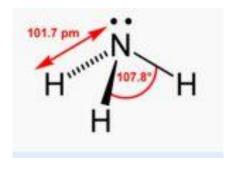
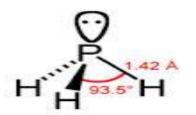
# Complex Systems. Types of systems and its dimensions: "static" and dynamical view

- boundary and approximation praise;
- intensive and extensive quantities;
- systems: isolated, closed, open;
- in statistical mechanics: canonical, microcanonical, grand canonical ensembles;
- thermodynamic equilibrium, local thermodynamic equilibrium and non-equilibrium;
- real, ideal and approximate systems.

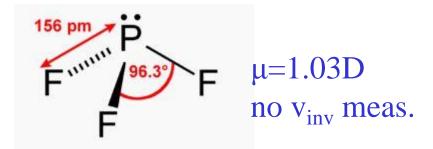
- **«More is different»**. P.W. Anderson (1923-): "More is different. Broken symmetry and the nature of the hierarchical structure of science", *Science* **177**, 393-397 (1972) (Nobel 1977), «. *The reductionist hypothesis may still a topic for controversy among philosophers, but among the great majority of active scientists I think it is accepted without question.*(p.393) [...] we can see how the whole becomes not only more than but very different from the sum of its parts (p.395».
- properties impossible to assign to a single component (water molecule, gold atom, carbon atom, ...): gas, liquid, solid, electrical conduction, thermal conduction (?)
- how many?
- how heavy?
- how big?
- C (diamond, graphite, fullerene, graphene), silicene, germanene, P(white, red, violet, black, phosphorene), B (borophene, borosphorene), ...

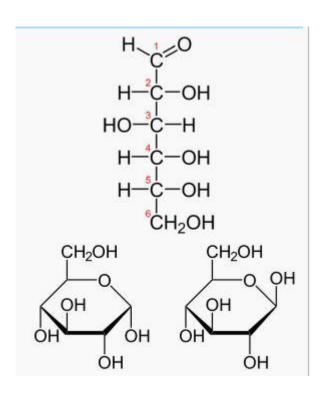


 $\mu$ =1.47D  $3x10^{10}$  inv/s



$$\mu$$
=0.58D  $\approx$ 10<sup>9</sup> inv/s

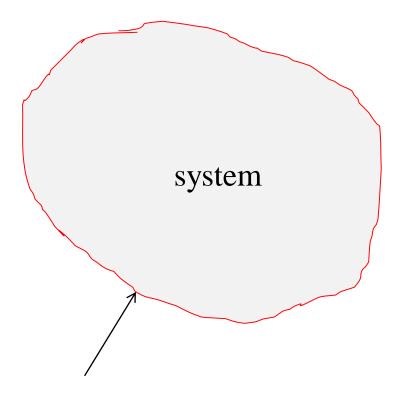




D-glucose  $(\alpha,\beta)$  closed forms

Broken symmetry

#### environment



Boundary (open, closed, isolated) – often semi-permeable membrane

- relationship between scaling and boundary (approximation)
- if fields are present?

System: "static" definition and choice *Static systems* are ones that are essentially still: we analyze them while they are at rest –before and after.

- Generic thermodynamic system: isolated, closed, open; microcanonical, canonical and grand canonical ensemble; intensive and extensive quantities; equilibrium and non-equilibrium
- Real, ideal and approximate systems: the systems that are typically subject of scientific research are never real systems; they are idealized and schematic systems, result of a complex conceptual processing, by separating it, so to speak, by side phenomena, generally referred as "perturbations".
- Before giving as complete as possible definition of what is a complex system, on which most researchers agree, it may be more useful to ask if the system I'm studying is a complex system. Is it possible the second question without answering the first?

- intensive and extensive quantities;
- isolated system: constant energy, lack of exchange of matter and energy with its surroundings; inside transient phenomena can occur until equilibrium is reached in which the *entropy* is maximum;
- closed system: it exchanges energy, but not matter with the outside environment; if P = const. and T = const., the state of equilibrium is reached when the Gibbs free energy, G, is minimal;
- open system: there are flows of the mass and energy through its borders and then you keep the non-equilibrium of the system (possible steady states);
- Local thermodynamic equilibrium (LTE): cold plasmas

The non-equilibrium transforms definitely matter properties: in equlibrium state the Matter is "blind", it become "to see" in non-equilirium state. [Prigogine]

- In statistical mechanics, a **microcanonical ensemble** is the statistical ensemble that is used to represent the possible states of a mechanical system which has an exactly specified total energy. The system is assumed to be isolated in the sense that the system cannot exchange energy or particles with its environment, so that (by conservation of energy) the energy of the system remains exactly known as time goes on. The system's energy, composition, volume, and shape are kept the same in all possible states of the system.
- In statistical mechanics, a **canonical ensemble** is the statistical ensemble (Gibbs) that represents the possible states of a mechanical system in thermal equilibrium with a heat bath at some fixed temperature. The system can exchange energy with the heat bath, so that the states of the system will differ in total energy.
- In statistical mechanics, a **grand canonical ensemble** is the statistical ensemble that is used to represent the possible states of a mechanical system of particles that is being maintained in thermodynamic equilibrium (thermal and chemical) with a reservoir. The system is said to be open in the sense that the system can exchange energy and particles with a reservoir, so that various possible states of the system can differ in both their total energy and total number of particles. The system's volume, shape, and other external coordinates are kept the same in all possible states of the system.

# System: its evolution

- *Dynamic systems* are ones that are moving in response to known, linear (or at least continuous) forces (complicated).
- Dynamical systems are ones that change in response to nonlinear, high dimension, and/or discontinuous forces (chaotic (deterministic), complex).

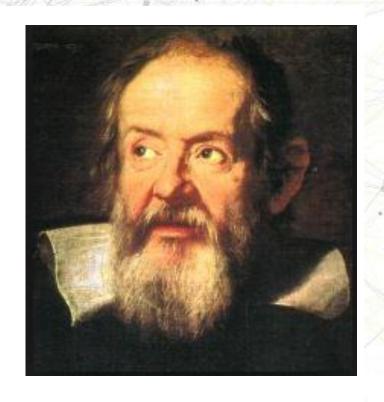
## Physics was born by studying simplified world

Causality principle (Galileo, Descartes, Newton)

Galileo supposes motions without friction: strange issues!

To sum up, physical science before 1900 was largely concerned with two-variable problems of simplicity [Weaver, 1948]

The ideal system imagined by the scientist does not allow generally easy conceptual considerations: strict deductions from the initial conditions, behaviour predictions in specific special cases and so on. It's necessary, then, to move forward, to introduce approximations which make the system "manageable".



Galileo Galilei (1564-1642)

# The model is more important than real system (!):Torricelli (Galileo's student)

Che i principii della dottrina de motu siano veri o falsi a me importa pochissimo. Poichè, se non son veri, fingasi che sian veri conforme habbiamo supposto, e poi prendansi tutte le altre specolazioni derivate da essi principii, non come cose miste, ma pure geometriche. Io fingo o suppongo che qualche corpo o punto si muova all'ingiù e all'insù con la nota proporzione et horizzontalmente con moto equabile.

Traducendo in linguaggio moderno "si muova in assenza di attrito atmosferico". (cfr.G.Parisi)

Quando questo sia io dico che seguirà tutto quello che ha detto il Galileo et io ancora. Se poi le palle di piombo, di ferro, di pietra non osservano quella supposta proporzione, suo danno, noi diremo che non parliamo di esse.



Physics began to study the motion of bodies taking into account friction, air resistance, to face increasingly complicated systems (damped pendulum).

Laplace' view: intelligenza." Essai philosophique sur les probabilitès

"Un'intelligenza che, per un istante dato, potesse conoscere tutte le forze da cui la natura è animata, e la situazione rispettiva degli esseri che la compongono, e che inoltre fosse abbastanza grande da sottomettere questi dati all'analisi,

abbraccerebbe nella stessa formula i

movimenti dei più grandi corpi dell'universo e quelli dell'atomo più leggero: nulla le risulterebbe incerto, l'avvenire come il passato sarebbe presente ai suoi occhi. Lo spirito umano offre, nella perfezione che ha saputo dare all'astronomia, una debole parvenza di questa.

Determinism and predictability (dynamic systems)



# Problems of Disorganized Complexity: Boltzmann Maxwell and Gibbs

Subsequent to 1900 and actually earlier, if one includes heroic pioneers such as Josiah Willard Gibbs, the physical sciences developed an attack on nature of an essentially and dramatically new kind. Rather than study

problems which. Involved variables or at most three or four, some imaginative minds went to the other extreme, and said: "Let us develop analytical methods which can deal with two billion variables." That is to say, the physical scientists, with the mathematicians often in the avanguard, developed powerful techniques of probability theory and of statistical mechanics to deal with what may he called problems of disorganized complexity. [Weaver, op. cit.]



- It is clear what is meant by a problem of *disorganized complexity*. It is a problem in which the number of variables is very large, and one in which each of the many variables has a behavior which is individually erratic, or perhaps totally unknown. However, in spite of this helter-skelter, or unknown, behavior of all the individual variables, the system as a whole possesses certain orderly and analyzable average properties. [cfr.Weaver]
- Boltzmann and Maxwell introduce the probability in the world description (for gases, average and standard deviation).
- Systems that are noisy or stochastic —showing randomness- are not dynamic systems and we need to apply probability to their analysis.

If we want study the evaporation or boiling, is not necessary to know the positions and velocities of all water molecules: at P=1 atm. it will boil always at 100°C!

The vapor pressure will be only f(T).

# Poincaré, phase space, initial conditions and chaotic systems

After two centuries of studies on three-body Problem, in order to state the stability of Solar system, H. Poincaré suggested a dramatic change in attitude for supporting rather the view of the impossibility of solving such a problem...Poincaré really did discovered chaos in his analysis of three-body problem.

Billiard case: rectangular, with curved sides, with spherical obstacles, Sinai



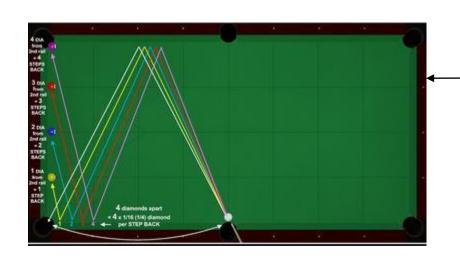
# Two-body problem

- All actions occur in a causal manner as effect of a sequential chain of events occurred previously; nothing happens by chance, but there is always cause and effect.
- A deterministic system is governed by a differential equation: assigned the initial conditions, the future is uniquely determined.

# Three-body problem

- A stochastic system is described by random processes or stochastic: the future of the system is indeterminate and you can only know it with a certain probability.
- Perturbation theory is used to determine an approximate solution of the equations of motion. (Laplace, Lagrange, Delaunay, Leverrier, Tisserand (XVIII-XIX century)

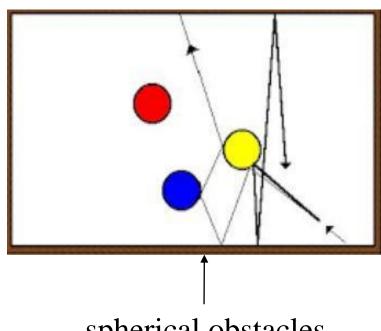
# **Billiards and Chaos**



rectangular sides

On a billiard, a displacement of 0.1 mm in the ball trajectory with respect to planned trajectory and hoped, it becomes 1 mm after the first bounce, 1 cm after the second, 10 cm after the third. At this point the subsequent rebounds have nothing to do with predictions.

Little change  $\longrightarrow$  Dramatic effect f(t)

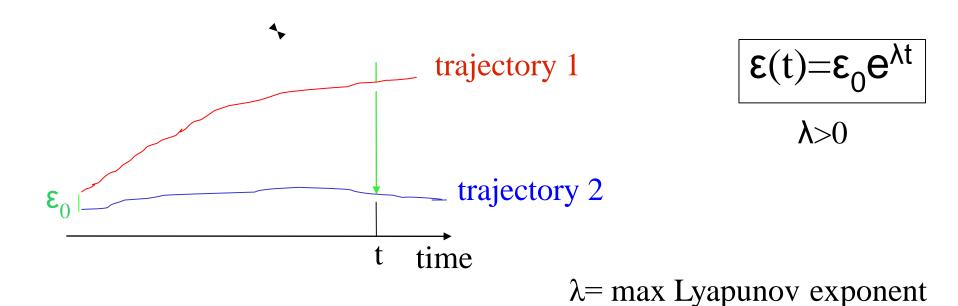


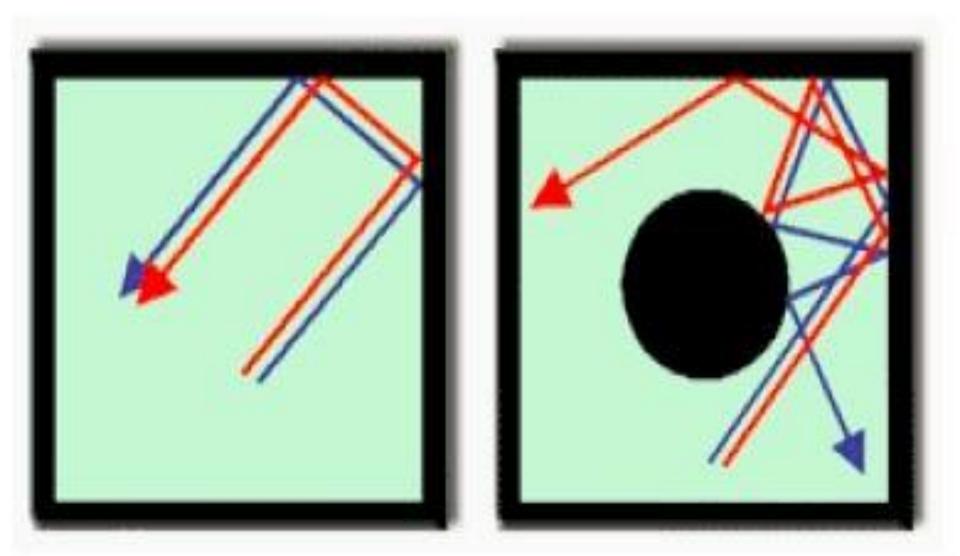
spherical obstacles

#### **Deterministic Chaos**

A phenomenon shows a *chaos deterministic* regime when:

- we have a very sensitive dependence on initial conditions
- initial uncertainty grows exponentially with time
- this results in a long-term unpredictability of its future evolution
- uncertainties about the initial conditions are deleted when you consider the average of quite long time.

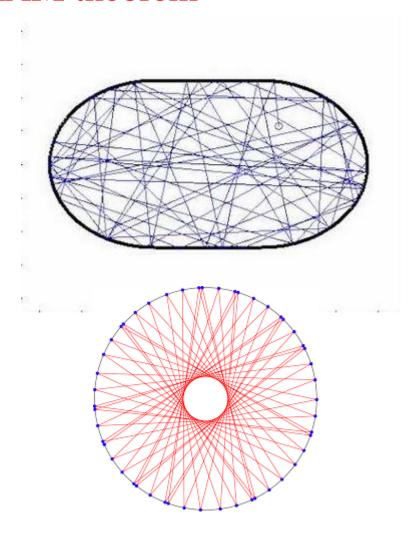




### Deterministic Chaos- KAM theorem

#### L.A.Bunimovich stadium

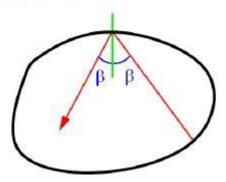




Y.G.Sinai (1935-) Abel Prize 2014

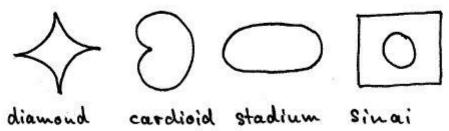
#### Billiards (classical)

particle moving in domain  $B \subset \mathbb{R}^2$ 



- motion on straight line with constant velocity
- reflection at boundary
   (angle of incidence = angle of reflection)

Billiards with 'irregular' boundary show chaotic behaviour.

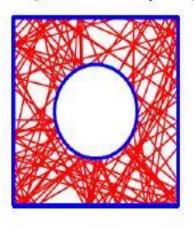


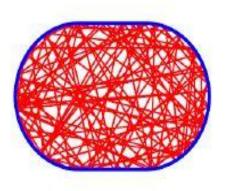
#### **Deterministic Chaos**

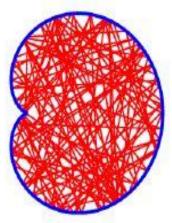
### (a) sensitive dependence on initial conditions

## (b) ergodicity

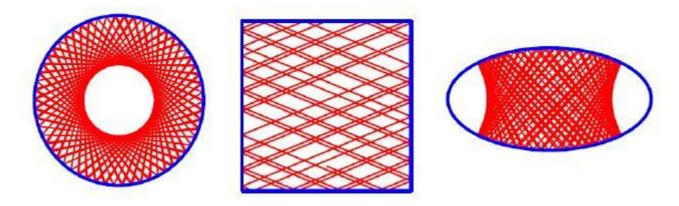
long trajectories fill the interior almost uniformly + all angles are equally likely







### billiards that are not ergodic:

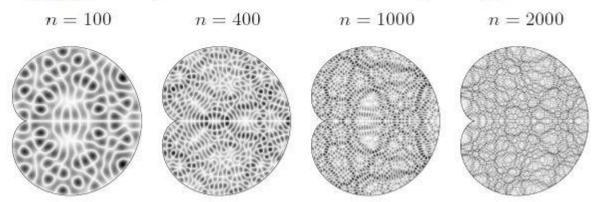


#### **Quantum Chaos**

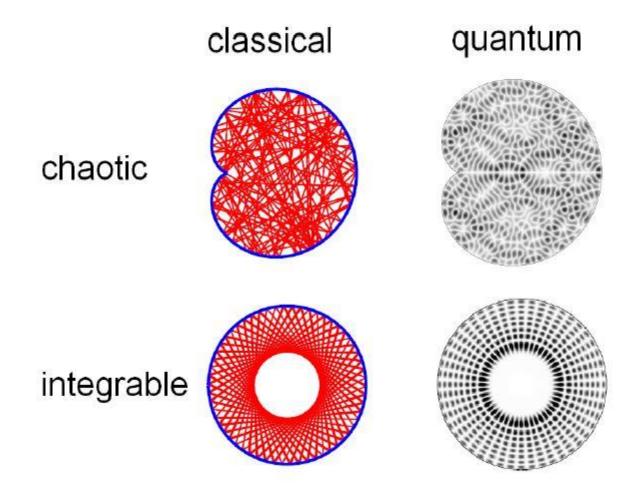
Quantum properties of systems that are classically chaotic

- (a) sensitive dependence on initial conditions? NO!, because Schrodinger equation is linear
- (b) energy eigenfunctions

plot  $|\psi_n(\mathbf{q})|^2$  for eigenfunctions with increasing energy:



eigenfunctions become more and more equidistributed (quantum ergodicity)



# KAM Theorem (Kolmogorov-Arnold-Moser)

A Hamiltonian system is integrable when its trajectories are periodic or quasiperiodic. The Solar system provides an important example of Hamiltonian system. When planetary interactions are neglected, the system reduces to the two-body problem Sun-Planet, whose integrability can be easily proved.

What about effect of perturbations?

KAM theorem implies that, even in the absence of global analytic integrals of motion, the perturbed system behaves similarly to the integrable one, at least for generic initial conditions. In conclusion, the absence of conserved quantities does not imply that all the perturbed trajectories will be far from the unperturbed ones, meaning that, also if

motion integrals do not exist, the trajectories of perturbated Hamiltonian system will be "close" to those of the integrable one.