Phase diagram of IBM-2 and catastrophe theory

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The model (I)

- Hamiltonian

$$H = x\left(n_{d_\pi} + n_{d_\nu}\right) - \frac{1-x}{N} Q^{(\chi_\pi,\chi_\nu)} \cdot Q^{(\chi_\pi,\chi_\nu)},$$

$$n_d = \sum_\mu d_\mu^\dagger d_\mu, \quad Q^{(\chi_\pi,\chi_\nu)} = \left(Q_\pi^{\chi_\pi} + Q_\nu^{\chi_\nu}\right)$$

$$Q_\kappa^\chi = \left[d_\kappa^\dagger \tilde{s}_\kappa + s_\kappa^\dagger \tilde{d}_\kappa\right]^2 + \chi_\kappa \left[d_\kappa^\dagger \tilde{d}_\kappa\right]^2$$

- Wave function

$$|N_\pi, N_\nu, \beta_\pi, \gamma_\pi, \beta_\nu, \gamma_\nu, \Omega\rangle = \frac{(\Gamma_\pi^\dagger)^{N_\pi} \hat{R}_3(\Omega) (\Gamma_\nu^\dagger)^{N_\nu}}{\sqrt{N_\pi! N_\nu!}} |0\rangle,$$

$$\Gamma_\kappa^\dagger = \frac{1}{\sqrt{1+\beta_\kappa^2}} \left[s_\kappa^\dagger + \beta_\kappa \cos\gamma_\kappa d_{\kappa 0}^\dagger + \frac{1}{\sqrt{2}} \beta_\kappa \sin\gamma_\kappa (d_{\kappa 2}^\dagger + d_{\kappa -2}^\dagger)\right]$$

The model (II)

- Energy per boson in the thermodynamical limit

$$E(\beta_\pi, \gamma_\pi, \beta_\nu, \gamma_\nu; \chi_\pi, \chi_\nu, x) = \frac{x}{2} \sum_{\kappa=\pi,\nu} \frac{\beta_\kappa^2}{1+\beta_\kappa^2}$$

$$- \quad \frac{1-x}{4} \sum_{\mu=0,\pm 2} \left[\sum_{\kappa=\pi,\nu} Q_\mu^2(\kappa) + 2 Q_\mu(\pi) Q_{-\mu}(\nu) \right]$$

$$Q_0(\kappa) = \frac{\left[2\beta_\kappa \cos\gamma_\kappa - \frac{2}{7}\beta_\kappa^2 \chi_\kappa \cos(2\gamma_\kappa)\right]}{1+\beta_\kappa^2} \,,$$

$$Q_2(\kappa) = \frac{1}{1+\beta_\kappa^2} \left[\sqrt{2}\beta_\kappa \sin\gamma_\kappa + \frac{1}{7}\beta_\kappa^2 \chi_\kappa \sin(2\gamma_\kappa) \right] .$$

The model (III)

- Order parameters

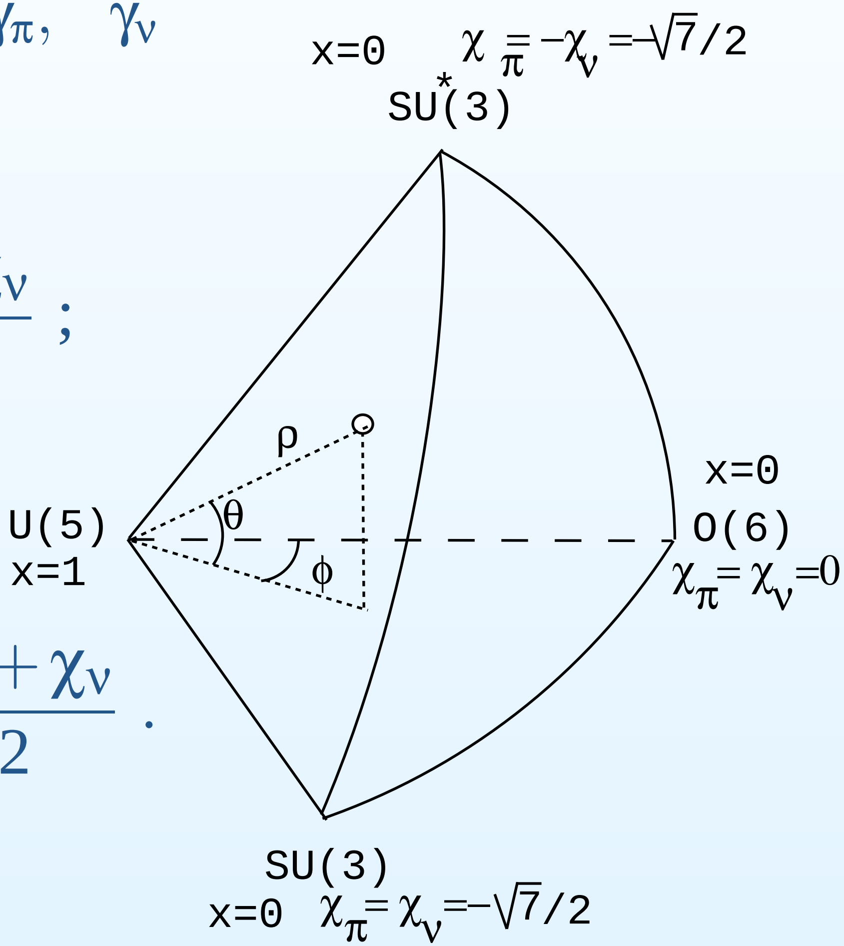
$$\beta_\pi, \quad \beta_\nu, \quad \gamma_\pi, \quad \gamma_\nu$$

- Control parameters

$$\rho = 1 - x \ ; \ \theta = -\frac{\pi}{3} \frac{\chi_\pi - \chi_\nu}{\sqrt{7}} \ ;$$

$$\phi = -\frac{\pi}{3} \frac{\chi_\pi + \chi_\nu}{\sqrt{7}}$$

$$\chi' = -\frac{\chi_\pi - \chi_\nu}{2} \ ; \ \chi = -\frac{\chi_\pi + \chi_\nu}{2} \ .$$



How to get the phase diagram

- Using a Hartree-Bose procedure

$$\sum_{\ell_2 m_2} h^{\kappa}_{\ell_1 m_1,\ell_2 m_2}\eta^{\kappa}_{\ell_2 m_2} = E_\kappa \eta^{\kappa}_{\ell_1 m_1},$$

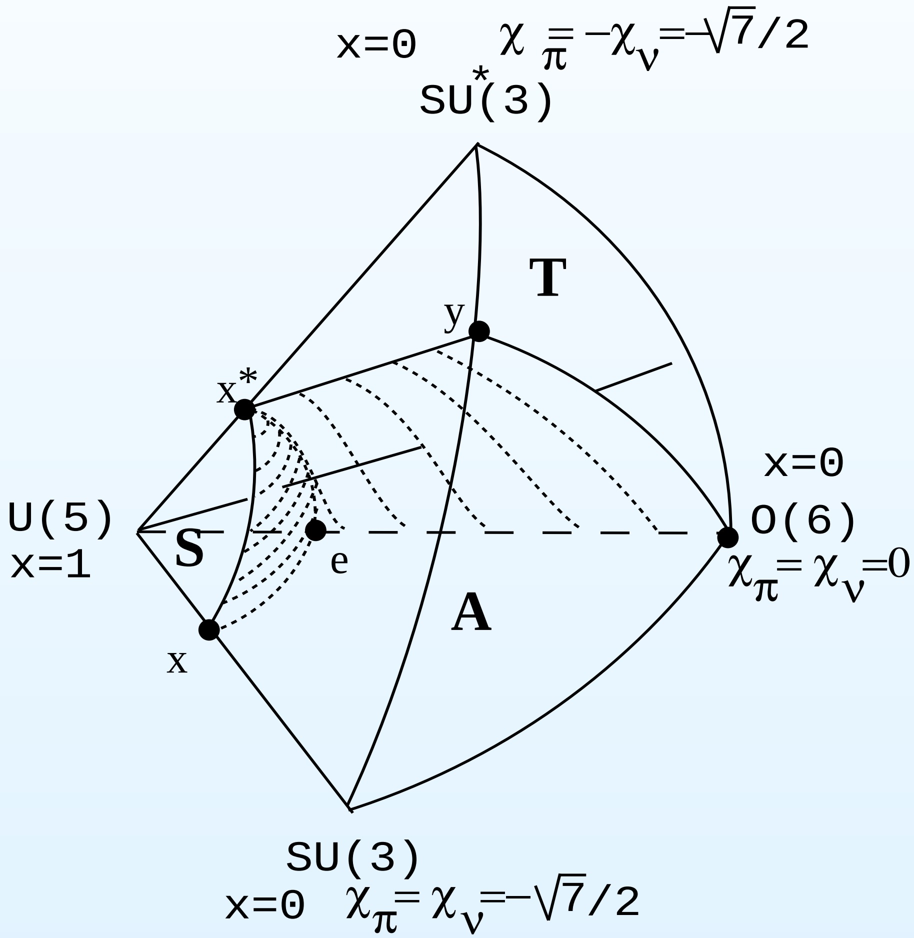
$$\begin{aligned} h^{\kappa}_{\ell_1 m_1,\ell_2 m_2} &= \frac{\varepsilon_{\ell_1\kappa}}{2}\delta_{\ell_1\ell_2}\delta_{m_1 m_2}\sum_{m_1}\eta^{*\kappa}_{\ell_1 m_1}\eta^{\kappa}_{\ell_1 m_1} \\ &+ 2\sum_{\ell_3 m_3 \ell_4 m_4 \kappa_2 \kappa_3 \kappa_4} V_{\ell_1 m_1 \kappa,\ell_3 m_3 \kappa_3,\ell_4 m_4 \kappa_4,\ell_2 m_2 \kappa_2}\frac{\eta^{*\kappa_3}_{\ell_3 m_3}\eta^{\kappa_4}_{\ell_4 m_4}\eta^{\kappa_2}_{\ell_2 m_2}}{4\eta^{\kappa}_{\ell_2 m_2}}. \end{aligned}$$

- Minimizing with *Mathematica*

$$FindMinimum[E(\beta_\pi,\gamma_\pi,\beta_\nu,\gamma_\nu;\chi_\pi,\chi_\nu,x)]$$

The phase diagram

- Three phases: spherical, axially deformed and triaxially deformed.



How to determine the order of a phase transition

- First order phase transition

$$\text{Discontinuity in } \frac{\partial E}{\partial \xi}$$

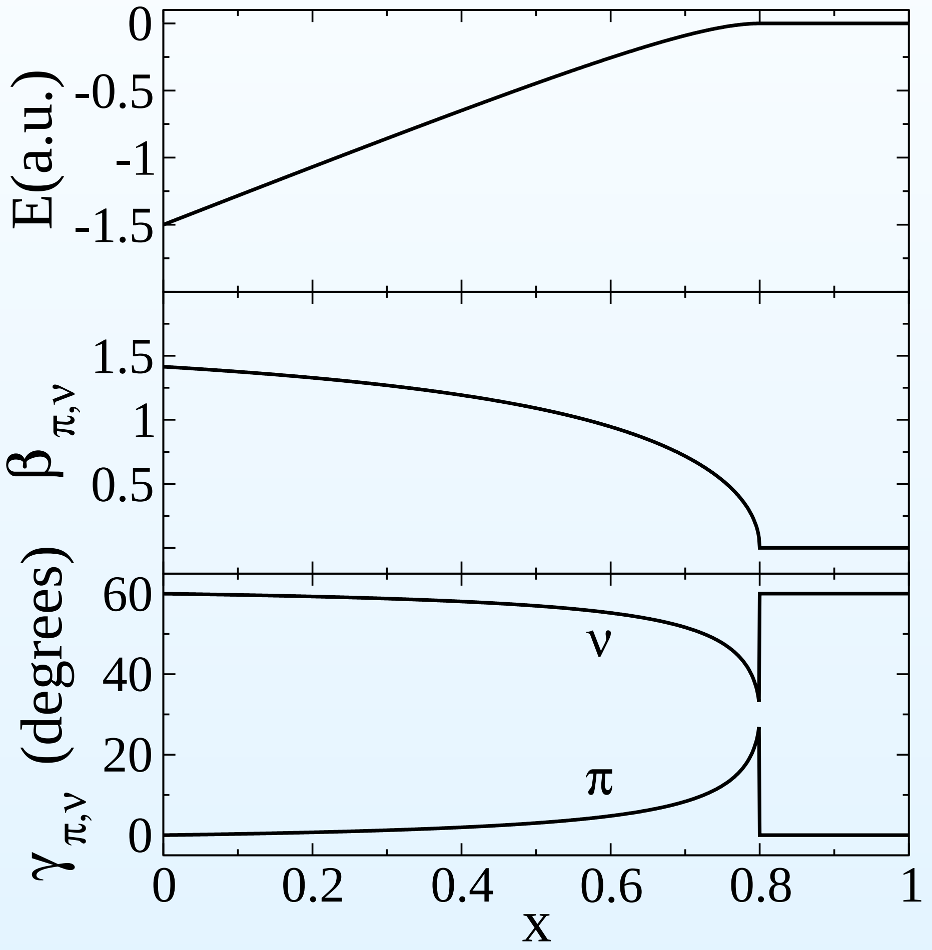
- Second order phase transition

$$\text{Discontinuity in } \frac{\partial^2 E}{\partial \xi^2}$$

- It seems very easy to determine the order of a phase transition!

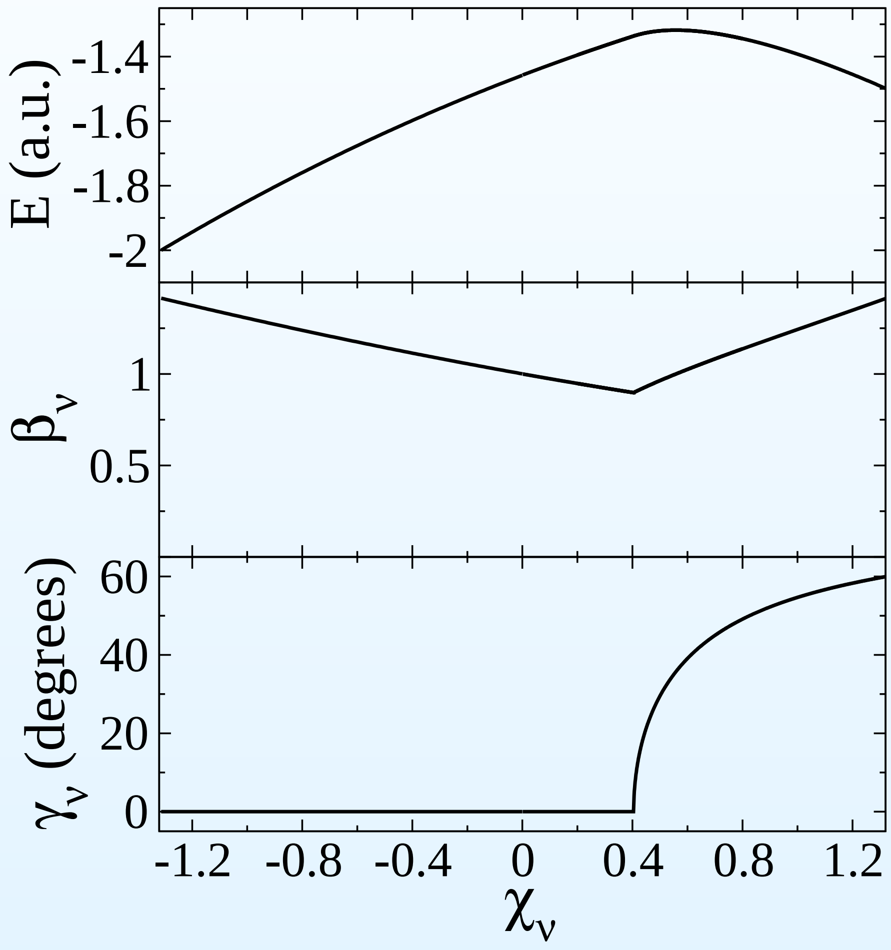
Transition $SU(3)$ to $SU(3)^*$

- Second order phase transition



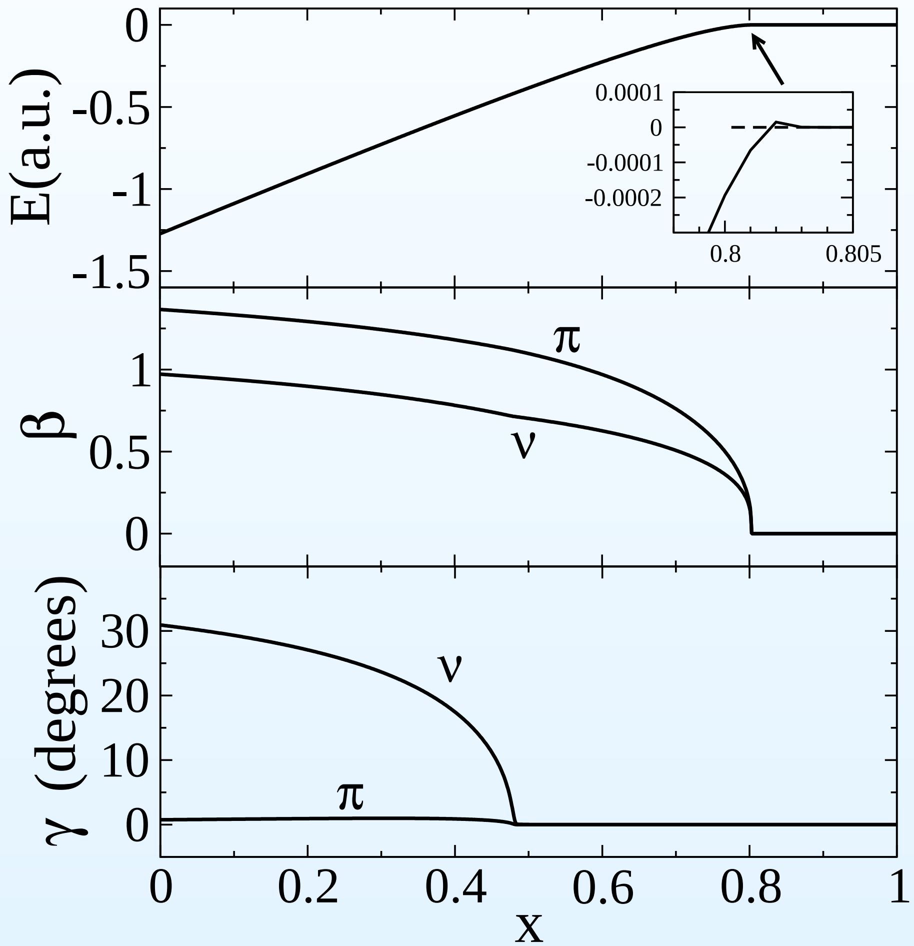
Transition $U(5)$ to $SU(3)^*$

- Second order phase transition



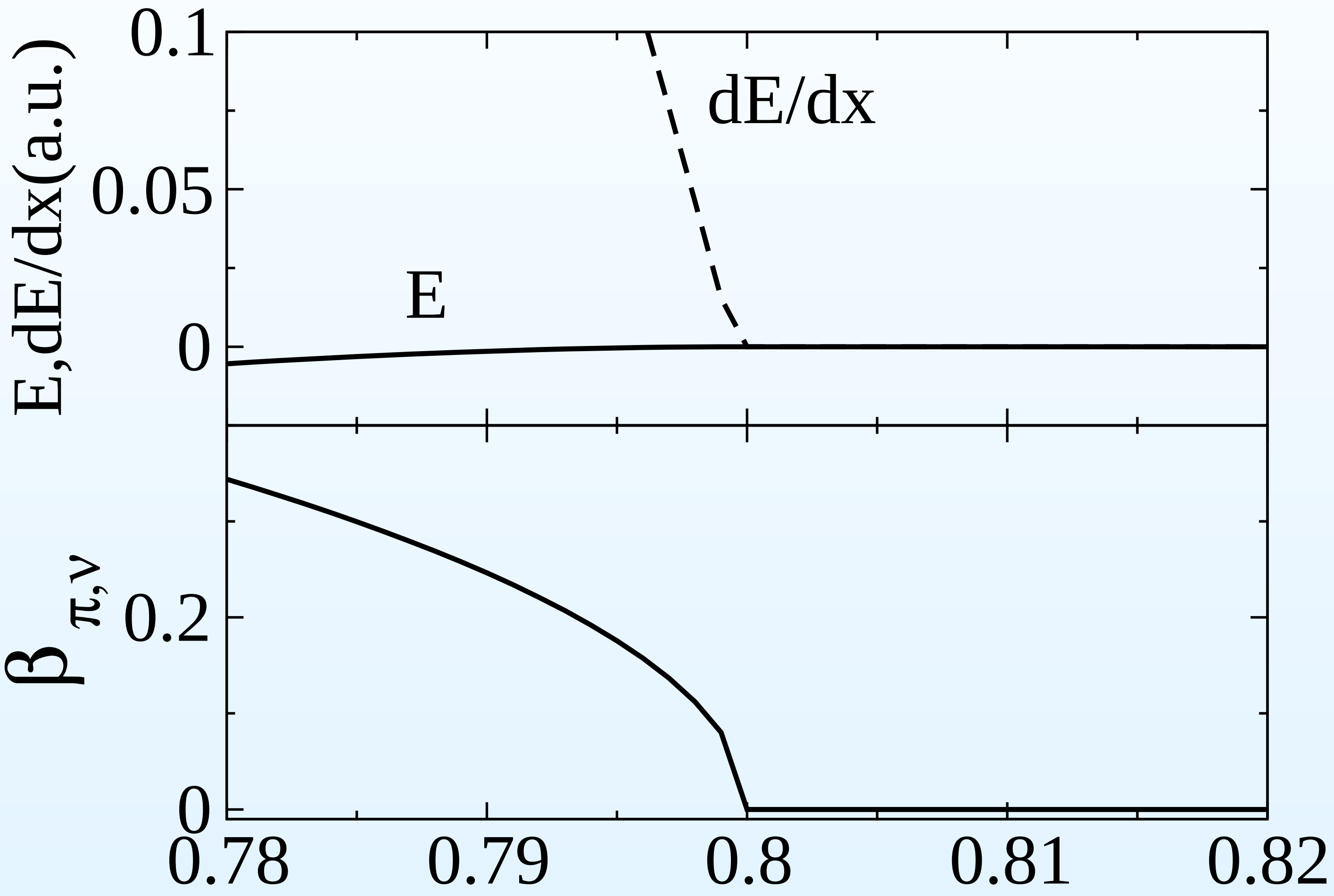
Transition $U(5)$ to triaxial shape

- Second and first order phase transition



Transition $U(5)$ to $SU(3)^*$ in detail

- Second order phase transition



Catastrophe theory

- First reference: René Thom, Stabilité Structurelle et Morphogénèse (1972).
- Catastrophe theory (CT) is framed in the theory of **singularities for differentiable mappings** and in the **theory of bifurcations**, therefore it deals with singularities of smooth real-valued functions and tries to classify such singularities.
- CT attempts to study how the qualitative nature of the solutions of equations depends on the parameters that appear in the equations (Gilmore 1981).
- CT explains how the state of a system can change suddenly under a smooth change in the control variables.

CT program

- Let us assume a system described by a real family of potentials:

$$V(\mathbf{x}, \lambda) \in \Re$$

  where $\mathbf{x} \in \Re^n$ are the state (order) variables and $\lambda \in \Re^r$ are the control parameters.
- In this family one can find three types of points:
  - Regular points: $\nabla V \neq 0$.
  - Morse points (isolated critical points):
    $\nabla V = 0$ and $|\mathcal{H}_{ij}| \neq 0$.
  - Non-Morse points (degenerated critical points):
    $\nabla V = 0$ and $|\mathcal{H}_{ij}| = 0$.

CT program (*Margalef-Roig, et al*)

- Definition of $h(\mathbf{x},\lambda) = V(\mathbf{x}+\mathbf{x^0},\lambda+\lambda^\mathbf{0}) - V(\mathbf{x^0},\lambda^\mathbf{0})$, where $(\mathbf{x^0},\lambda^\mathbf{0})$ correspond to a degenerated critical point.
- Definition of the germ: $g(\mathbf{x}) = h(\mathbf{x},\mathbf{0})$.
- Calculation of the determinacy and the codimension of $g(\mathbf{x})$ through the k-jet of $g(\mathbf{x})$ (truncated Taylor expansion with k term).
- Study the k-transversality of $g(\mathbf{x})$ in order to establish the isomorphism between $h(\mathbf{x},\lambda)$ and a canonical unfolding of $g(\mathbf{x})$.
- Note that it is only possible to prove the existence of an isomorphism but this DOES NOT provides the necessary change of coordinates.

What people do with CT

- Taylor expansion around a degenerated critical point. If possible, around the most degenerated critical point.
- Arrangement of the control parameters in order to annihilate the lower order terms in the Taylor expansion.
- The term that survives after the arrangement is the germ.
- The number of canceled terms corresponds to the number of essential parameters (equivalent to the codimension ...).

What people do with CT

- Substitution of $V(\mathbf{x},\lambda)$ by a truncated Taylor expansion $V(\mathbf{x},\lambda)_{pol}$, being the germ the higher order term (the order of the Taylor expansion is the determinacy...).
- Establish the mapping between $V(\mathbf{x},\lambda)_{pol}$ and a canonical form through a nonlinear change of variables (it should be calculated the transversality...).
- Work out $V(\mathbf{x},\lambda)_{pol}$ for getting the bifurcation and the Maxwell set.

Relevant theorems

- Implicit function theorem for regular points.

$$V(\mathbf{x}) \longrightarrow \mathbf{x}$$

- Morse lemma for isolated critical points.

$$V(\mathbf{x}) \longrightarrow \mathbf{x}^2$$

- Thom theorem for degenerated critical points.

$$V(\mathbf{x}) \longrightarrow g(\mathbf{x}) + \text{unfolding}$$

- Splitting lemma for potential with several variables.

$$V(\mathbf{x}) \longrightarrow g(\mathbf{x}) + \text{unfolding} + \mathbf{y}^2 - \mathbf{z}^2$$

Misunderstandings on Catastrophe theory

- In many cases, CT cannot provide quantitative results and indeed needs the help of numerical results to start with the CT program.
  About this Thom said: "...as soon as it became clear that the theory did not permit quantitative prediction, all good minds ... decided it was of no value..."
- CT does not consist in getting the bifurcation and the Maxwell sets.
- The interest of CT focus on the clasification of germs of a family of potentials and on giving universal unfoldings, *i.e.* general perturbations.

Region $U(5)-O(6)-SU^*(3)$ (I)

- Restrictions:

$$\chi_\pi = -\chi_\nu = \chi$$
$$\beta_\pi = \beta_\nu = \beta$$
$$\gamma_\pi = \pi/3 - \gamma_\nu = \gamma$$

- Energy surface:

$$\begin{aligned} E(\beta,\gamma,\chi,x) &= \frac{-1}{14\,(1+\beta^2)^2}\Big(\beta^2\,\big(42x-28-14\beta^2+14\,(1-x)\,\beta^2+2\,(1-x)\,\beta^2\chi^2 \\ -\ & 2\sqrt{14}\,(1-x)\,\beta\chi\,\cos(\gamma)+14\,(1-x)\,\cos(2\gamma)-4\sqrt{14}\,(1-x)\,\beta\chi\,\cos(3\gamma) \\ +\ & (1-x)\,\beta^2\chi^2\,\cos(4\gamma)+2\sqrt{42}\,(1-x)\,\beta\chi\,\sin(\gamma)+14\sqrt{3}\,(1-x)\,\sin(2\gamma) \\ -\ & \sqrt{3}\,(1-x)\,\beta^2\chi^2\,\sin(4\gamma)\big)\Big) \end{aligned}$$

Region $U(5)-O(6)-SU^*(3)$ (II)

- Taylor expansion around $\beta=0$ and $\gamma=\pi/3(\gamma-\pi/6\rightarrow\gamma)$:

$$
\begin{aligned}
E \sim & \left((5x-4)+4(1-x)\gamma^2-\frac{4(1-x)\gamma^4}{3}+\Theta(\gamma)^5\right)\beta^2 \\
+ & \left(-8\sqrt{\frac{2}{7}}(1-x)\chi\gamma+\frac{4\sqrt{14}(1-x)\chi\gamma^3}{3}+\Theta(\gamma)^5\right)\beta^3 \\
+ & \left((8-9x)-\frac{8(1-x)\left(7+\chi^2\right)\gamma^2}{7}+\frac{8(1-x)\left(7+4\chi^2\right)\gamma^4}{21}+\Theta(\gamma)^5\right)\beta^4+\Theta(\beta)^5
\end{aligned}
$$

- Reduction to a polynomial

$$
E_{pol}=(8-9x)\beta^4+\beta^2\left(5x-4+4(1-x)\gamma^2\right)-8\sqrt{\frac{2}{7}}(1-x)\beta^3\gamma\chi
$$

- Codimension, determinacy and transversality should be calculated!

Region $U(5)-O(6)-SU^*(3)$ (III)

- Critical points of E_{pol}:

$$\gamma=-\frac{\sqrt{5x-4}\chi}{\sqrt{63x-56+8(1-x)\chi^2}},\ \beta=-\frac{\sqrt{\frac{7}{2}}\sqrt{5x-4}}{\sqrt{63x-56+8(1-x)\chi^2}},$$

$$\gamma=\frac{\sqrt{5x-4}\chi}{\sqrt{63x-56+8(1-x)\chi^2}},\ \beta=\frac{\sqrt{\frac{7}{2}}\sqrt{5x-4}}{\sqrt{63x-56+8(1-x)\chi^2}},$$

$$\beta=0,$$

$$\beta=0.$$

- No coexistence region $\rightarrow$ second order phase transition.

Region $X(5) - E(5) - X^*(5)$ (I)

- Restrictions: $\gamma_\pi = \gamma_\nu = 0$
- Energy surface:

$$E(\beta_\pi, \beta_\nu, \chi_\pi, \chi_\nu, x) = \frac{x}{2}\left(\frac{{\beta_\nu}^2}{1+{\beta_\nu}^2} + \frac{{\beta_\pi}^2}{1+{\beta_\pi}^2}\right)$$

$$- \quad \frac{1-x}{196\left(1+{\beta_\nu}^2\right)^2\left(1+{\beta_\pi}^2\right)^2}\left(-14\beta_\nu\left(1+{\beta_\pi}^2\right) + \beta_\pi\left(-14+\sqrt{14}\beta_\pi\chi_\pi\right)\right.$$

$$\left. + \quad {\beta_\nu}^2\left(-14\beta_\pi + \sqrt{14}\chi_\nu + \sqrt{14}{\beta_\pi}^2\left(\chi_\nu+\chi_\pi\right)\right)^2\right)$$

Region $X(5) - E(5) - X^*(5)$ (II)

- Hessian matrix in $\beta_\pi = \beta_\nu = 0$:

$$\mathcal{H} = \begin{pmatrix} 3x-2 & 2x-2 \\ 2x-2 & 3x-2 \end{pmatrix}$$

- Eigenvalues and eigenvectors:

$$\begin{aligned} \lambda_1 &= 5x-4, & \beta_1 &= \tfrac{1}{2}(\beta_\pi + \beta_\nu) \\ \lambda_2 &= x, & \beta_2 &= \tfrac{1}{2}(-\beta_\pi + \beta_\nu) \end{aligned}$$

- β_1 is the essential and β_2 is the unessential variable.

Region $X(5)-E(5)-X^*(5)$ (III)

- Reduction of the energy to a polynomial:

$$E_{pol} = x\beta_2^2 + (5x-4)\,\beta_1{}^2$$
$$+ \quad 4\sqrt{\frac{2}{7}}(1-x)\chi\beta_1{}^3 + \left(9x - 8 - \frac{2(1-x)\chi^2}{7}\right)\beta_1{}^4,$$

- Because of the cubic terms there exists a region where two minima coexist $\rightarrow$ first order phase transition.
- Codimension, determinacy and transversality should be calculated!

Summary and conclusions

- We have presented a phase diagram for IBM-2 where a spherical, an axially deformed and a triaxial shape region can distinguish.
- We have established numerically the order of the phase transitions in the IBM-2 phase diagram.
- The ambiguity of the purely numerical results indicates that CT is a valuable tool for this problem.
- We have presented the main features of CT.
- We have established analytically (using CT) the order of the phase transitions in the IBM-2 phase diagram.