Quantum phase transitions in simple two-level systems and Catastrophe Theory

José-Enrique García-Ramos

Departamento de Física Aplicada, Universidad de Huelva, Huelva, Spain
enrique.ramos@dfaie.uhu.es

Index

- Parte I: Phase transitions
  - The Lipkin Model
  - Mean field: an approach to the quantum problem
  - Phase transitions: a) Classic transitions, Landau theory. b) Quantum Phase Transitions
  - Phase diagram of the Lipkin model
- Parte II: Catastrophe Theory
  - Motivation: the Zeeman catastrophe machine
  - Definitions
  - Relevant theorems
  - “The mathematical way.”
  - “The physical way.”
  - Application to the Lipkin model
  - Misunderstandings of CT

Macroscopic/Classical Phase Transitions

Definition of phase and phase transition

- Phase: state of matter that is uniform throughout, not only in chemical composition but also in physical properties.
- Phase Transition: abrupt change in one or more properties of the system.

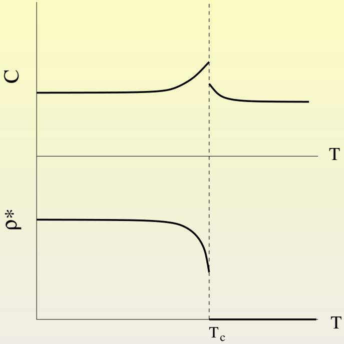
The phase of the system

- Most stable phase of matter is the one with the lowest thermodynamical potential Φ. This is a function of some parameters that are allowed to change (F(T,V), F(T,B); G(T,p), G(T,M)).
- Φ is analogous to the potential energy, V(x), of a particle in a one dimensional well. The system looks for the minimum energy going into the bottom of the potential.

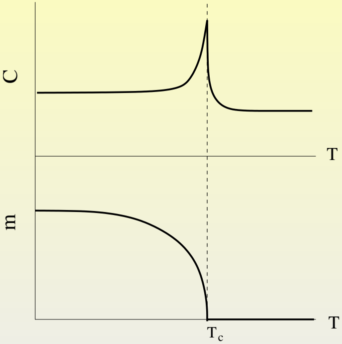
Macroscopic/Classical Phase Transitions

- Control parameter: variable that affects the system, it can be changed smoothly and "arbitrarily".
- Order parameter: observable that changes as a function of the control parameter and that defines the "phase" of the system.
- Ordered and disordered phases correspond to a value of the order 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: first, continuous (second order).

Examples of Macroscopic Phase Transitions

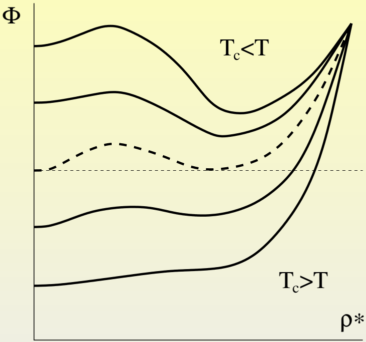


First order phase transition.
Liquid-gas

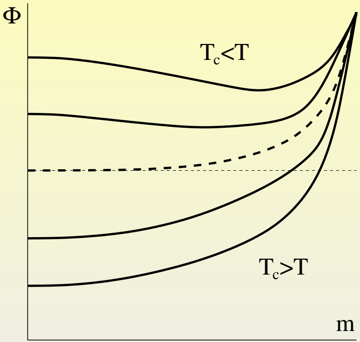


Second order phase transition.
Paramagnetic-ferromagnetic

What is happening at the phase transition point?



First order phase transition

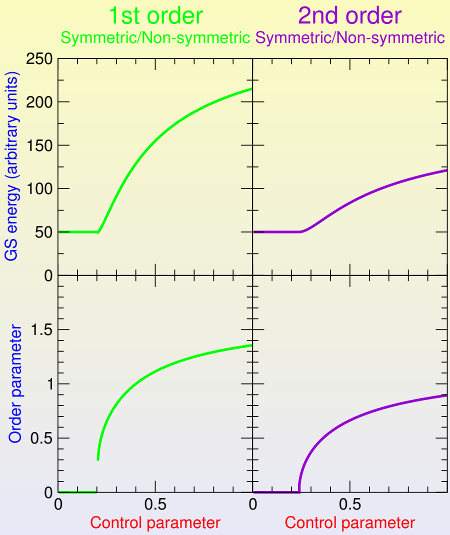


Second order phase transition

Φ in the Landau theory

$$\Phi = A(T, ...)\beta^4 + B(T, ...)\beta^2 + C(T, ...)\beta$$

The variation of the order parameter



Quantum Phase Transitions

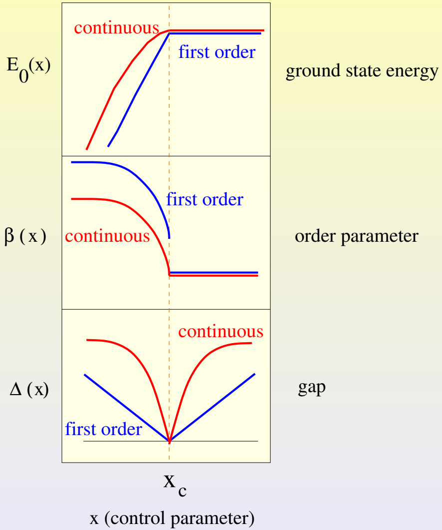
QPT occurs at some critical value, x_c, of the control parameter x that controls an interaction strength in the system's Hamiltonian $H(x)$. It is implicit a zero temperature.

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

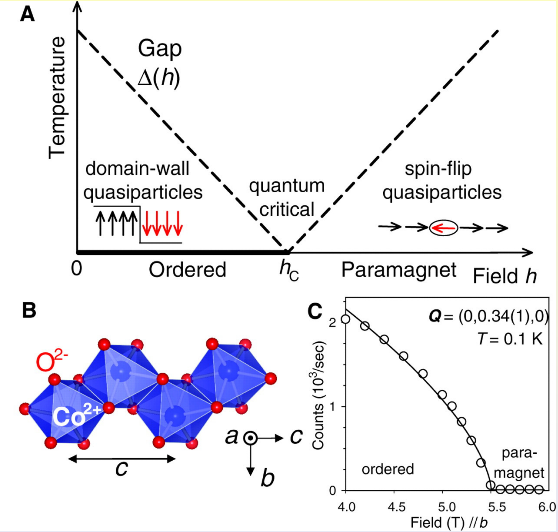
At the critical point:

- The ground state energy is nonanalytic.
- The gap Δ between the first excited state and the ground state vanishes.

Quantum Phase Transitions



QPT: experimental example for an Ising chain



R. Coldea et al., Science 327, 177-180 (2010).

QPT: Lipkin model

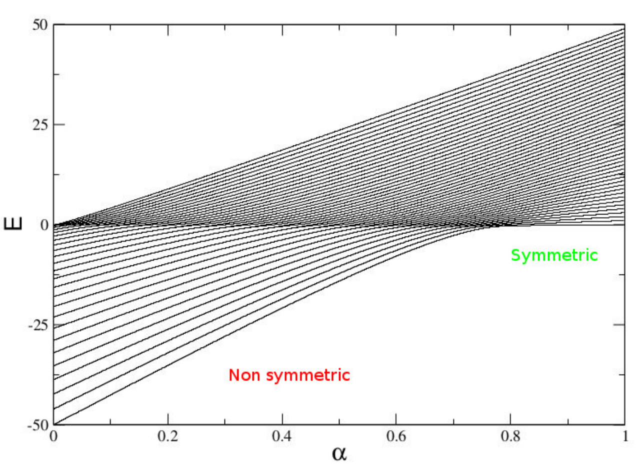


Figure: Energy spectrum (per boson) for a Lipkin model with $N = 50$, $\alpha = x$ and $y = 0$.

QPT: Lipkin model

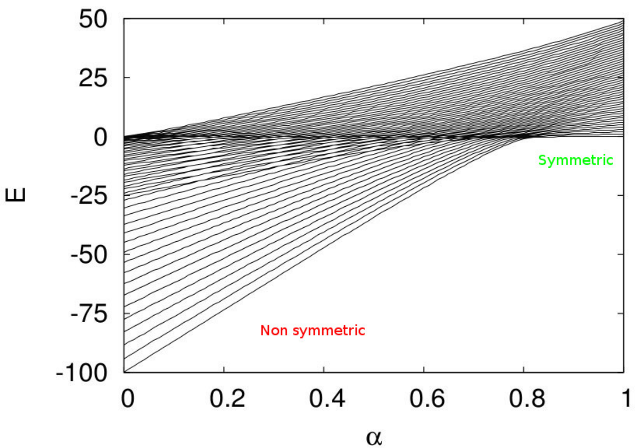


Figure: Energy spectrum (per boson) for a Lipkin model with $N = 50$, $\alpha = x$ and $y = 1/\sqrt{2}$.

Phase diagram of the Lipkin model

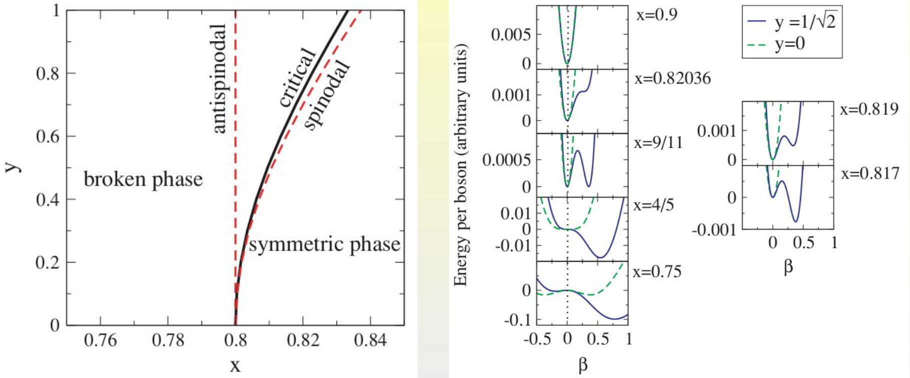


Figure: Phase diagram and energy curves for selected values of the control parameters.

QPT: Lipkin model

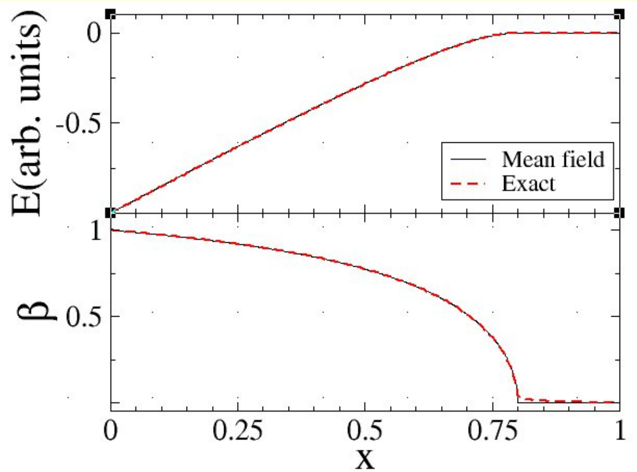


Figure: Comparison of exact ($N = 1000$) and mean-field results for $y = 0$ as a function of x.

QPT: Lipkin model

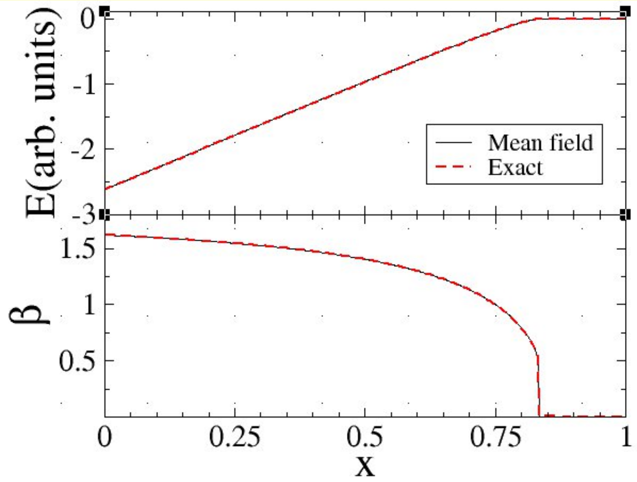


Figure: Comparison of exact ($N = 1000$) and mean-field results for $y = 1$ as a function of x.

The Zeeman Catastrophe machine

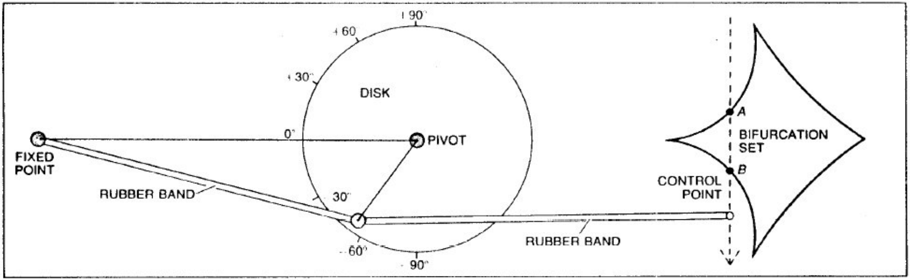


Figure: Schematic view of the Zeeman Catastrophe machine.

Zeeman machine: energy curves

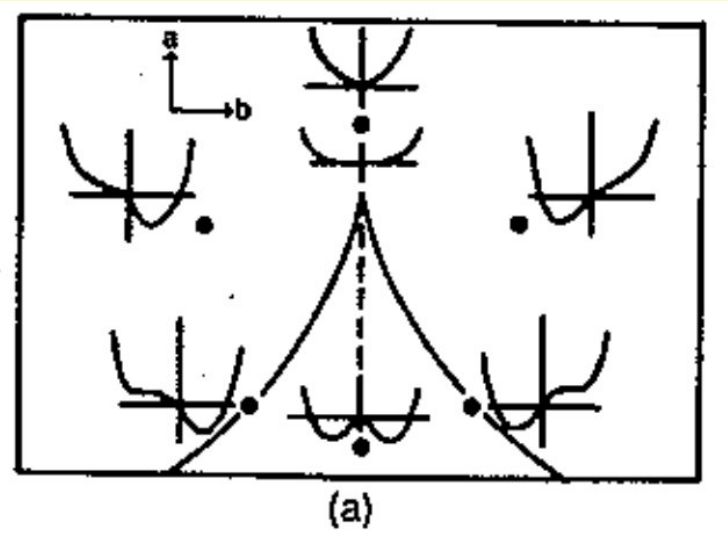
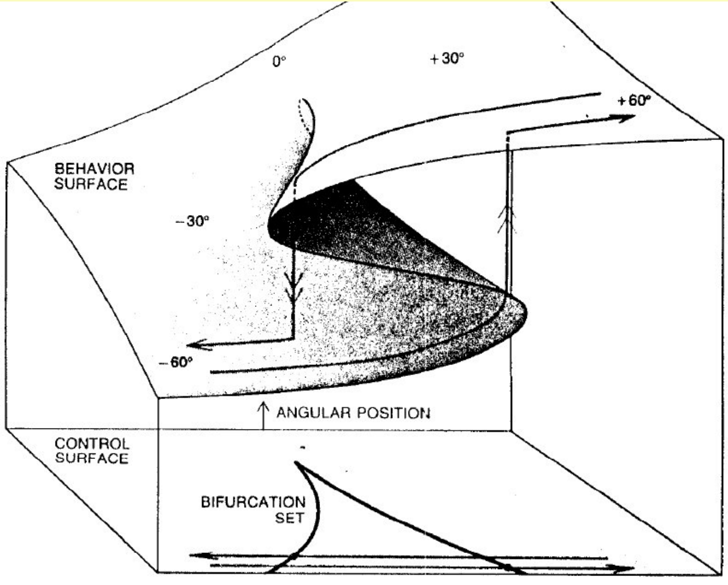


Figure: Parameter space and energy curves

Cusp diagram



What is for Catastrophe Theory?

Some notes

- 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.

Definitions and background

- Structural stability.
- Codimension: number of essential parameters.
- Corank: *essentia*l and *non-essential* variables.
- k-jet/k-determinacy
- Catastrophe germ.
- Universal unfolding.

Relevant theorems

- Implicit function theorem for regular points.

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

- Morse lemma for isolated critical points.

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

- Thom theorem for degenerated critical points.

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

- Splitting lemma for potential with several variables.

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

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 $|\mathcal{H}_{ij}| = 0$.

The mathematical way (*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.

The physical way

- 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.

The seventh elementary catastrophe

Catastrophe germs and unfolding

- Fold, A_2: $x^3 + a_1 x$
- Cusp, $A_{\pm 3}$: $\pm x^4 + a_1 x + a_2 x^2$
- Swallowtail, A_4: $x^5 + a_1 x + a_2 x^2 + a_3 x^3$
- Butterly, $A_{\pm 5}$: $x^6 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4$
- Elliptical umbilic, D_{-4}: $x^2 y - y^3 + a_1 x + a_2 y + a_3 y^2$
- Hyperbolic umbilic, D_{+4}: $x^2 y + y^3 + a_1 x + a_2 y + a_3 y^2$
- Parabolic umbilic, D_{+5}: $x^2 y + y^4 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2$

Application to the Lipkin Model

- Lipkin energy surface:

$$\frac{E(x,y,\beta)}{N} = x\frac{\beta^2}{1+\beta^2} - \frac{1-x}{4}\left(\frac{1}{(1+\beta^2)^2}(2\,\beta + y\,\beta^2)^2\right)$$

- Taylor expansion:

$$\begin{aligned}\frac{E(x,y,\beta)}{N} &= (5x-4)\beta^2 + 4(x-1)y\beta^3 \\ &+ \left(8-9x+y^2(x-1)\right)\beta^4 + \Theta(\beta^5)\end{aligned}$$

- Why do we stop at β^4?

Application to the Lipkin Model

Simple conclusion, but not trivial

- $y = 0$ implies second order phase transition.
- $y \neq 0$ implies first order phase transition.
- This is this while β^4 coefficient remains positive.

Phase diagram of the Lipkin model

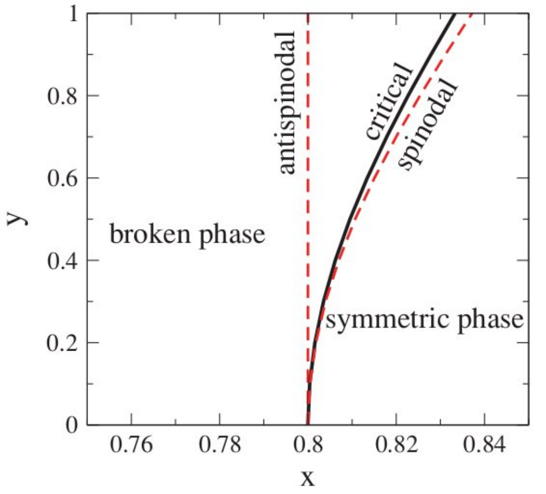


Figure: Phase diagram.

Two variables

- Energy surface:

$$
\begin{aligned}
& E(\beta_\pi, \beta_\nu, \chi_\pi, \chi_\nu, x) = \frac{x}{2} \left(\frac{{\beta_\nu}^2}{1+{\beta_\nu}^2} + \frac{{\beta_\pi}^2}{1+{\beta_\pi}^2} \right) \\
- \quad & \frac{1-x}{196\,(1+{\beta_\nu}^2)^2\,(1+{\beta_\pi}^2)^2} \left(-14\,\beta_\nu\,\left(1+{\beta_\pi}^2\right) + \beta_\pi\,\left(-14+\sqrt{14}\,\beta_\pi\,\chi_\pi\right) \right. \\
+ \quad & \left. {\beta_\nu}^2\,\left(-14\,\beta_\pi + \sqrt{14}\,\chi_\nu + \sqrt{14}\,{\beta_\pi}^2\,(\chi_\nu+\chi_\pi)\right)^2 \right)
\end{aligned}
$$

Two variables

- 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:

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

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

Two variables

- Reduction of the energy to a polynomial:

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

- Because of the cubic terms there exists a region where two minima coexist → first order phase transition.

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.
- A numerical calculation is always very valuable.

References

- R. Thom, Structural Stability and Morphogenesis, Benjamin, Reading, 1975.
- T. Poston, I.N. Stewart, Catastrophe Theory and Its Applications, Pitman, London, 1978.
- R. Gilmore, Catastrophe Theory for Scientists and Engineers, Wiley, New York, 1981.
- P.T. Saunders, An introduction to Catastrophe Theory, Cambridge University Press, 1980.