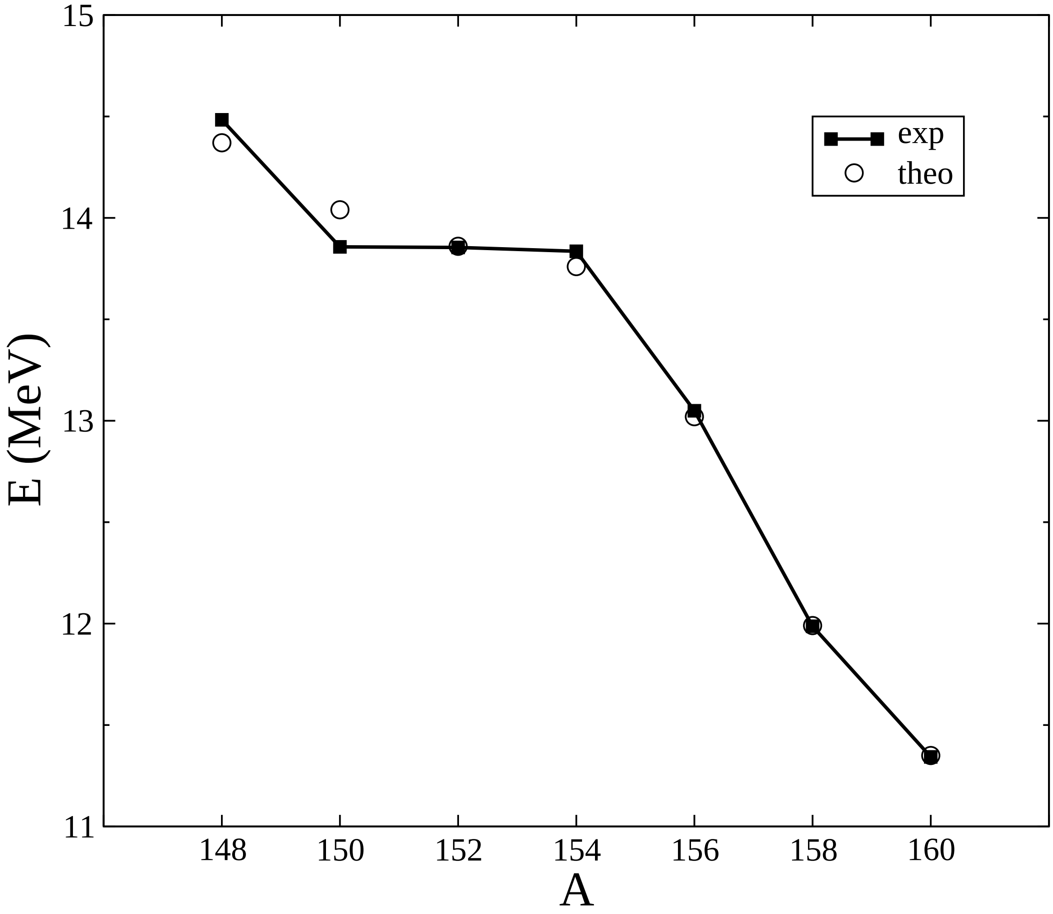
Application: Sm isotopes. Excitation energies



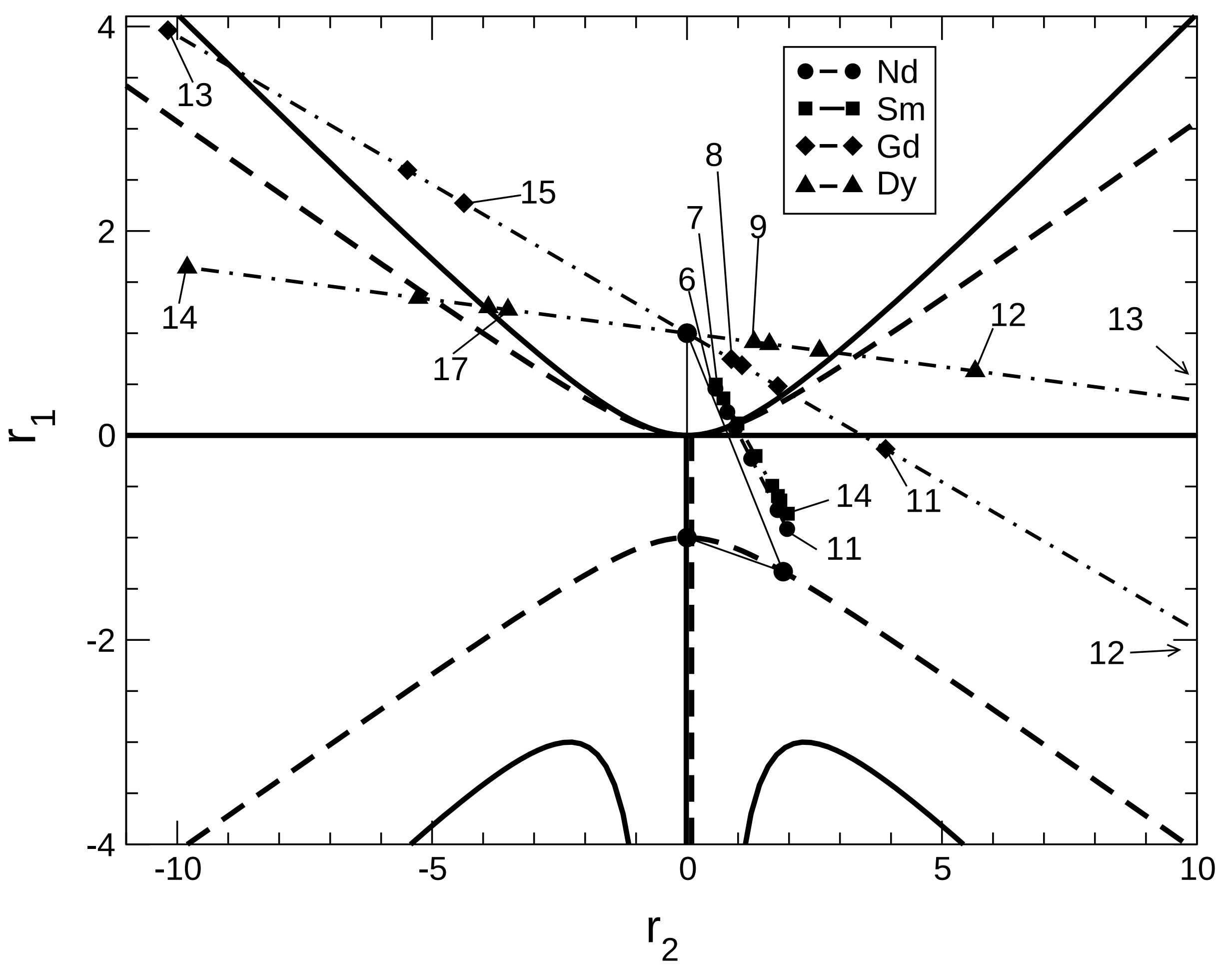
Application: Sm isotopes. Transition rates



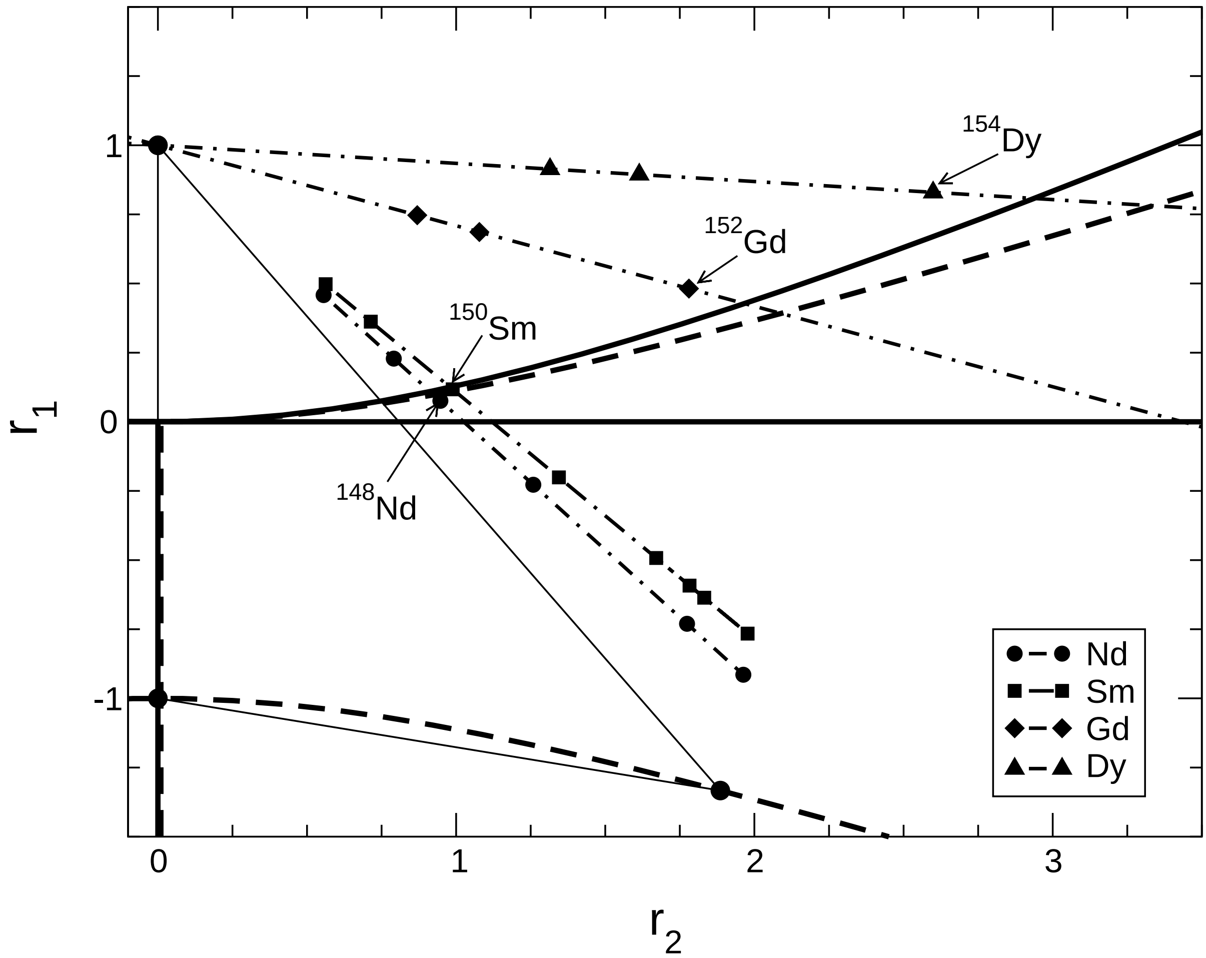
Application: Sm isotopes. S_{2n} values



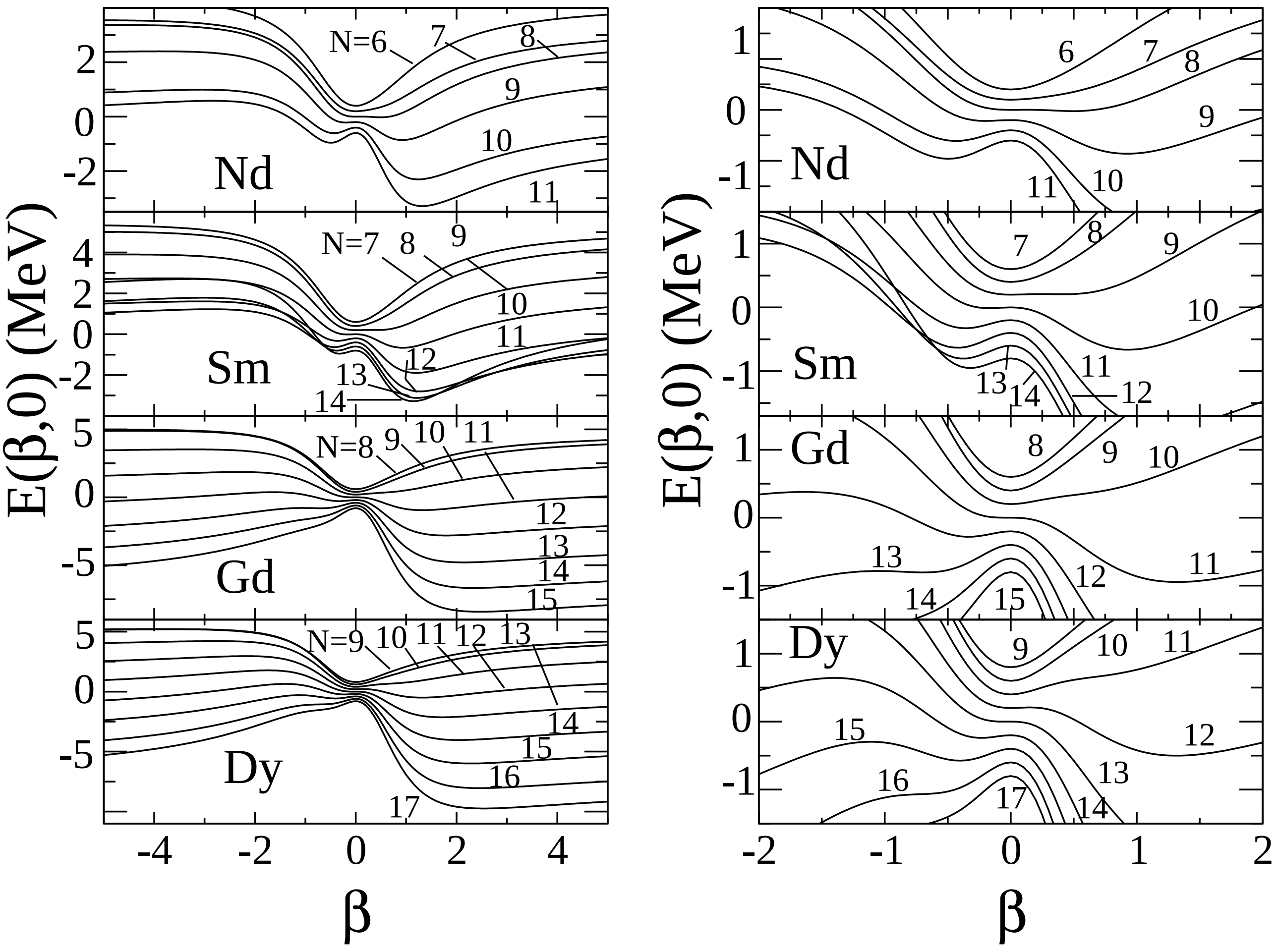
Rare-earths in the separatrix plane



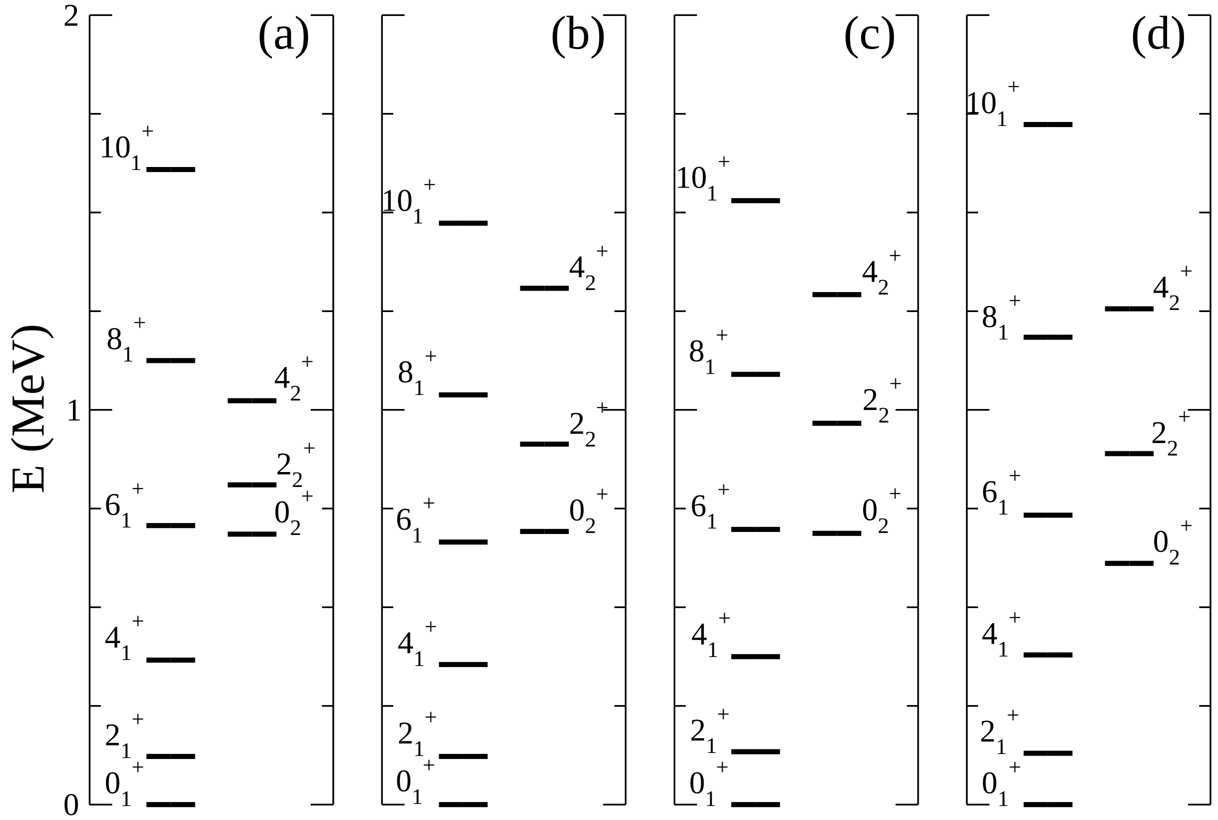
Rare-earths in the separatrix plane (closer view)



Energy surfaces of rare-earths



The ^{152}Sm case: energies



(a) experimental, (b) X(5) symmetry, (c) this work, and (d) using CQF.

The ^{152}Sm case: $B(E2)$

	Exp.	$X(5)$	This work	CQF
$B(E2:2_1^+ \to 0_1^+)$	144	144	128	144
$B(E2:4_1^+ \to 2_1^+)$	209	228	193	216
$B(E2:6_1^+ \to 4_1^+)$	245	285	215	242
$B(E2:8_1^+ \to 6_1^+)$	285	327	218	248
$B(E2:10_1^+ \to 8_1^+)$	320	376	210	242
$B(E2:0_2^+ \to 2_1^+)$	33	91	53	57
$B(E2:2_2^+ \to 4_1^+)$	19	52	14	20
$B(E2:2_2^+ \to 2_1^+)$	6	13	5	11
$B(E2:2_2^+ \to 0_1^+)$	1	3	0	0.1
$B(E2:4_2^+ \to 6_1^+)$	4	40	7	14
$B(E2:4_2^+ \to 4_1^+)$	5	9	2	8
$B(E2:4_2^+ \to 2_1^+)$	1	13	0	0.1

In w.u.

Conclusions and remarks

- There is a deep connection between macroscopic and quantum phase transitions.
- More work should be done for determining the observables that denote the existence of a critical point.
- Catastrophe theory turn to be a very useful tool for determining the dynamical behavior of complex Hamiltonians.
- The critical character of a nucleus depend (partially) on the used Hamiltonian.
- It should be found a way for avoiding the non biunivocal relation between energy spectra and energy surface.