A physicist lost in the wonderland of complex systems

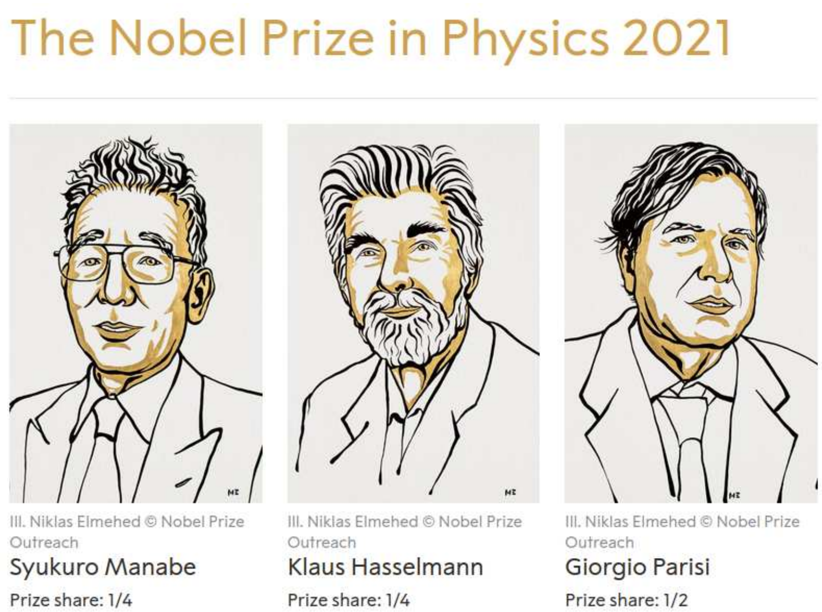
Alessandro Torcini

alessandro.torcini@cyu.fr

LPTM

CY Cergy Paris Université

Nobel Prize in Physics 2021



The Nobel Prize in Physics 2021 was awarded "for groundbreaking contributions to our understanding of complex systems" with one half jointly to Syukuro Manabe and Klaus Hasselmann "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming" and the other half to Giorgio Parisi "for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales."

The ceremony will take place on 10th December, 2021

Scientific Motivations

Scientific Background on the Nobel Prize in Physics 2021

"FOR GROUNDBREAKING CONTRIBUTIONS TO OUR UNDERSTANDING OF COMPLEX PHYSICAL SYSTEMS"

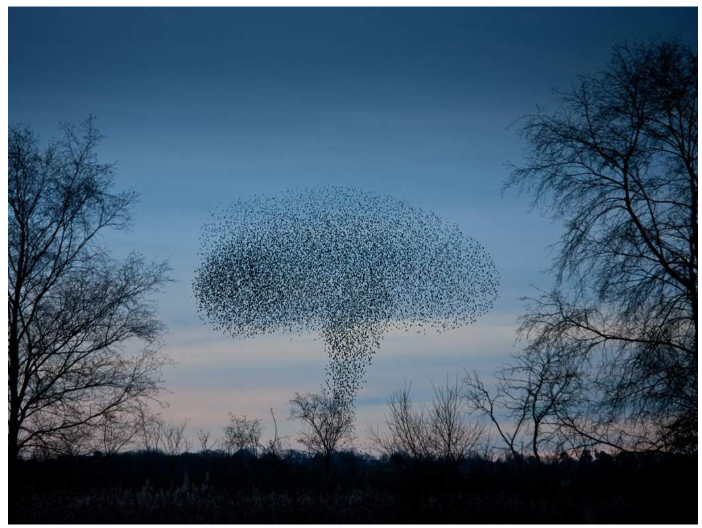
The Nobel Committee for Physics

This year's Nobel Prize in Physics focuses upon the complexity of physical systems, from the largest scales experienced by humans, such as Earth's climate, down to the microscopic structure and dynamics of mysterious and yet commonplace materials, such as glass . . .
A central emphasis is on the physical reality that the variability in the basic processes, from climate dynamics to frustrated materials, leads to the emergence of multiple length and time scales . . .

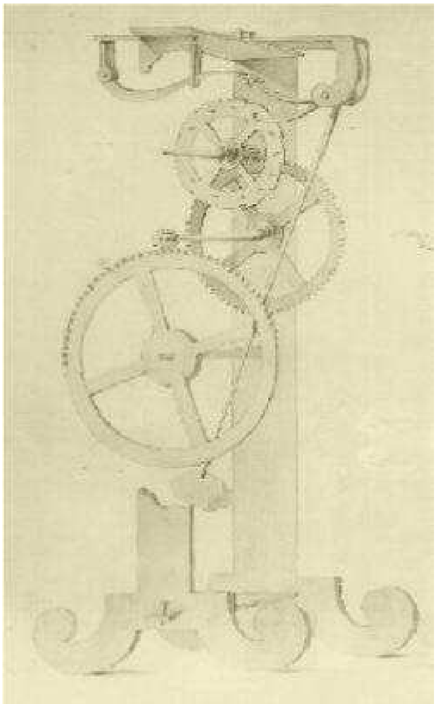
What is it a Complex System ?

Two different view of a complex system :

- A quite simple system that can give rise to a very complex behaviour : e.g. a pendulum
- A system made of a large number of interacting elements, so that the collective behaviour of those elements goes far beyond the simple sum of the individual behaviours.
  - schools of fishes
  - swarm of birds FILM



A clock



Galileo Gailei was the first who had the idea to exploit the regularity of pendulum oscillations to realize a clock, however was the Dutch scientist Christian Huygens to realize it in 1656.

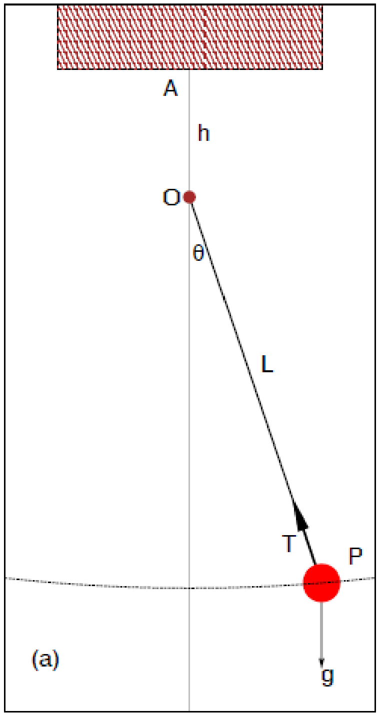
The first clock had an error less than 1 minute per day, an incredible good accuracy at the time.

Everyone will safely affirm that the oscillations of a pendulum are regular (predictable), but as we will see this is completely FALSE

From pendulum to chaos

Deterministic (Newton's law) $\neq$ Predictable

The pendulum



Planar Pendulum

- **Mass M**
- **attached to a Pivot O**
- **via a massless and inextensibile wire of length L**
- **2 forces acting on the mass :**
  - **gravity** $\mathbf{F_g} = M\mathbf{g}$
  - **wire tension** $\mathbf{T} = M g \cos\theta$

By applying the Newton's second law (F=ma) it emerges that the system can be described simply by the angle θ between the wire and the vertical axis and by the angular velocity $d\theta/dt$, the equation of motion turns out to be independent of the mass

$$\frac{d\theta^2}{dt^2} = -\frac{g}{L}\sin\theta$$

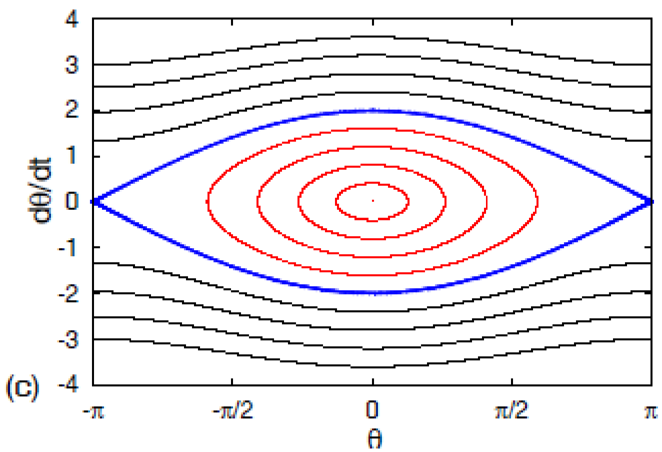
This is a NONLINEAR ordinary differential equation (ODE), difficult to solve.

Trajectories' visualization

Since the nonlinear ODE for large oscillations cannot be solved analytically

$$\frac{d\theta^2}{dt^2} = -\frac{g}{L}\sin\theta \qquad ,$$

but only numerically we plot the dynamics graphically in the Phase Space $\left(\theta; \frac{d\theta}{dt}\right)$



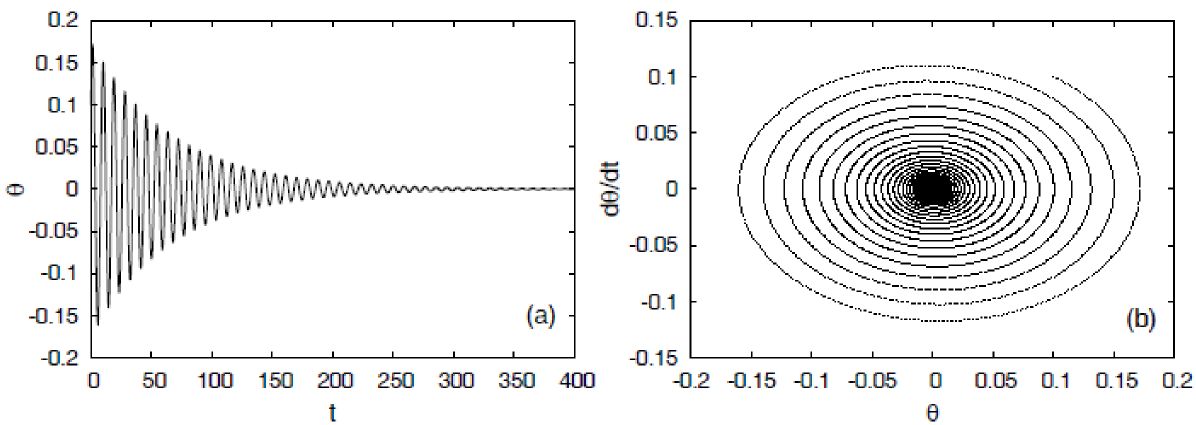
Each curve in the Phase Space is called a trajectory

- Oscillations (closed orbits)
- Rotations (open orbits)
- The separatrix corresponds to the pendulum starting with zero velocity from the unstable equilibrium position $\theta = \pi$ and returning to it with zero velocity in an infinite time.
  ($\theta = \pi$ and $\dot{\theta} = 0$ – $E_{sep} = 2mgL$)
- The motion continues for ever, the system is conservative, its energy is constant
- The motion repeats periodically

The damped pendulum

The previous picture is not realistic, the friction due to the air drag on the pendulum is always present. This force is proportional to the velocity $d\theta/dt$ and it acts against the motion (Stokes' law):

$$\frac{d\theta^2}{dt^2} = -\gamma \frac{d\theta}{dt} - \frac{g}{L}\sin\theta \qquad \gamma \text{ is the damping constant}$$



The energy is no more conserved, the friction dissipates energy, and the pendulum ends up always in the resting state $\theta = 0$ In mathematical language:

- **the system is dissipative**
- **the rest state $(\theta, d\theta/dt) = (0, 0)$ is an attractor for the dynamics : a stable fixed point**

The driven damped pendulum

O Botafumeiro - Santiago de Compostela

A giant censer of 53 kg (1.60 mt height) hanging from the vault of the Cathedral by a rope of 20 meter.

Due to dissipation the pendulum tends to stop, by varying periodically the length of the rope it is possible to maintain it in motion: parametric energy pumping !

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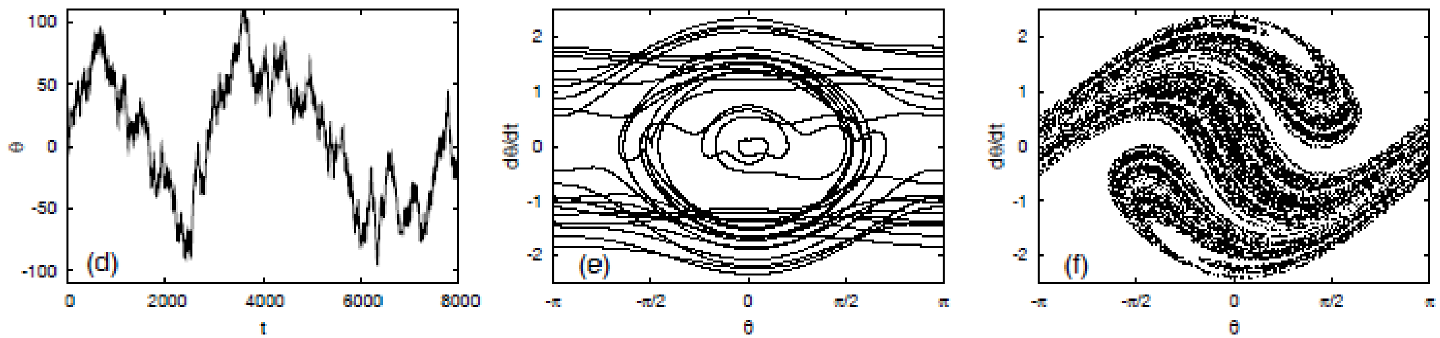
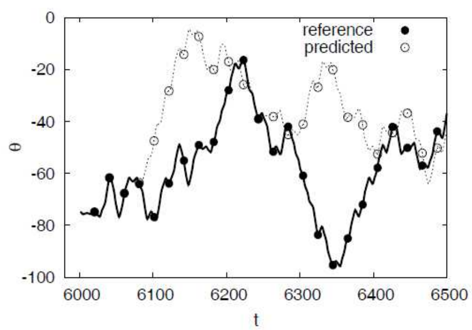
The driven damped pendulum

For a certain choice of parameters L, h_0, ω



- (d) The dynamics is always irregular
- (e) The Phase Plane is almost filled
- (f) The stroboscopic observation reveals a Chaotic Attractor

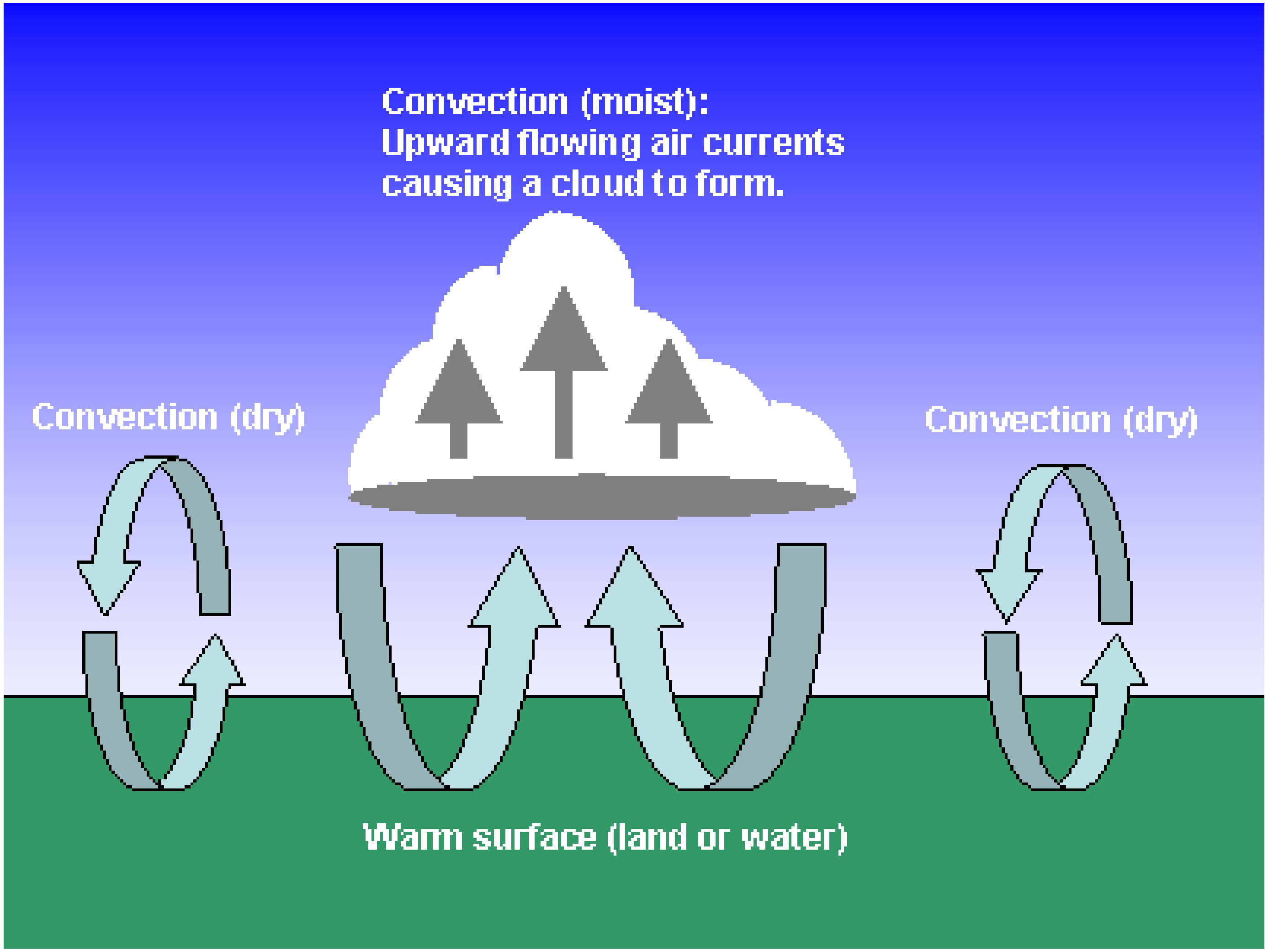


Two initial conditions differing less than 1 part/100,000 give rise to different trajectories :

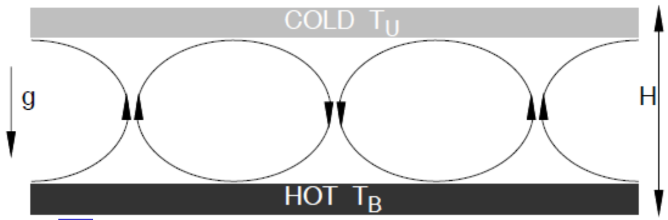
Sensitivity to Initial Conditions (SIC)

Deterministic but NOT predictable : chaotic

Atmospheric Convection



Fluid Convection



- The fluid density depends on the temperature
- Forces : Buoyancy (Spinta di Archimede) vs Viscosity
- The dynamics is controlled by the Rayleigh number

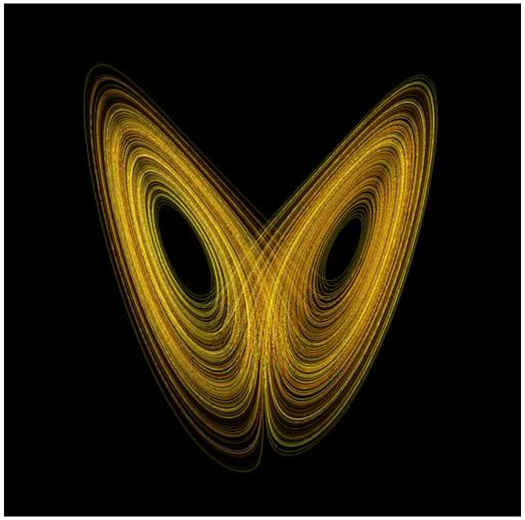
$$R_a = \frac{\rho_0 g \alpha H^3 \Delta T}{k\nu} \qquad \Delta T = T_U - T_B$$

  - g is the gravity constant
  - $\rho(\Delta T) = \rho_0(1 - \alpha\Delta T)$, α thermal dilatation coefficient
  - k thermal diffusivity - Heat equation $\dot{T} = K\nabla^2 T$
  - ν fluid viscosity
- If $Ra > Ra_c$ the heat conduction is replaced by the convective motions
- If $Ra >> Ra_c$ the steady convection state is replaced by erratic dynamics

Rayleigh-Bénard convection is fundamental for atmosphere, stars, earth magmatic mantile etc.

Lorenz Model 1960

A three dimensional truncation of the Galerkin expansion of the equations for Rayleigh-Benard convection for the description of convective motions in a fluid



$$\frac{dX}{dt} = \sigma(Y - X)$$
$$\frac{dY}{dt} = -XZ + rX - Y$$
$$\frac{dZ}{dt} = XY - bZ$$

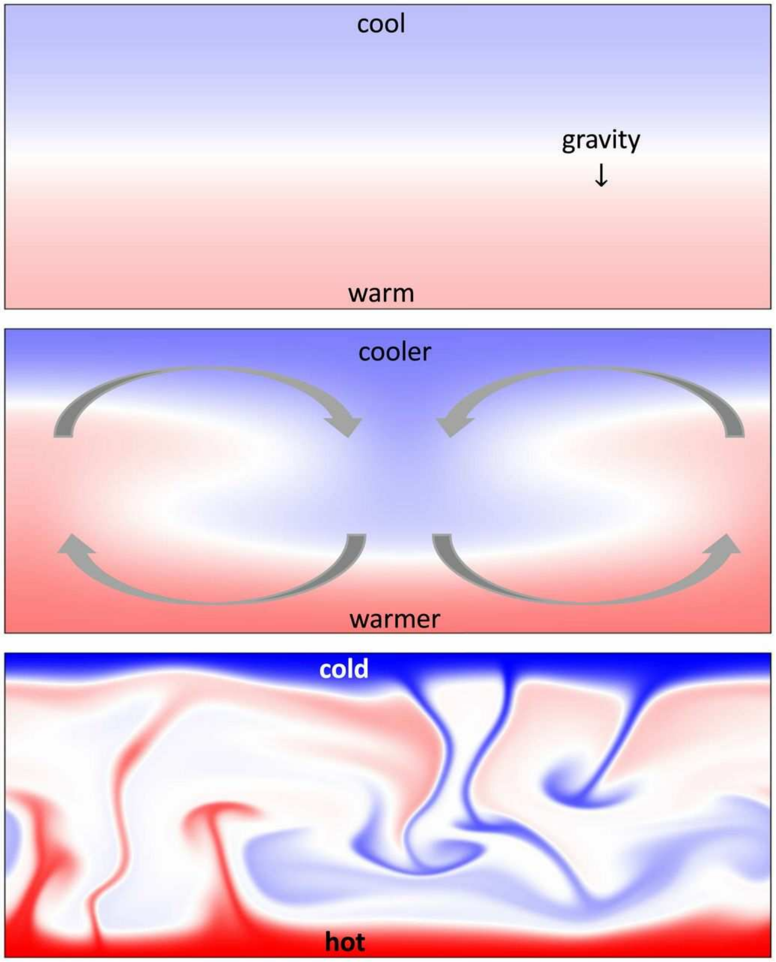
- $X(t)$ **is the amplitude of the convective motion**
- $Y(t)$ **is the temperature difference between ascending and descending fluid**
- $Z(t)$ **is the deviation from the linear temperature profile**

The parameters have physical meaning

$$r = \frac{Ra}{Ra_c} \qquad \sigma = \frac{\nu}{k}$$

b **is a geometrical factors linked to the rolls wave lenght**

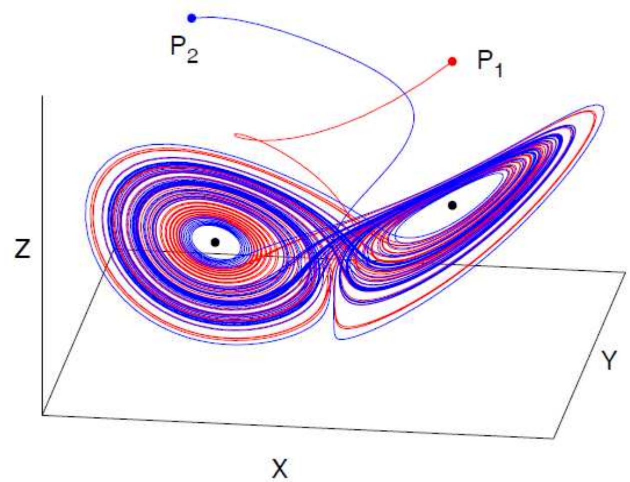
Lorenz Model 1960



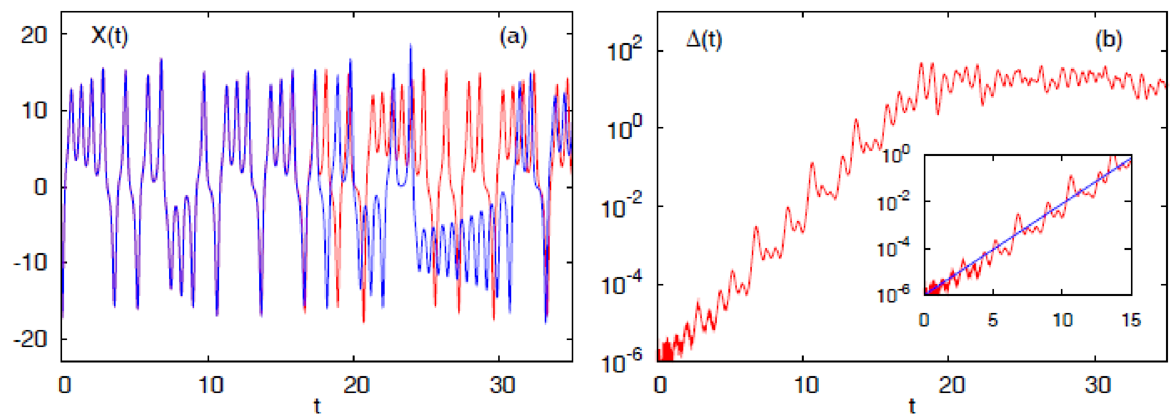
- $r = \frac{Ra}{Ra_c} < 1$ **Ony one stable fixed point** $R_0^* = (x^*, y^*, z^*) = (0, 0, 0)$ **- Heat Conduction**
- $1 < r = \frac{Ra}{Ra_c} < r_c$ **two stable fixed points** $R_\pm^* = (\pm\sqrt{b(r-1)}, \pm\sqrt{b(r-1)}, r-1)$ **- Heat Convection -** $+$ **(-) clockwise (anti-clockwise) rotation of the convection rolls**
- $r > r_c$ **- Temporal Chaos - Lorentz Model - Low Dimensional**
- $r >> r_c$ **- Spatio-temporal Chaos (Turbulence) – Other High Dimensional Models**

Lorenz Model 1960

Distant initial points **The motion is bounded in a finite portion of the space (Attractor)**



Nearby initial conditions **Exponential divergence of nearby orbits (SIC)**



Turbulent Convection

For very large Rayleigh number

$$R_a = \frac{\rho_0 g \alpha H^3 \Delta T}{k\nu} \qquad \Delta T = T_U - T_B$$

the dynamics is completely different if observed at small or large spatial scales and also at short or long temporal scales.

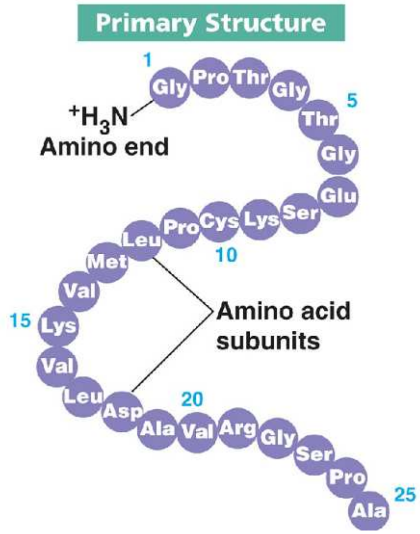
- A system is complex if it displays a dynamics at a microscopic level (time scale and/or spatial scale) completely different from that at the macroscopic level (e.g. the atmosphere, but also proteins and glasses) (Giorgio Parisi)

FILM

Vorticity is a vector measuring fluid rotation, the curl of the fluid velocity $\mathbf{v}$: $\mathbf{w} = \nabla \times \mathbf{v}$

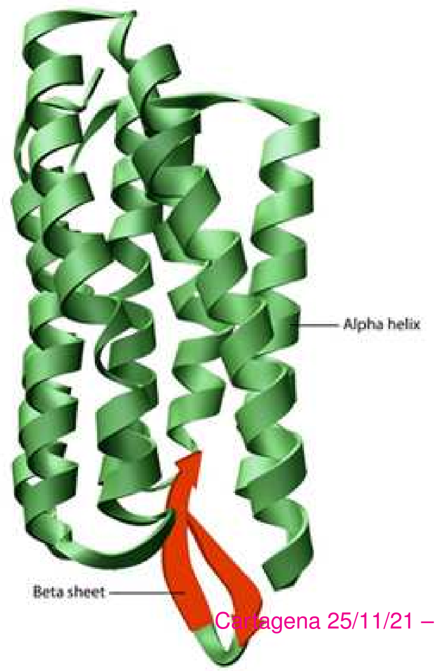
Proteins as Complex Systems

- Proteins are fundamental for the life on the earth, for Eukaryotes (cells with nucleus) they are made of 20 aminoacids linked together via peptide bonds.
- The sequence of aminoacids forming a certain protein is called Primary Structure
- The primary structure of a protein drives the folding and intramolecular bonding of the linear amino acid chain, which ultimately determines the protein's unique three-dimensional shape. (Anfisen's Dogma)



Amino Acid	Abbreviations
Alanine	Ala; A
Arginine	Arg; R
Asparagine	Asn; N
Aspartic acid	Asp; D
Cysteine	Cys; C
Glutamic acid	Glu; E
Glutamine	Gln; Q
Glycine	Gly; G
Histidine	His; H
Isoleucine	Ile; I
Leucine	Leu; L
Lysine	Lys; K
Methionine	Met; M
Phenylalanine	Phe; F
Proline	Pro; P
Serine	Ser; S
Threonine	Thr; T
Tyrosine	Tyr; Y
Tryptophan	Trp; W
Valine	Val; V

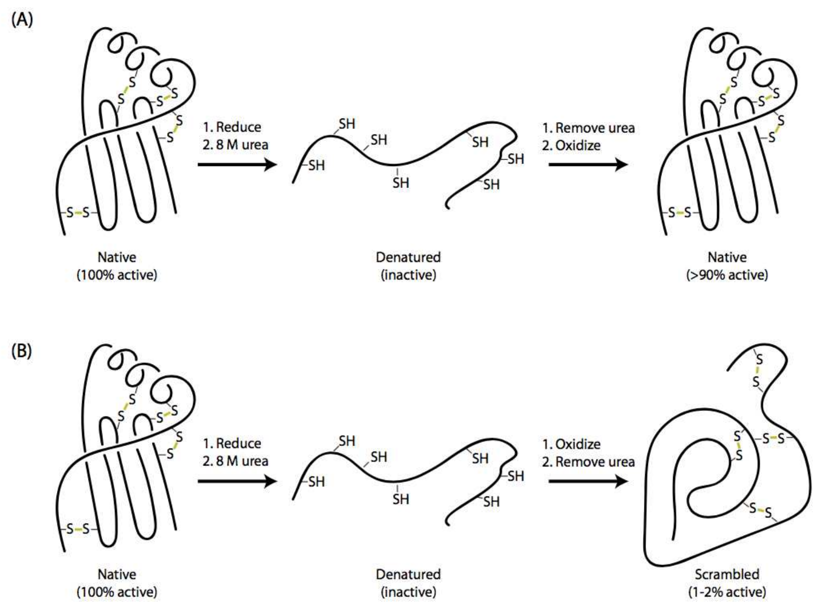
Bacteriorhodopsin



Proteins as Complex Systems

Anfisen's Dogma (Nobel Laureate in 1972 in Chemistry)

- Anfinsen shown experimentally that the information required to fold a protein into its native (lowest free-energy conformation) is entirely contained within its sequence of amino acids.
- The final shape adopted by a newly synthesized protein is typically the most energetically favorable one. As proteins fold, they test a variety of conformations before reaching their final form, which is unique and compact.



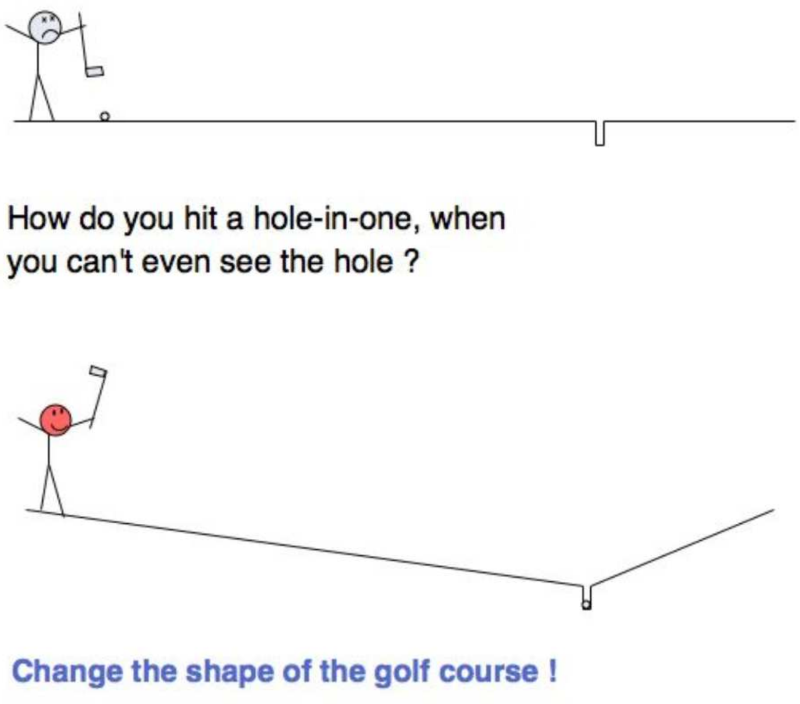
Proteins as Complex Systems

Levinthal's Paradox (1968)

- Let us consider a protein made of 100 aminoacids, each bond between aminoacids can have several states, let us say 3 states;
- The number of different conformations is $3^{100} = 5 \times 10^{47}$;
- If the protein chain changes its conformation every picosecond 10^{-12} sec = the time of thermal vibration, the fastest physical process at room temperature;
- The protein in order to find the native configuration (the global minimum) should sample all the possible conformations, this will take $\simeq 10^{28}$ years.
- The Protein tipically folds *in vitro* on a time scale of a few seconds or less and *in vivo* on a scale of the the order of 0.1 sec (These are long times with respect to protein diffusion time $\simeq 20$ ms over a characteristic cell distance $1\mu m$)

Proteins as Complex Systems

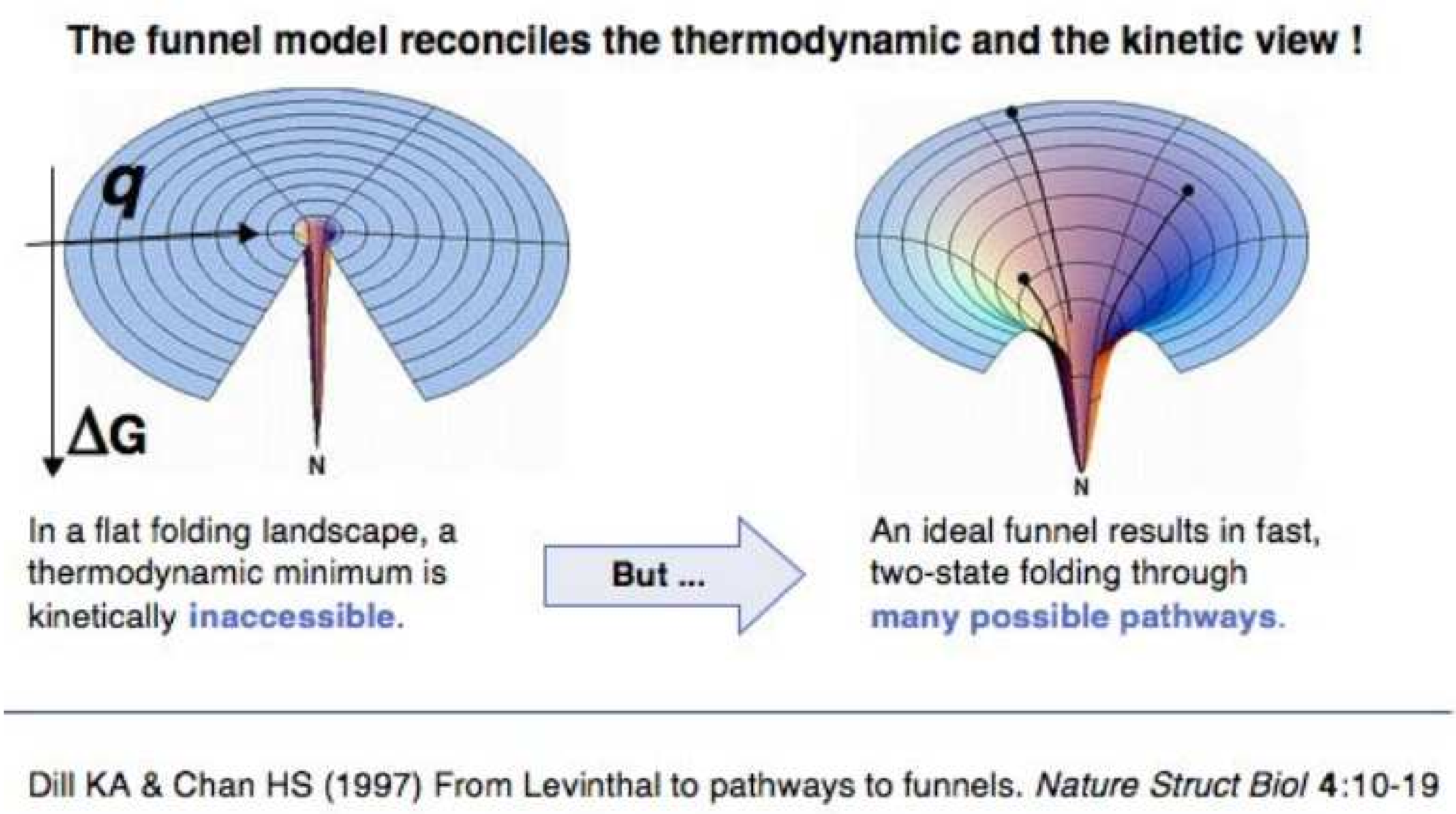
The Blind golfer



This is too simple, only one sequence of conformal changes would lead to the native state, it does not allow for fluctuations on the protein shape before reaching the native state

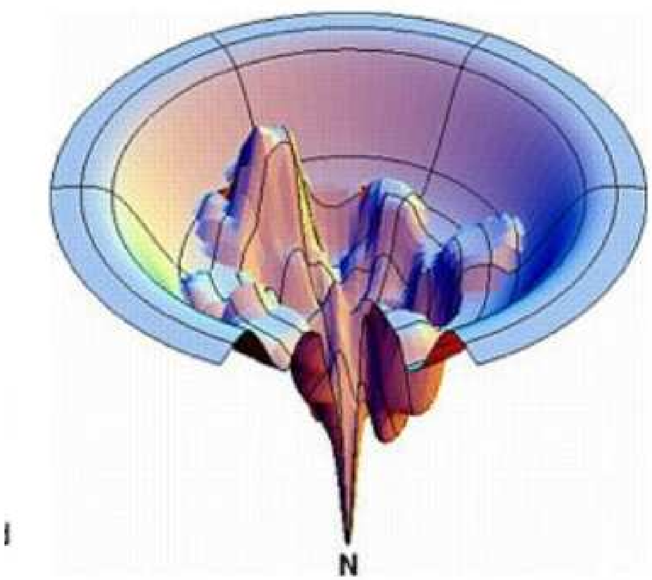
Proteins as Complex Systems

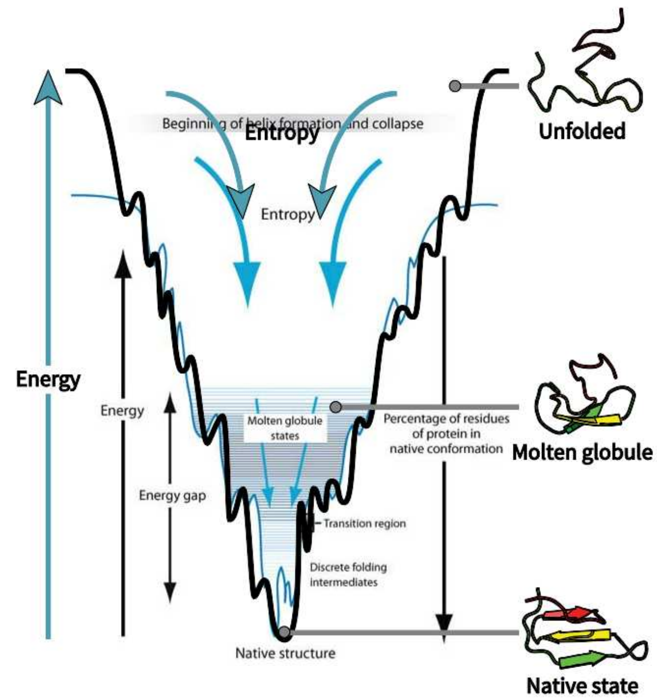
The Folding Funnel (embudo)



Proteins as Complex Systems

The Folding Funnel





At the first stages of folding the protein has many possible configurations (large entropy) and a quite high energy, at later stages the number of possible configurations (entropy) reduces as well an its energy. The global minimum is a free energy minimum, where the free energy is funnel shaped (en forma de embudo)

THE VIDEO !

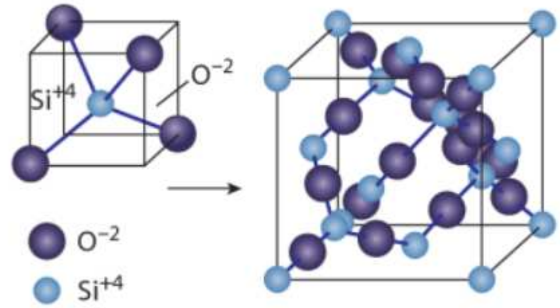
Glasses

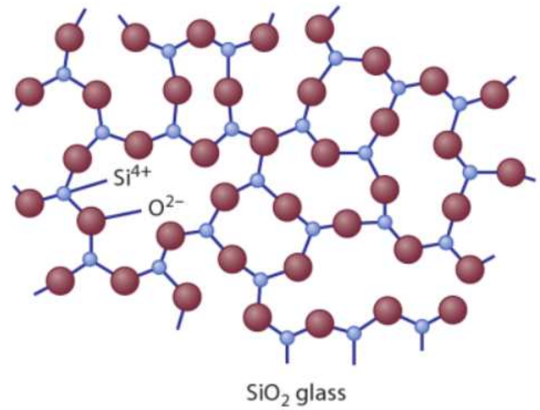
Silica (SiO_2) can exist in different forms in nature:

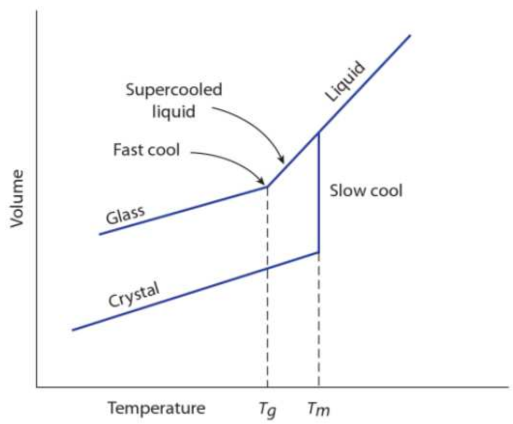
- Crystalline Quartz
- Amorphous Glass

The formation of quartz or glass depends on the cooling rate :

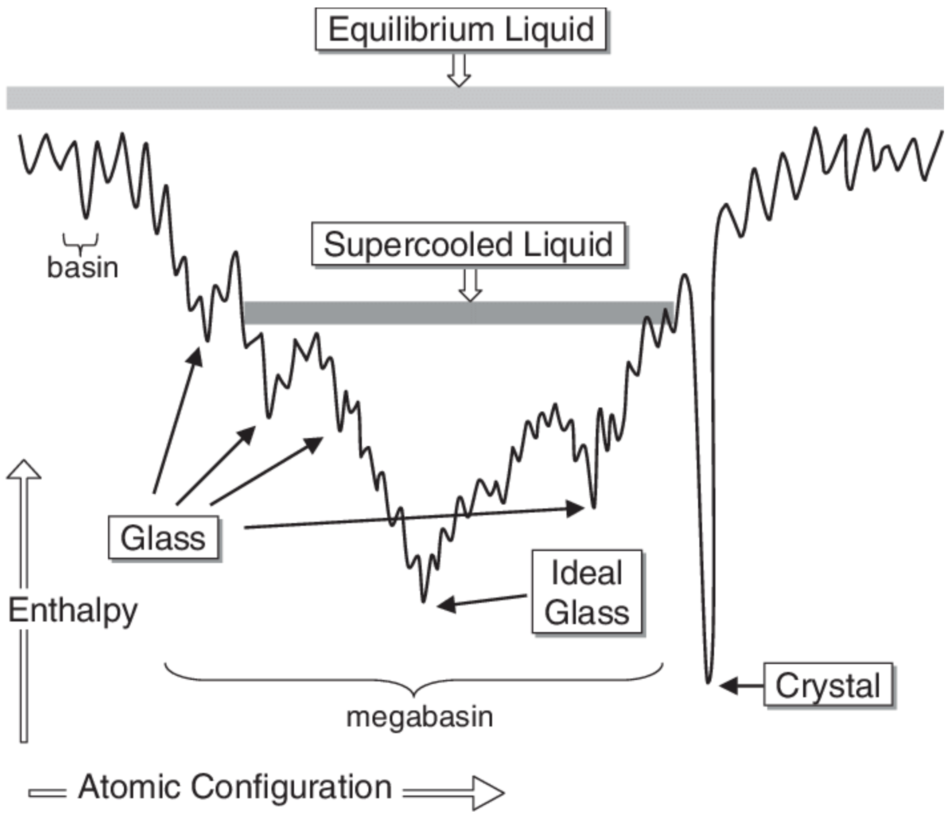
- slow ==> quartz (the earth slowly cooled, we have abundance of quartz)
- fast ===> glass (the eruption of a volcano leads to formation of glass from silica)







The Glass Energy Landscape

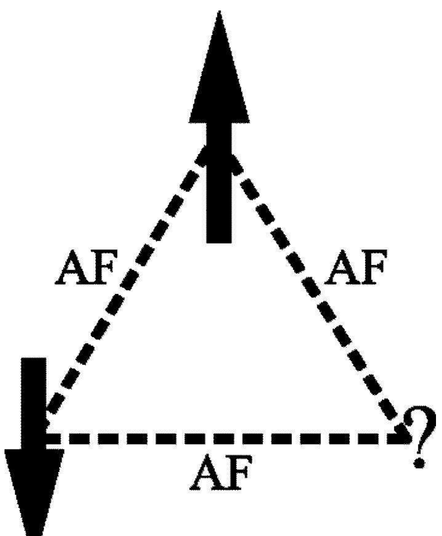


- A glass can exist in many different configurations
- All these configuration at room temperature are stable for extremely long times
- These are all coexisting quasi-equilibria for the system

Spin Glasses

Magnetic spins are the orientation of the north and south magnetic poles in three-dimensional space

- In ferromagnetic solids, the magnetic spins all align in the same direction below a certain temperature: this is analogous to what happens in a crystal
- A spin glass is a disordered magnetic systems , with ferromagnetic and antiferromagnetic interactions, that appeared to have a phase transition to a state in which each magnetic atom was stably aligned, but where the alignment direction varies randomly between atoms.



In a spin glass the spins cannot have an unique orientation due to frustration

- Consider 3 spins at the vertices of a triangle with antiferromagnetic interactions: any adjacent pair must have the opposite orientation.
- When 2 magnets satisfy the constraint, 2 others do not. The system is "frustrated".

Spin Glasses

Sherrington and Kirkpatrick (1975) introduced a simple Ising model for the spin glasses

$$E = -\sum_{i,j} J_{ij} S_i S_j - h \sum_i S_i$$

where $S_i = \pm 1$ are the spin orientations, the couplings J_{ij} are Gaussian random variables with a zero meand and a variance $\propto 1/N$.
The equilibrium solution of this model was found by Giorgio Parisi in 1979 with the replica method.
Parisi noticed that in contrast to ferromagnets which have only two “pure states” (up/down) in the ordered phase, there must be an infinite number of such states within the ordered phase of the spin glass.

Millennium Bridge

London, 07 January 2015

More in the next talk by Juan Gabriel Restrepo

Further Readings

- Scientific Background on the Nobel Prize in Physics 2021
  The Nobel Committee for Physics (2021)
- Chaos: From Simple Models to Complex Systems
  Vulpiani, A., Cecconi, F., & Cencini, M. (World Scientific, 2009)
- Theory of protein folding
  Onuchic, J. N., & Wolynes, P. G. (Current opinion in structural biology, 2004)
- Supercooled liquids and the glass transition
  Debenedetti, P. G., & Stillinger, F. H. (Nature, 2001).
- Spin glass theory and beyond: An Introduction to the Replica Method and Its Applications
  Mézard M, Parisi G, Virasoro M. (World Scientific, 1987)