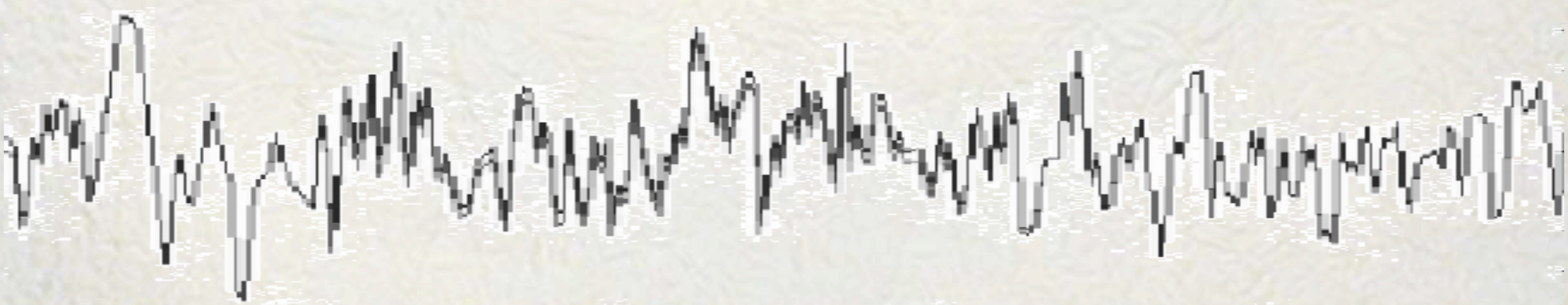
Rumore e dinamica non-lineare: **Risonanza Stocastica** e altri fenomeni "sorprendenti"

Luca Gammaitoni
N.i.P.S Laboratory, Dipartimento di Fisica - Università degli Studi di Perugia and INFN Perugia

N.i.P.S Laboratory
Noise in Physical Systems

Things should be made as simple as possible, but not any simpler.

A. Einstein



» list of contents

A. What do we mean with **noise**

B. Noise and non-linearity: a simple cartoon

C. The strange case of the **Stochastic Resonance** phenomenon

D. Other “surprising” noise induced phenomena

E. Stochastic nonlinear dynamics at the nanoscale: modeling protein dynamics

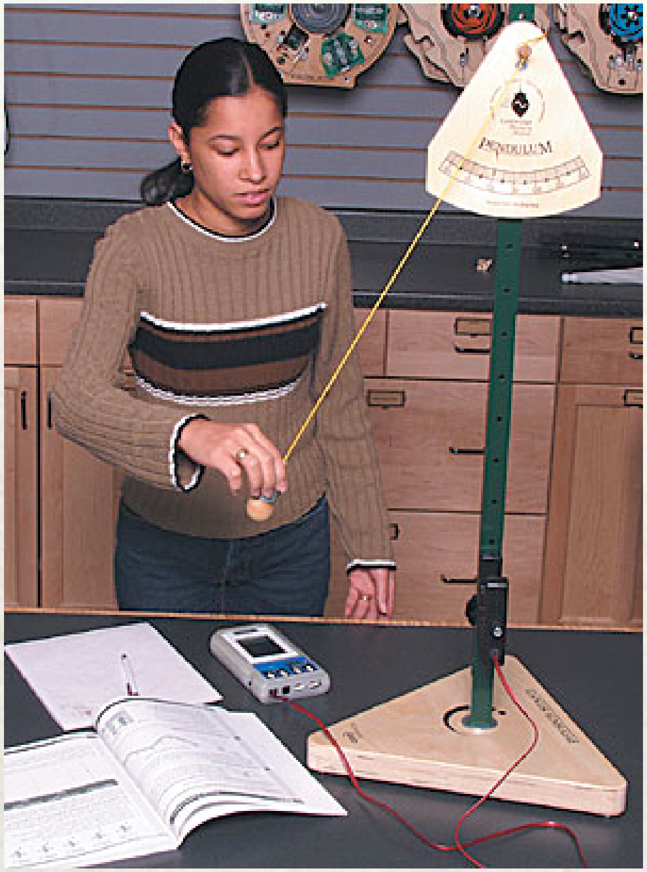
A) What do we mean with noise

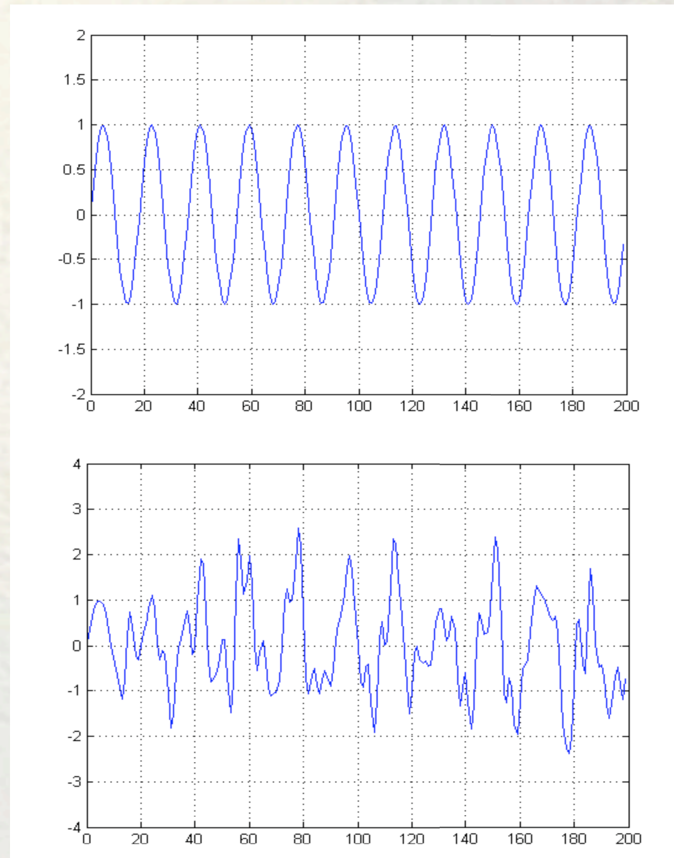
Noise in Physics means:
A disturbance, especially a random and persistent disturbance, that obscures or reduces the clarity of a signal.

Noise becomes relevant when we try to measure a physical quantity with high **precision**

"**Precision** is the ability of an instrument to produce the same value or result, given the same input"

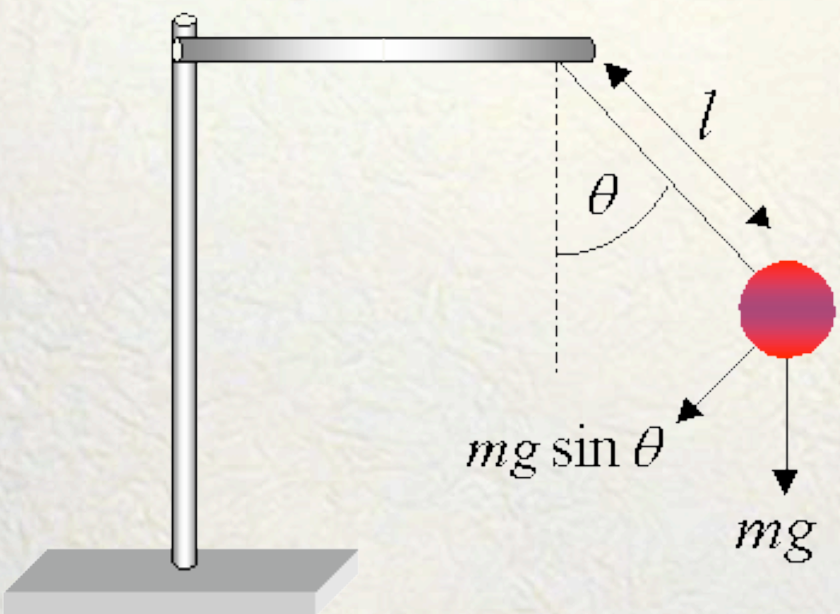
Example: the measurement of the pendulum position





Where does this noise comes from?

The almost “simple” pendulum

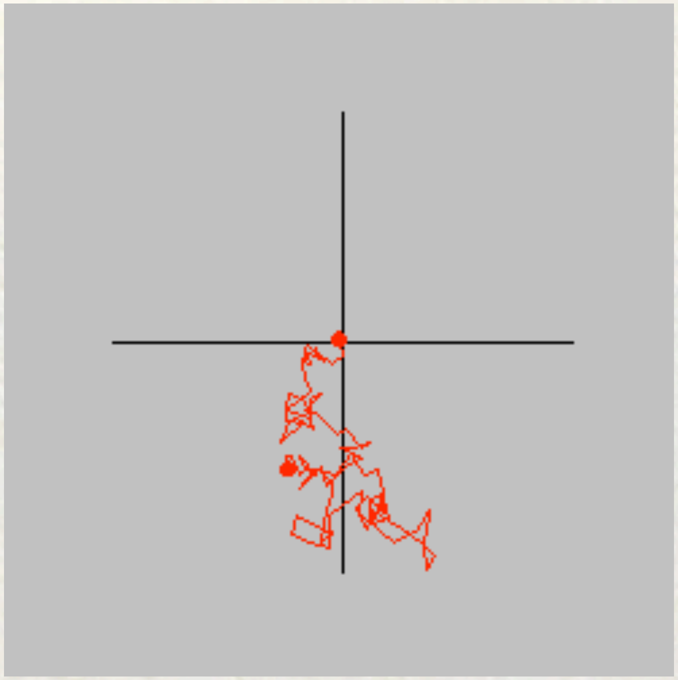


Motion equation

$$m l^2 \frac{d^2\theta}{dt^2} + m g l \sin\theta = 0$$

What if we wait long enough ?

The very small oscillation limit.
Let the pendulm swing freely…

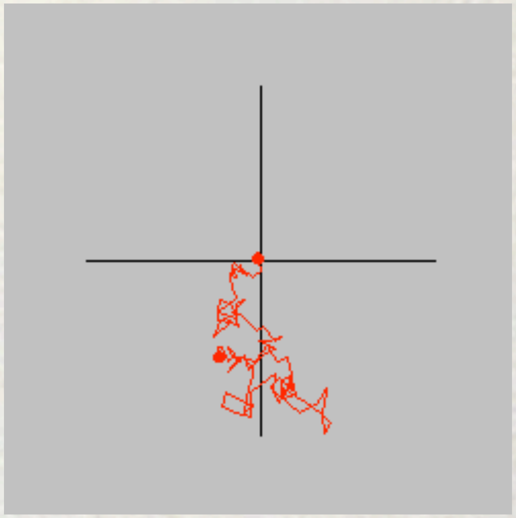


Example: the real measurement of a free swinging pendulum

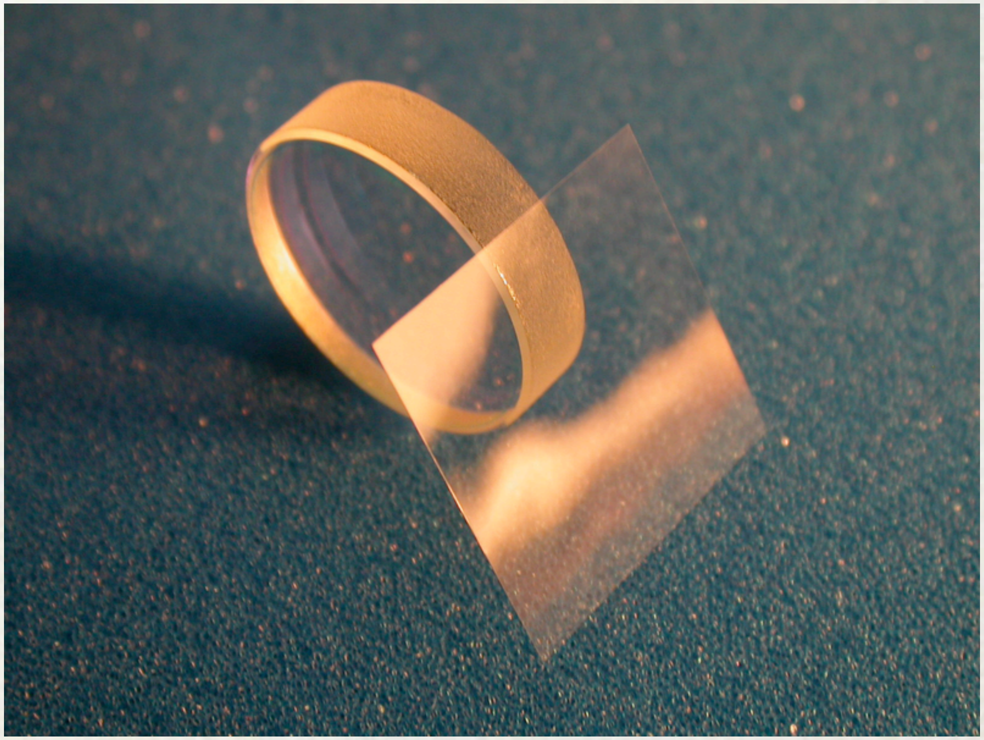
Mass m= 1 Kg
Length l = 1 m
rms motion = 2 10^{-11} m

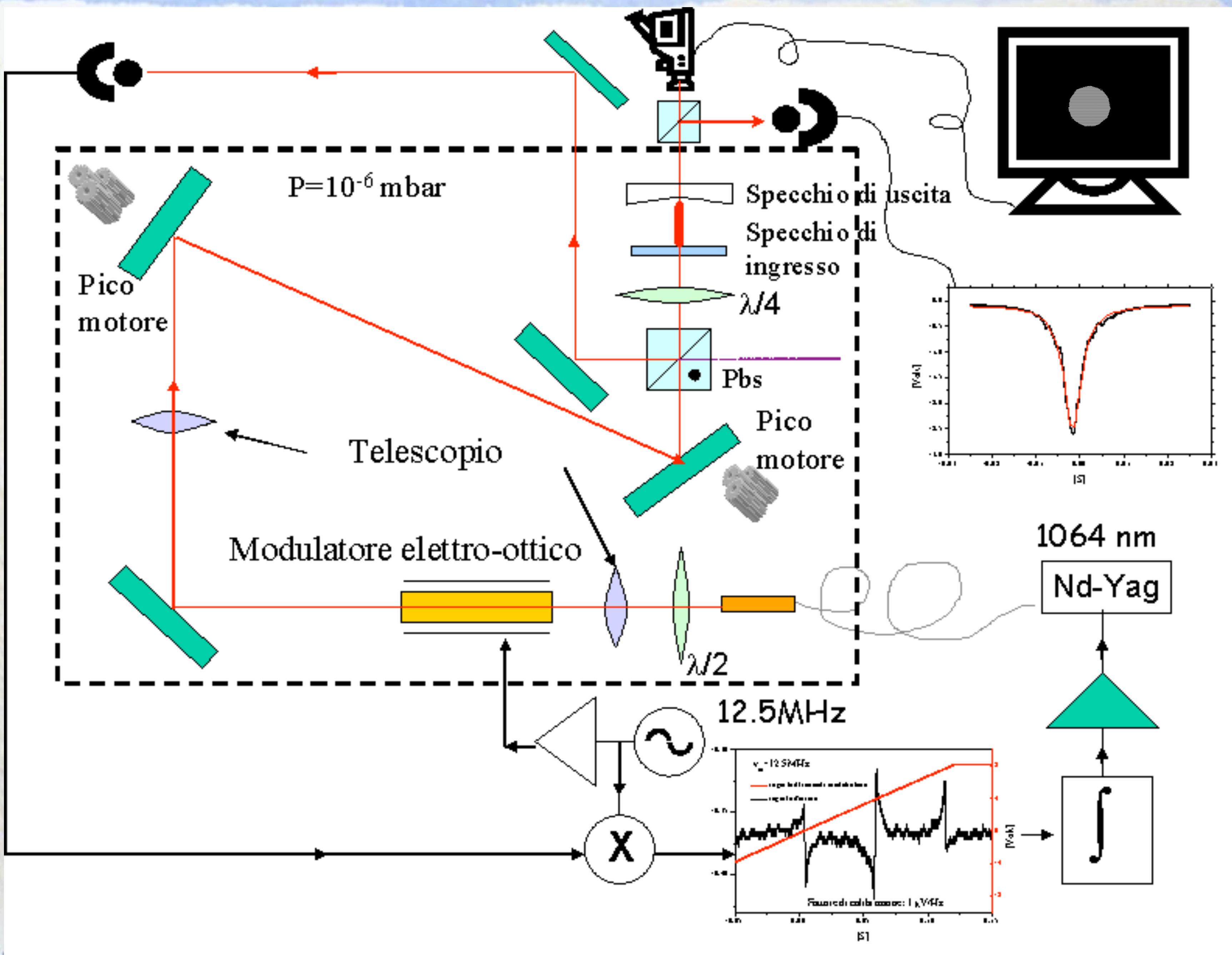
Mass m= 1 g
Length l = 1 m
rms motion = 6 10^{-10} m

Mass m= 10^{-6} g
Length l = 1 m
rms motion approx 1 mircon

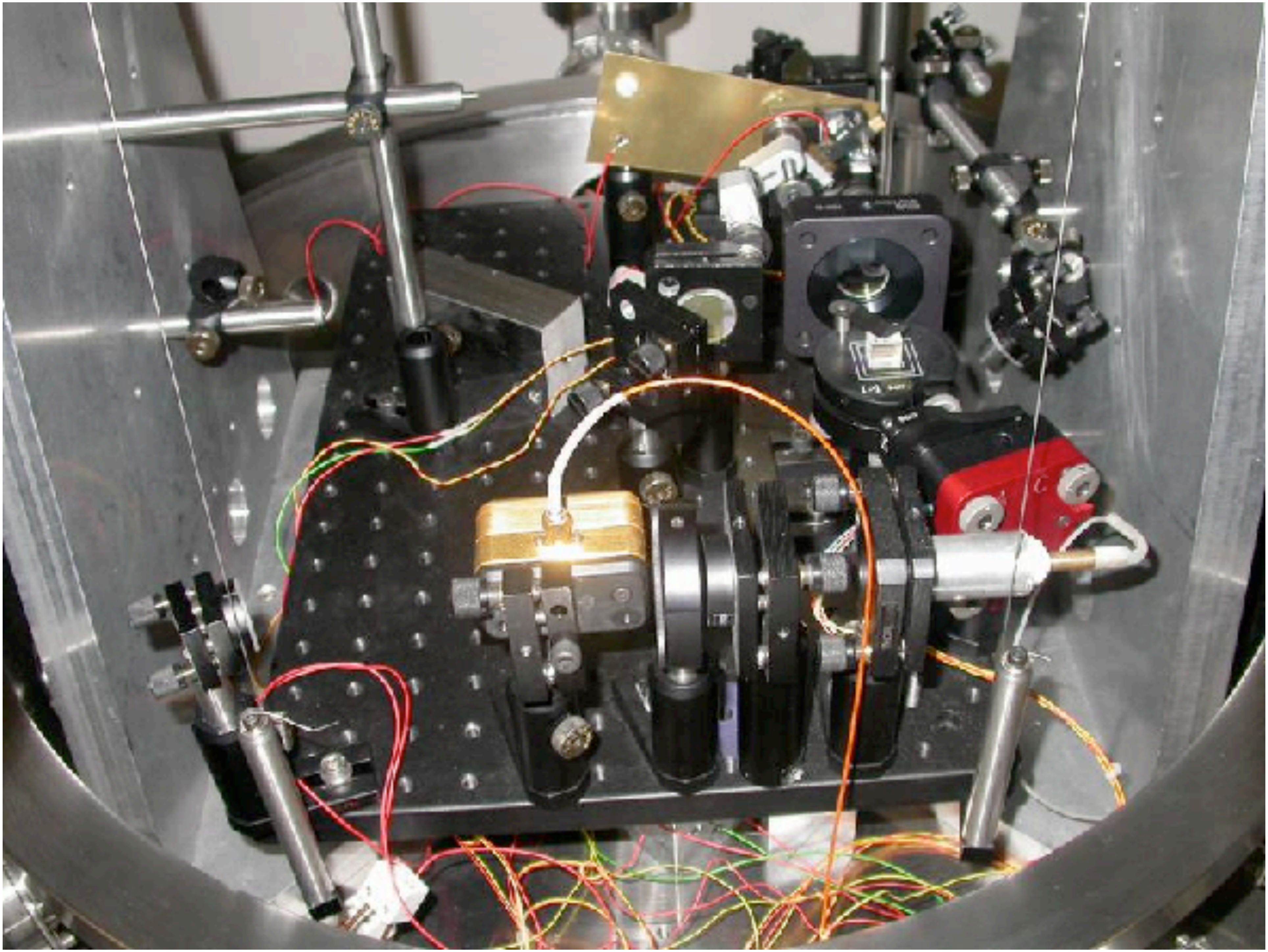


Direct measurement of internal vibration on a thin fused silica slab

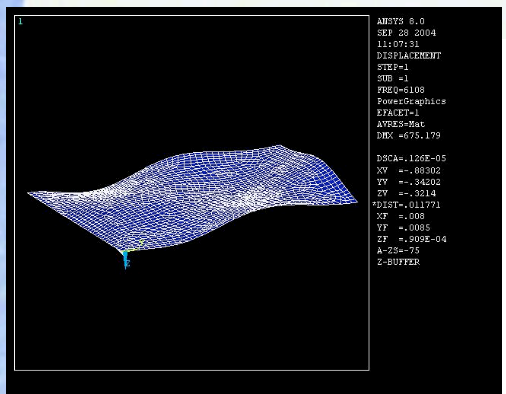




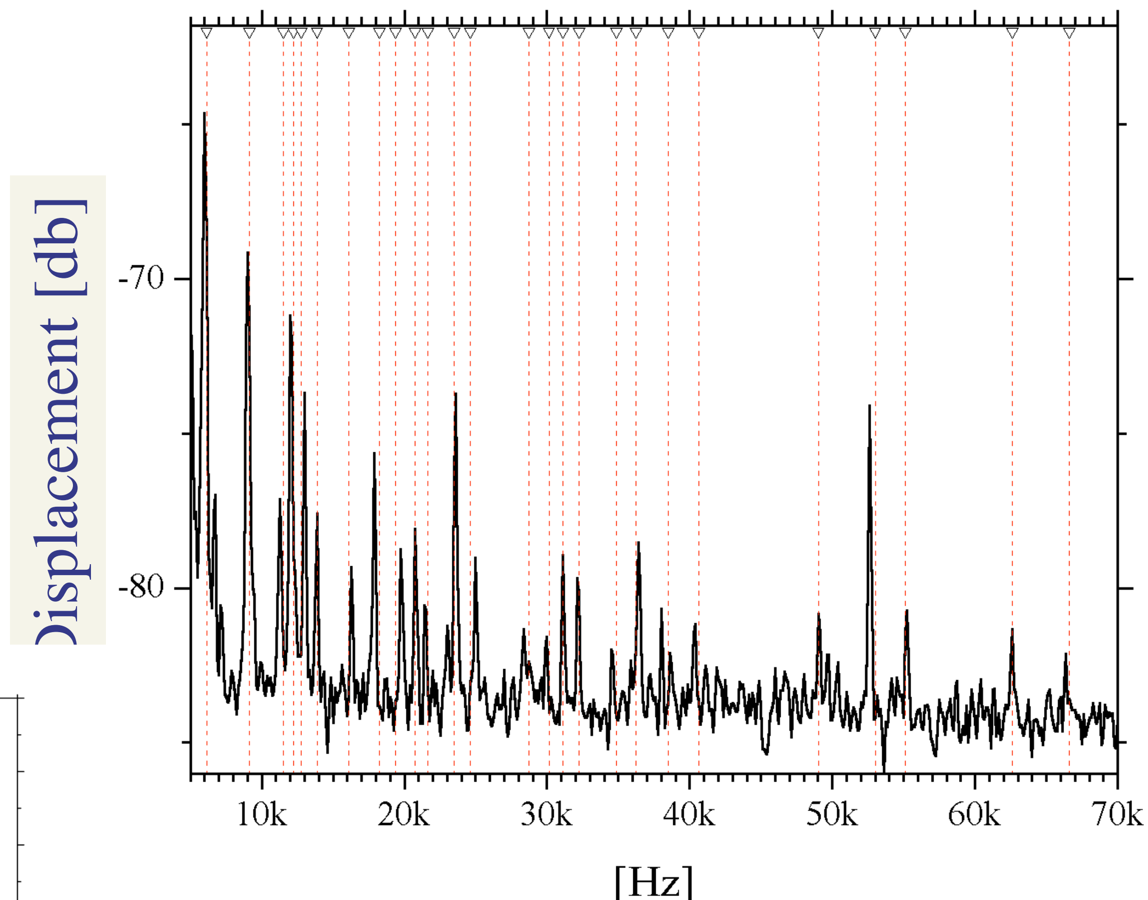
P=10-6 mbar
Specchio di uscita
Specchio di ingresso
λ/4
Pbs
Pico motore
Pico motore
Telescopio
Modulatore elettro-ottico
λ/2
1064 nm
Nd-Yag
12.5MHz
X
∫

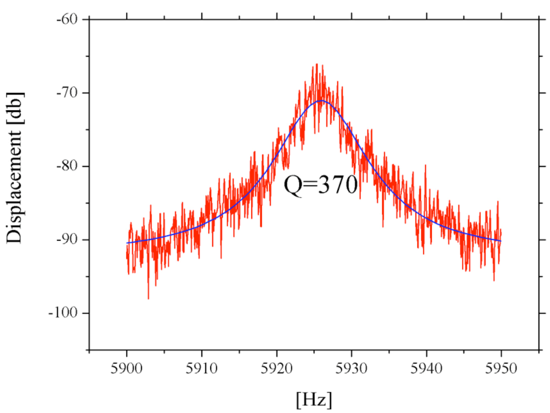


FEM mechanical characterization



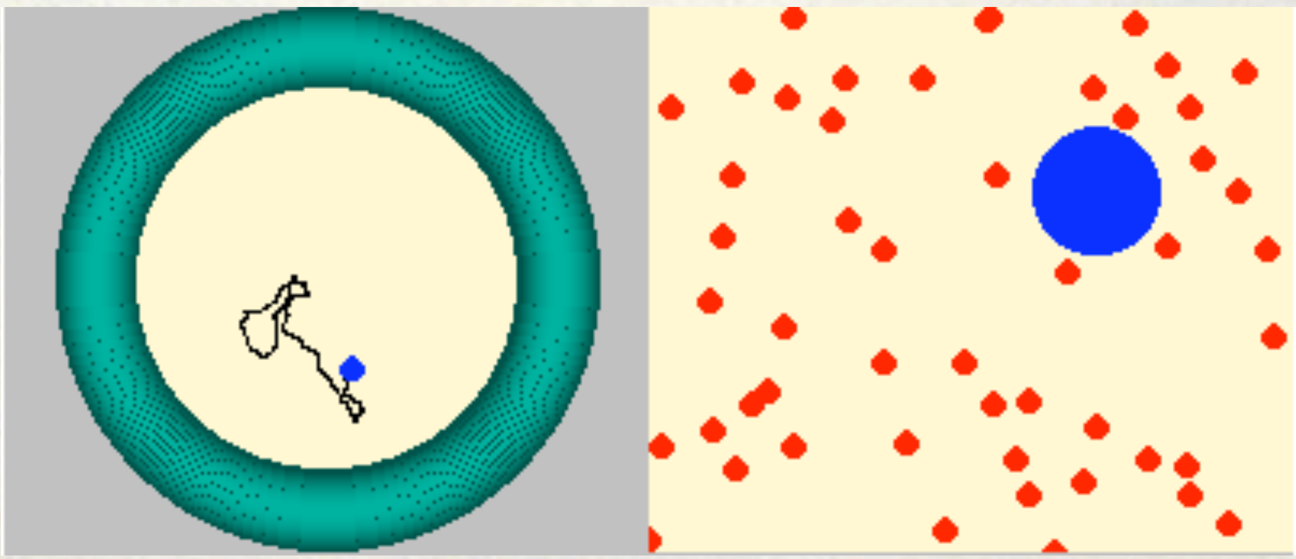
20 layer
quarter wave
TiO2-SiO2
(SILO)





Where all these fluctuations come from?

1828 R. Brown
1905 A. Einstein



The mother of all noises: **thermal noise**

Brownian motion → thermal noise

thermal noise is the name commonly given to fluctuations affecting a physical observable of a macroscopic system at thermal equilibrium with its environment.

The internal energy of a macroscopic apparatus at thermal equilibrium is <u>shared between all its degrees of freedom</u> or, equivalently, <u>between all its normal modes</u> each carrying an average energy kT, where T is the equilibrium temperature.

This is true also for such modes as the oscillations of springs, pendula, needles, etc. Such an **energy** manifests itself as a **random fluctuation** of the relevant observable experimentally perceived as the noise affecting its measured value.

How to model thermal noise

To describe such a dynamics it is necessary to introduce a statistical approach

a) Fokker-Plank equation
b) Langevin Equation

The usual equation of motion (Newton f = ma) should be changed in order to accomodate non deterministic forces. What we get is called **Langevin equation**:

The are two kind of forces acting on the pollen grain:

1) A viscous drag (motion in a fluid) $-6\pi \eta a \dot{x}$

2) A fluctuating force (representing the incessant impact of the molecules) $\zeta(t)$

$$m \ddot{x} = -6\pi \eta a \dot{x} + \zeta(t)$$

Generalization:

The viscous drag expression can be generalized in order to describe a wider class of damping functions

$$-m\int_{-\infty}^{t}\gamma\,(t-\tau)\,\dot{x}\,d\tau$$

Generalized Langevin equation

$$m\,\ddot{x} = -m\int_{-\infty}^{t}\gamma\,(t-\tau)\,\dot{x}\,d\tau + \zeta(t)$$

$\zeta(t)$ Is the stochastic force with known statistical properties:
Probability density function, moments, correlations, ...

For the pendulum we get:

$$\ddot{x} = -\omega_p^2\, x - \int_{-\infty}^{t} \gamma\,(t-\boldsymbol{\tau})\,\dot{x}\,d\boldsymbol{\tau} + \frac{\zeta(t)}{m}$$

The arbitrariness in our choice of the damping function and the stochastic force is constrained by the so-called Fluctuation-Dissipation theorem which suffices to enforce the energy equipartition

$$\langle \zeta(t)\zeta(0)\rangle = k\,T\;m\gamma\,(|t|)$$

In the spectral domain, for a linear system, is always possible to write its response to an external force like:

$$X(\omega) = H(\omega)F(\omega)$$

Where H is the system transfer function.

$$H(\omega) = H'(\omega) + i\, H''(\omega) = \left|H(\omega)\right| e^{i\phi(\omega)}$$

The F-D Theorem can be written here as:

$$S_x(\omega) = -\,4\,k\,T\,\frac{H''(\omega)}{\omega}$$

The dissipative properties of the dynamical system are thus directly related to the equilibrium fluctuations.

Fluctuation-Dissipation theorem

The **dissipative properties** of the dynamical system are thus directly related to the equilibrium fluctuations.

Physical connection:

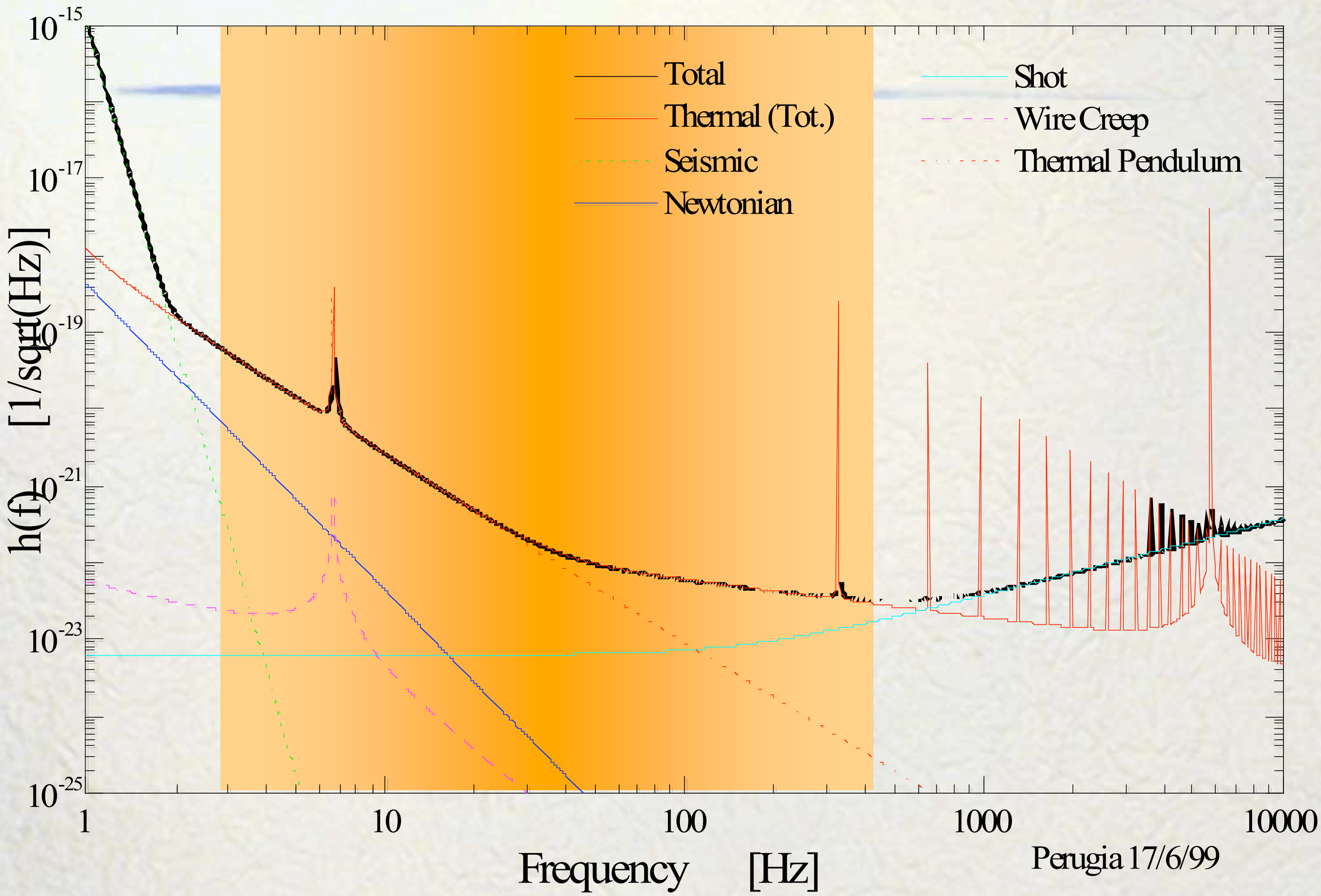
the source of the fluctuations is the very same of the source of the dissipation

Why should we bother with thermal noise ?

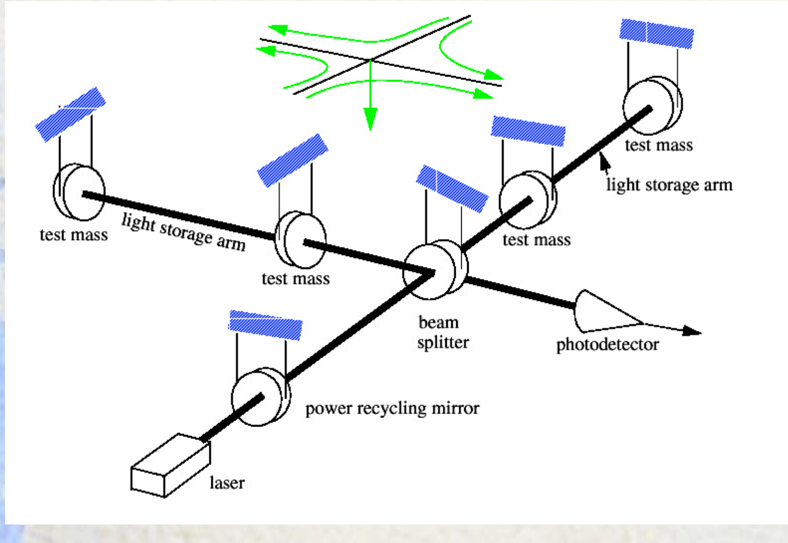
Physics is like sex.
Sure, it may give some practical results,
but that's not why we do it.

Richard Feynman

A very sensitive displacement measurement device…



Gravitational wave interferometric detector !!!



Where are we !?

» list of contents

B) Noise and non-linearity: a simple cartoon

Langevin Equation for the linear pendulum

$$\ddot{x} = -\omega_p^2 \, x - \int_{-\infty}^{t} \gamma(t-\tau) \, \dot{x} \, d\tau + \frac{\zeta(t)}{m}$$

For the generic physical dynamic system we can use the "potential" description (conservative forces):

$$\ddot{x} = -V'(x) - f(\dot{x}) + \zeta(t)$$

Where we set m=1 and introduced the dissipation function

B) Noise and non-linearity: a simple cartoon

Langevin Equation for the linear pendulum

$$\ddot{x} = -\omega_p^2 \, x - \int_{-\infty}^{t} \gamma(t-\tau) \, \dot{x} \, d\tau + \frac{\zeta(t)}{m}$$

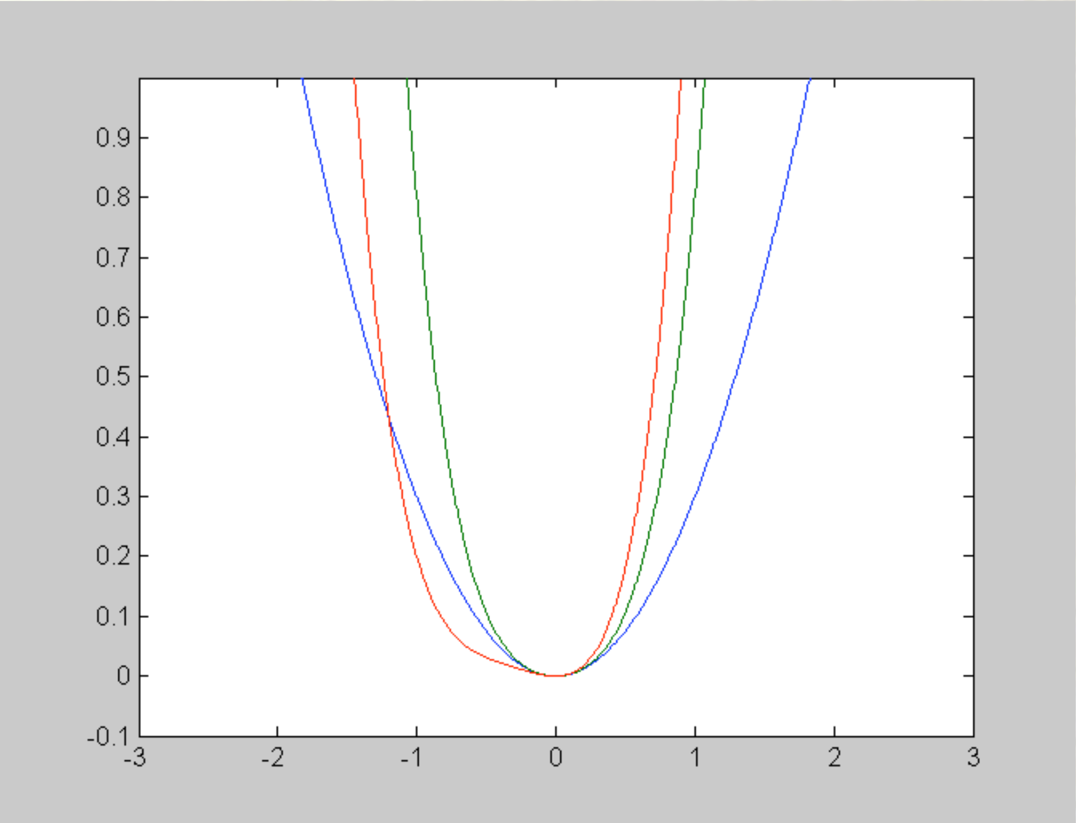
For the linear pendulum = harmonic oscillator

$$V(x) = \frac{1}{2} m \omega_p^2 x^2$$

The potential of a linear system is a parabolic one!

nonlinear dynamics in **nonlinear** potential

We can change the shape of the curve by adding terms to the polinomial expression of the potential



Monostable nonlinear potential

Bistable (nonlinear) potential

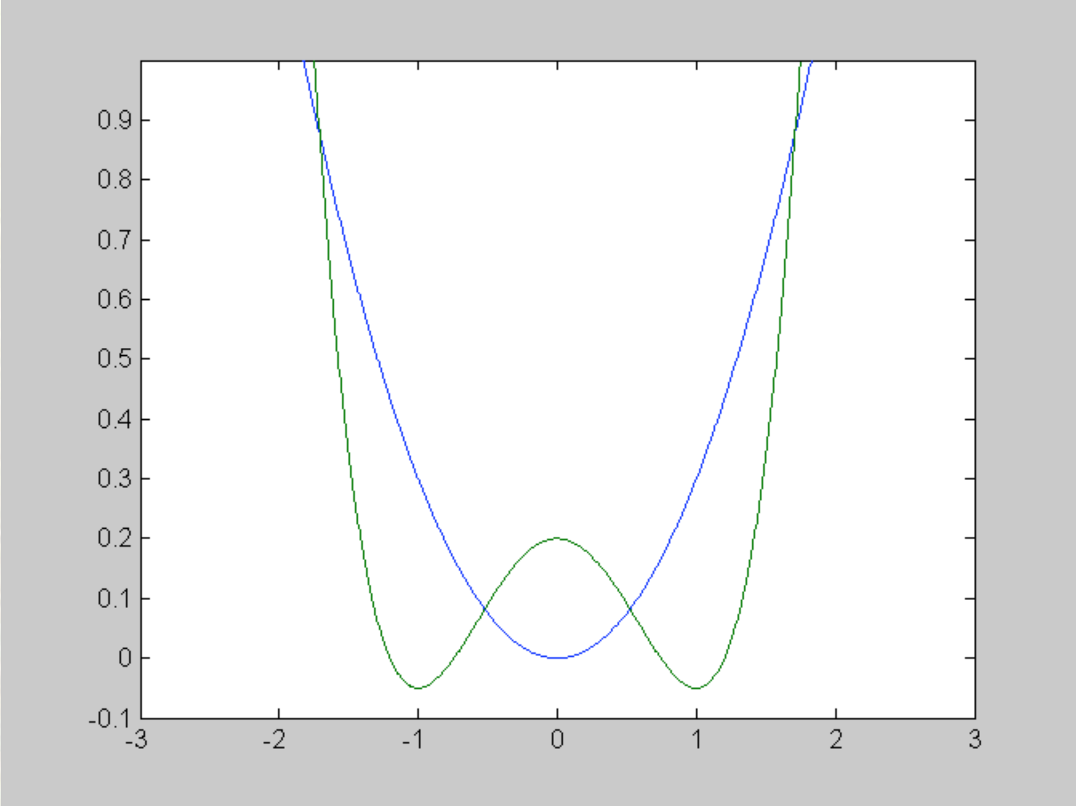
$$V(x) = -\frac{1}{2}ax^2 + \frac{1}{4}bx^4$$

Bistable …

Add cubic term

Add quartic term

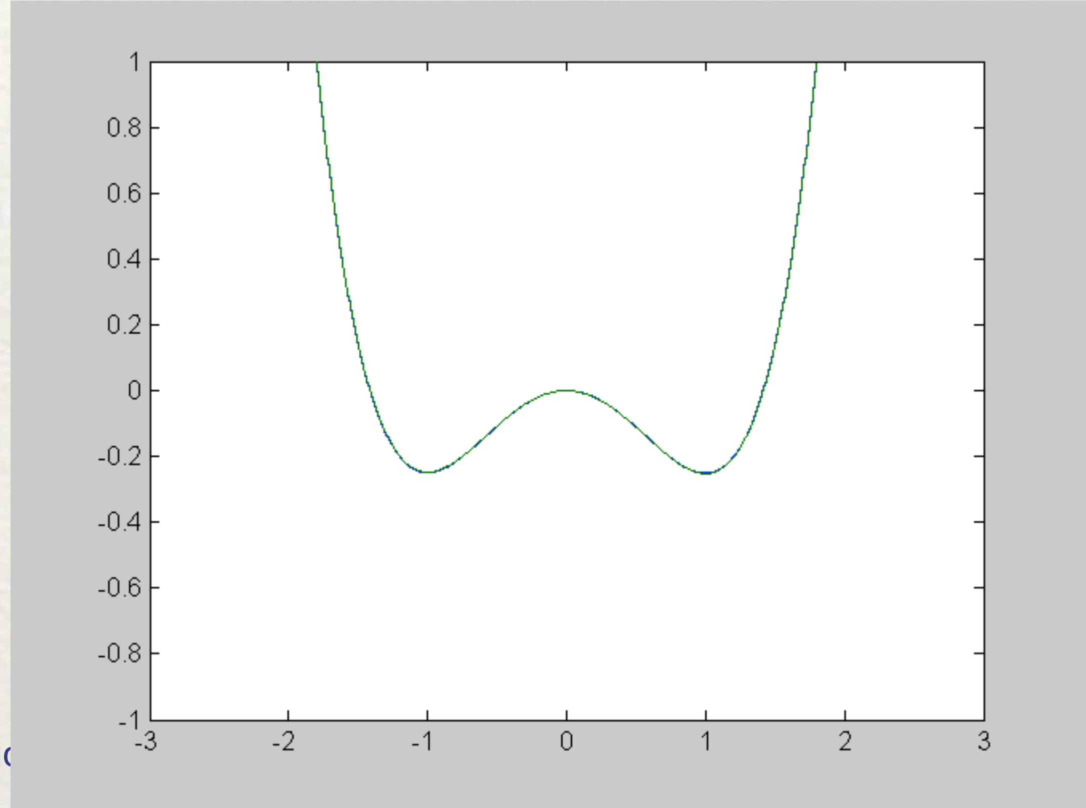
symmetric
quartic



What if …

I introduce the time dependent part into the potential ?

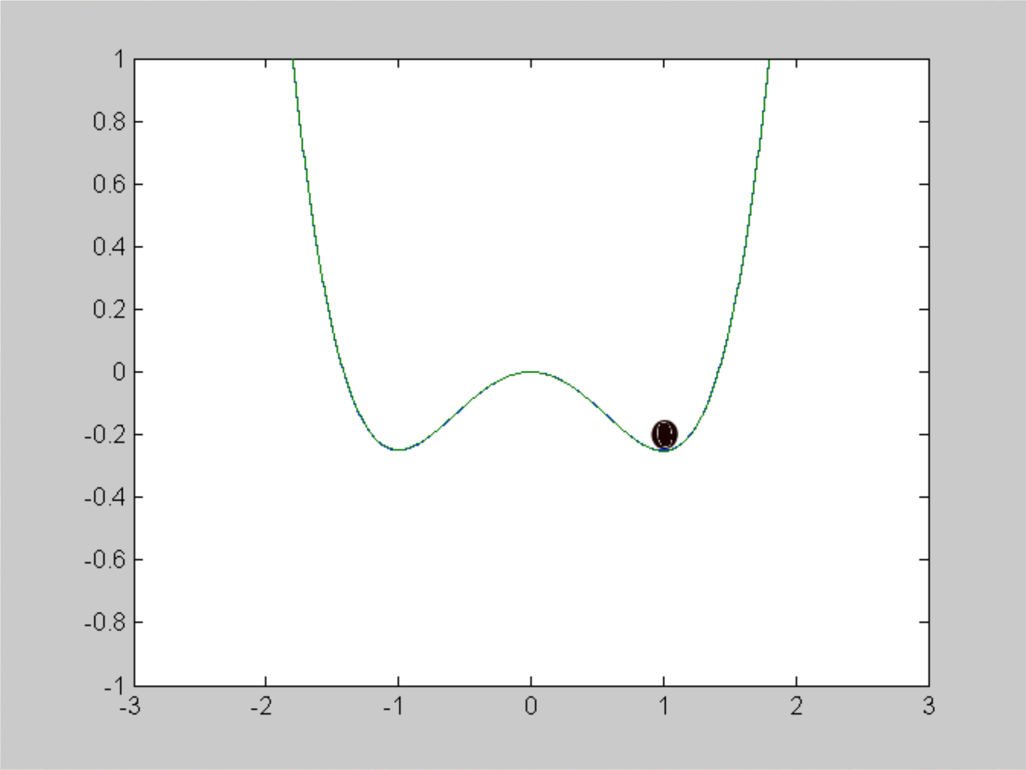
$V(x,t) = V(x) + A(t) \qquad A(t) = A \sin(\omega t)$



Marble in a cartoon: let's play dynamics!

$$\ddot{x} = -V'(x) - \gamma\dot{x} + A(t)$$

$$V(x) = -\frac{1}{2}ax^2 + \frac{1}{4}bx^4 \qquad A(t) = A\sin(\omega t)$$



Where are we !?

» **list of contents**

C) The strange case of the **Stochastic Resonance** phenomenon

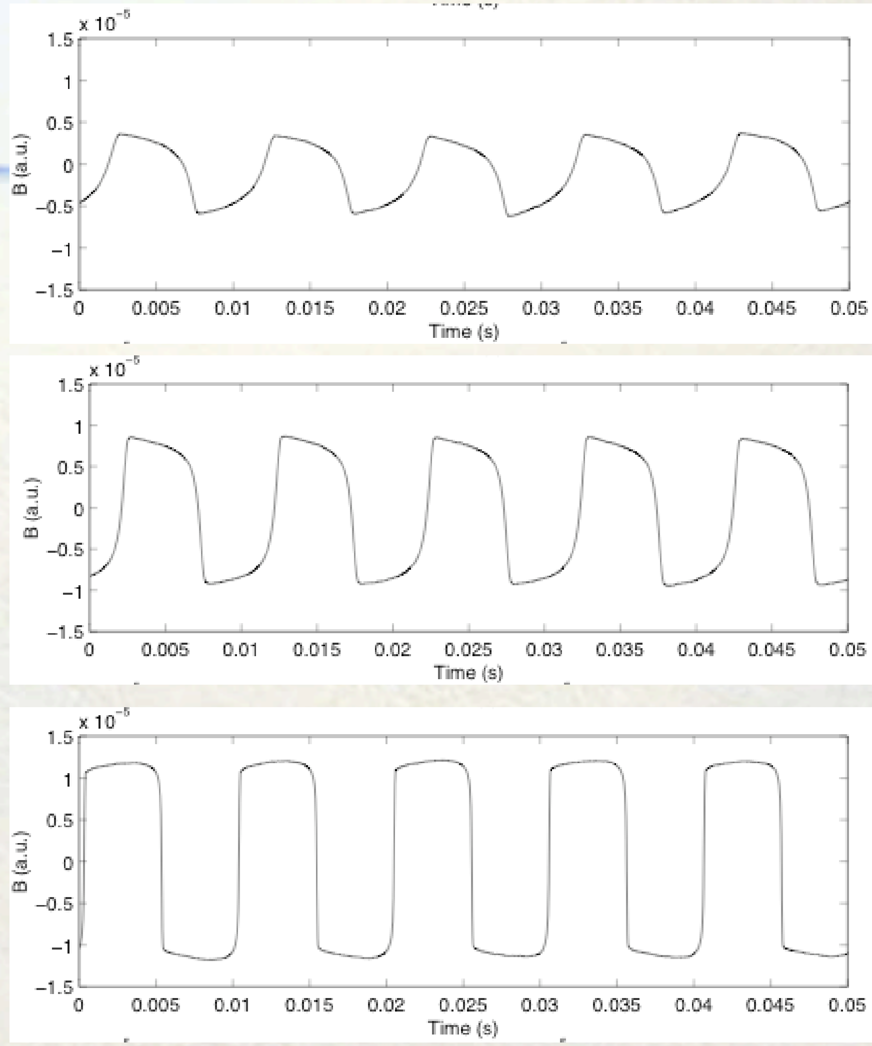
Let’s consider our very basic ingredients:

$$\ddot{x} = -V'(x) - \gamma \dot{x} + A(t)$$

$$V(x) = -\frac{1}{2} a x^2 + \frac{1}{4} b x^4 \qquad \mathrm{A(t) = A\ sin(\omega t)}$$

Let’s look for the time evolution of x(t)

How does it look?

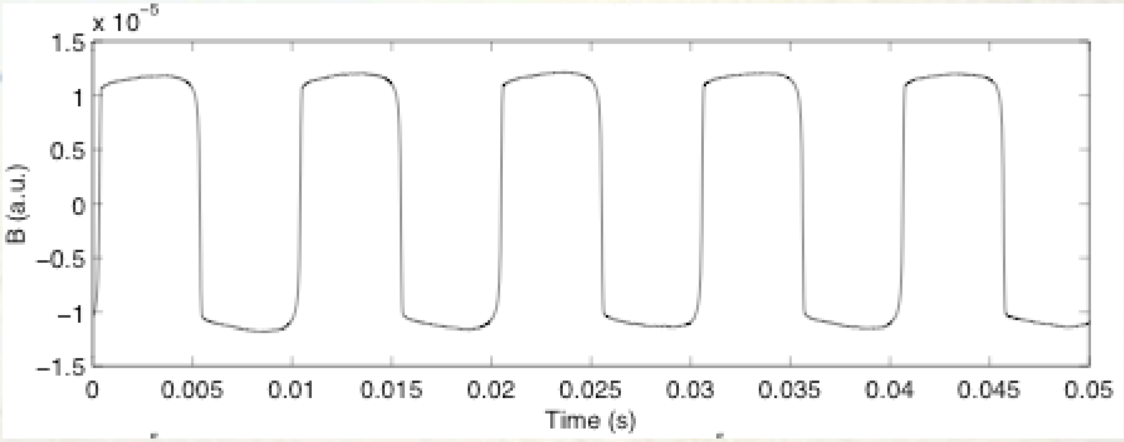


A = 3

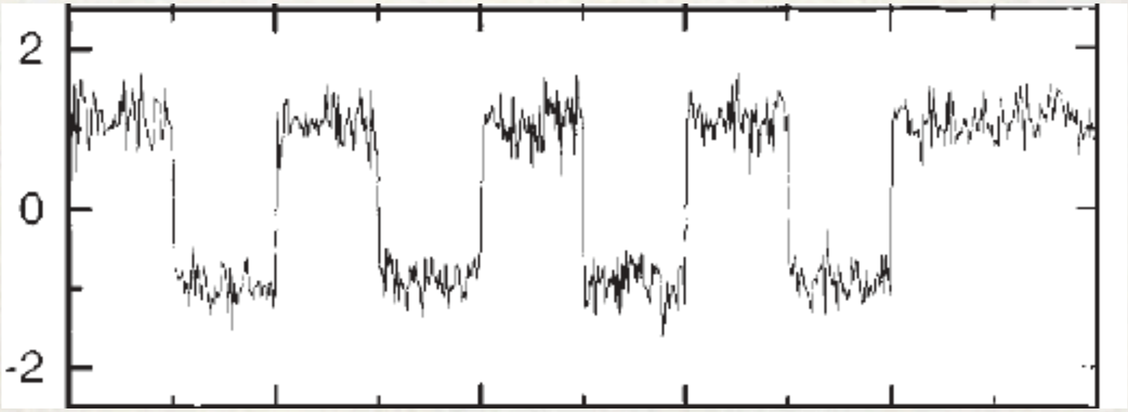
A= 4

A= 5

What if we add the noisy force?



No noise

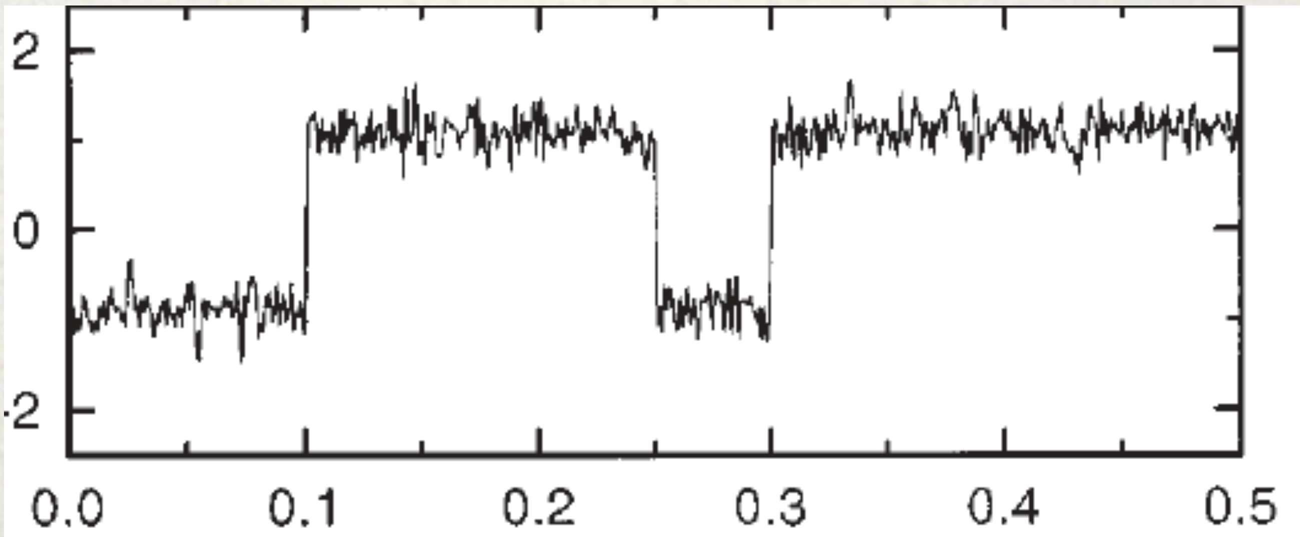


With noise

What if the periodic driving is to small to let the marble to jump??

The marble would stay trapped into one well unless The noise provide some help…

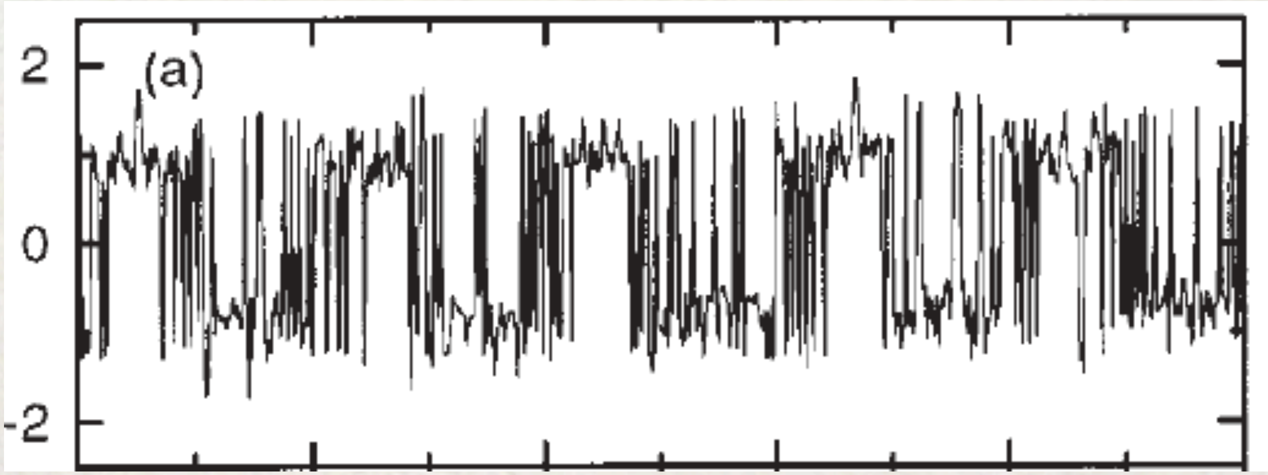
For **small** noise we will have **occasional** jumps



What if the periodic driving is to small to let the marble to jump??

The marble would stay trapped into one well unless The noise provide some help…

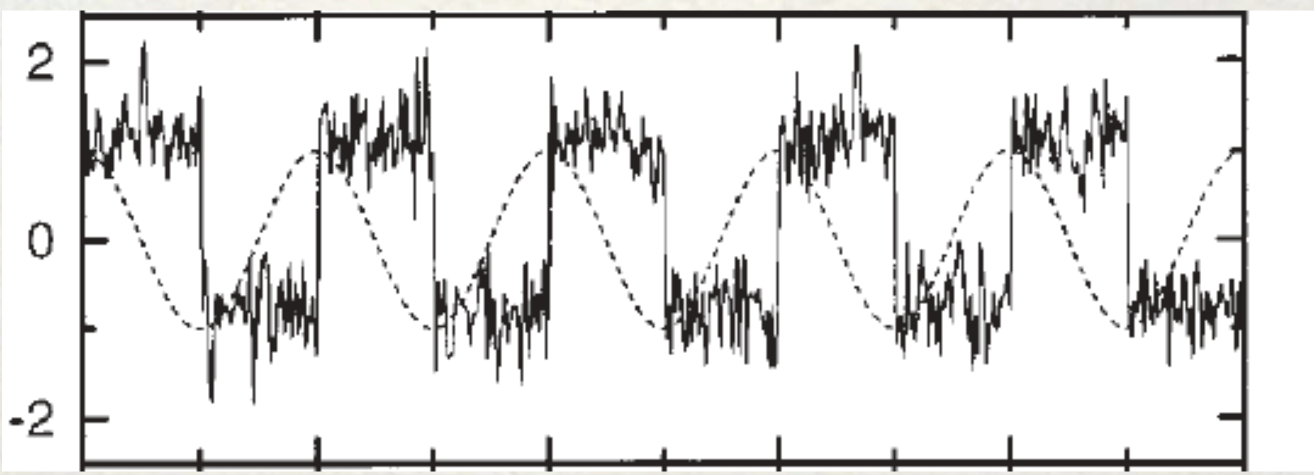
For **large** noise we will have **frequent** jumps



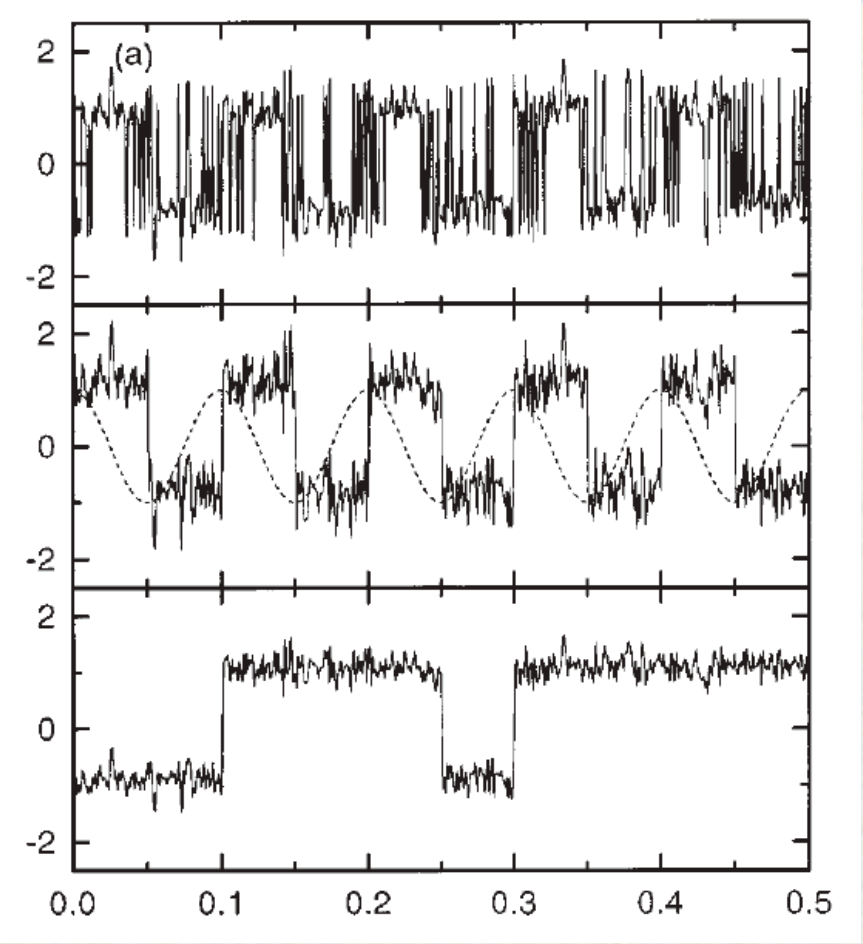
What if the periodic driving is to small
to let the marble to jump??

And in between ?

It exists an optimal noise intensity that produces the Jumps in synchrony with the forcing !!!



The **Stochastic Resonance** Phenomenon

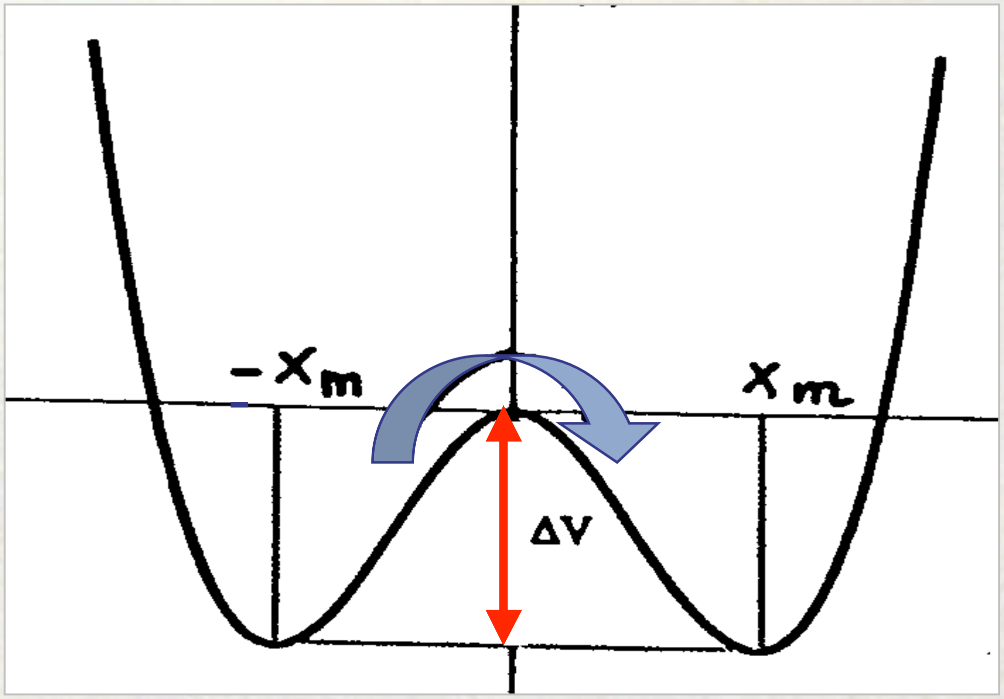


Large noise

Optimal noise

Small noise

Why such a peculiar behavior?



SR is the matching of two different time scales:

deterministic t.s. $\longleftrightarrow$ **stochastic t.s.**

Quantitative description:

approximations	
$A_0 x_m << \Delta V$	bistability
$A_0 x_m << D$	modulation as a perturbation
$\omega << \mu_k(D)$	adiabatic approximation

- **Kramers' mechanism:** rate

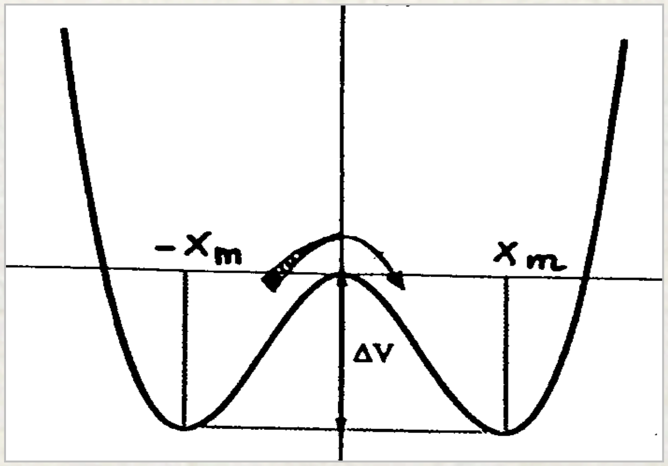
$$\mu_K(D) = (a\sqrt{2}/\pi)\ \left[1 - 3/8\ (D/\Delta V) + \ldots\right] e^{-\Delta V/D} \quad (D << \Delta V)$$

$$= 2 \times (\text{escape time})^{-1} \quad \pm x_m \rightarrow 0$$

SR is the matching of two different time scales:

deterministic t.s. $\longleftrightarrow$ **stochastic t.s.**

$$T_K = \mu_K^{-1} \qquad T_K = \frac{T_\omega}{2}$$

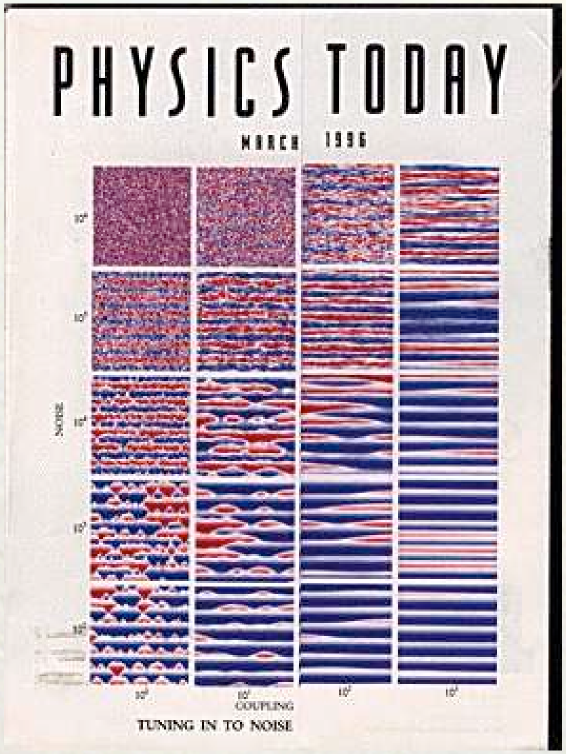


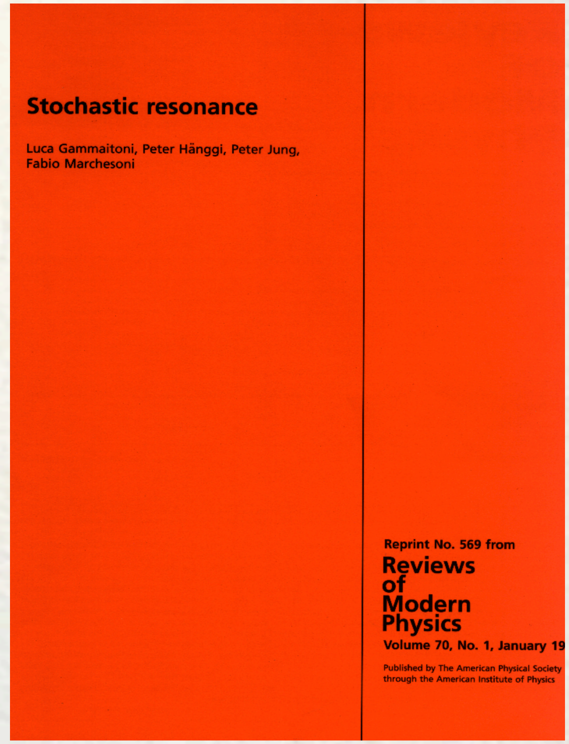
This was SR approximately 10 year ago

Since then a huge number of extensions of the very basic idea of SR where proposed and the situation got… slightly out of hand…

Risultati **1** - **10** su circa **228.000** per **"stochastic resonance"** . (**0,12 s)**

The **Stochastic Resonance** Phenomenon





A. R. Bulsara, L. Gammaitoni,
Physics Today Vol. 49, NO. 3, p. 39, 1996

L. Gammaitoni, P. Hanggi, P. Jung, F. Marchesoni
Rev. Mod. Phys. 70, 225 (1998)

Where are we !?

» list of contents

A. What do we mean with **noise**

B. Noise and non-linearity: a simple cartoon

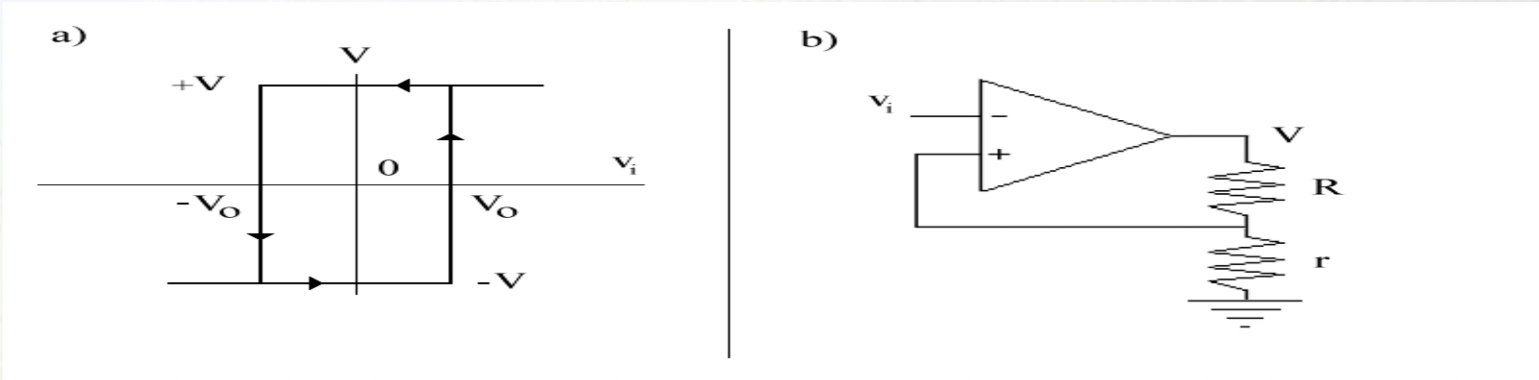
C. The strange case of the **Stochastic Resonance** phenomen

D. Other "surprising" noise induced phenomena

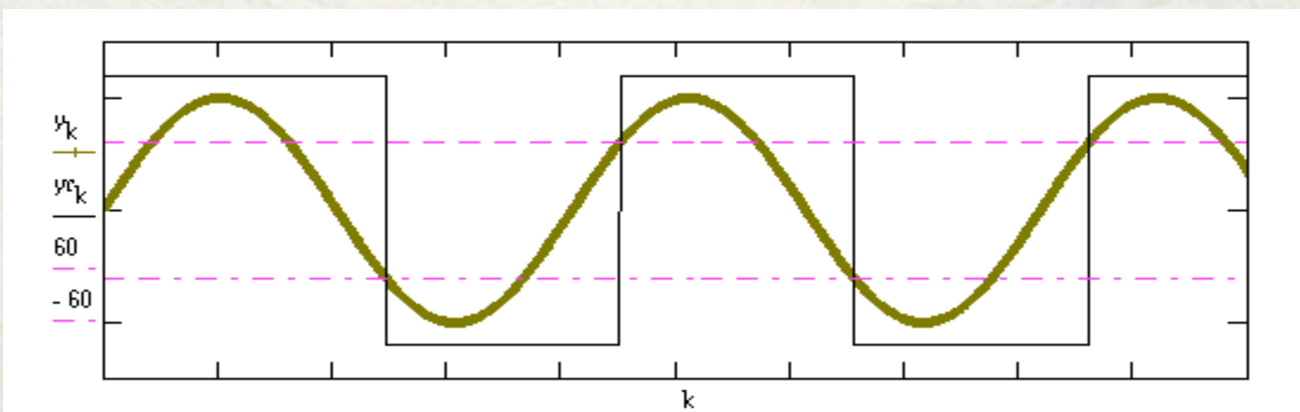
E. Stochastic nonlinear Dynamics at the nanoscale: modelling protein dynamics

C) Other "surprising" noise induced phenomena

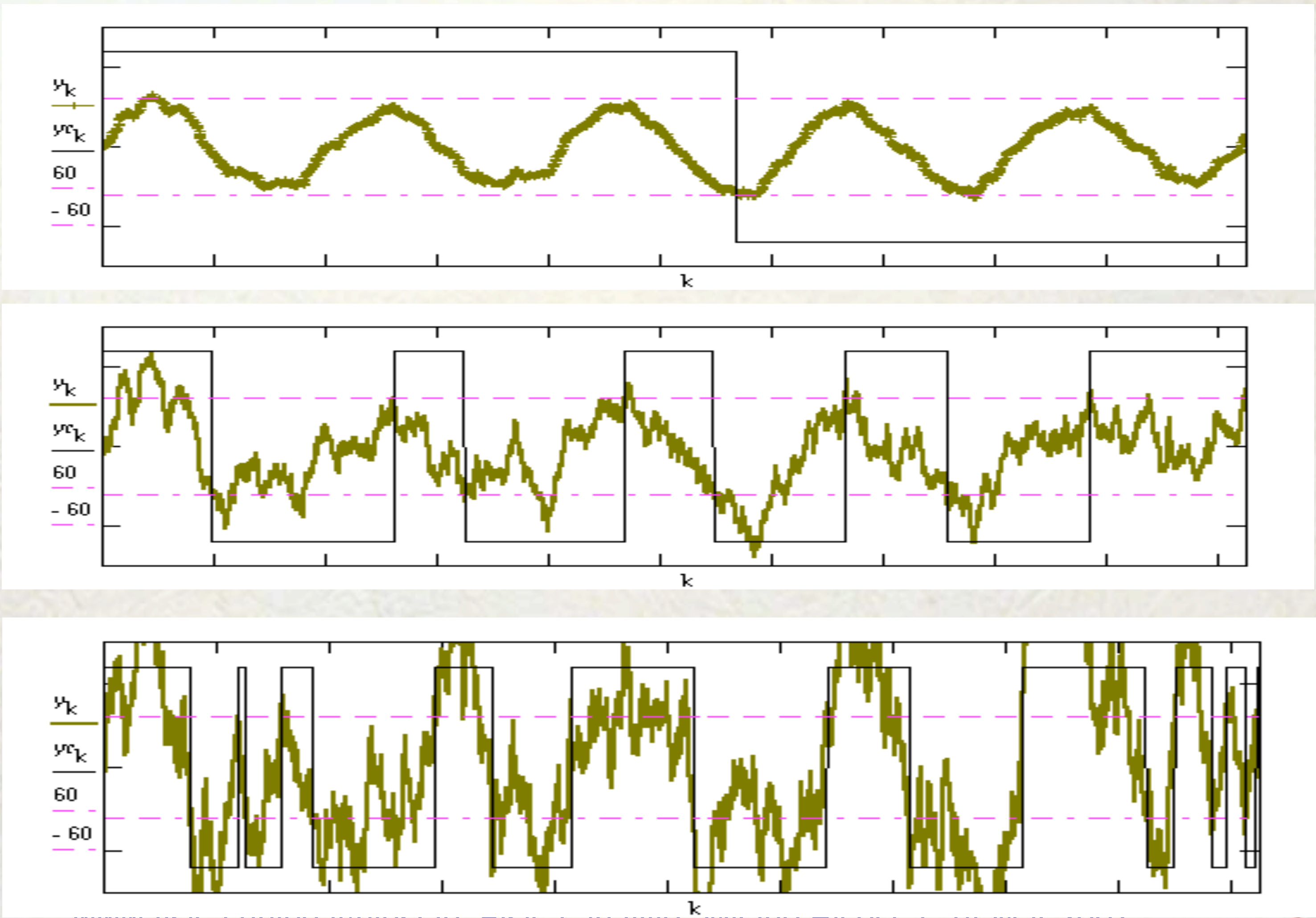
1. **Resonant Trapping**
2. Dithering Effect
3. Resonant Activation
4. Brownian Ratchet
5. Resonant crossing
6. …



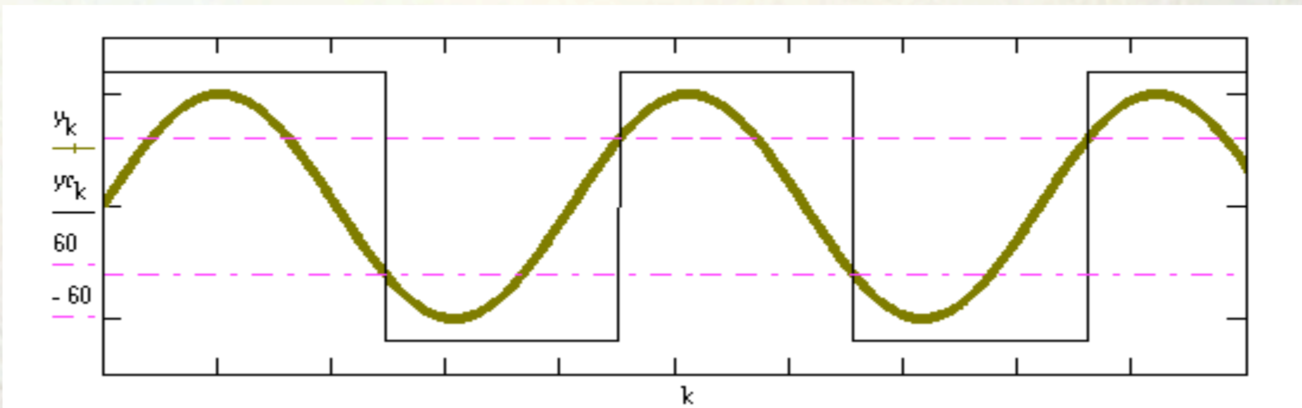
SCHMIDT TRIGGER: trasformation of a sinusoid



Stochastic Resonance in ST (after S. Fauve and F. Heslot - Phys. Lett. 97A 5 (1983))



SCHMIDT TRIGGER in the SUPRA-THRESHOLD regime



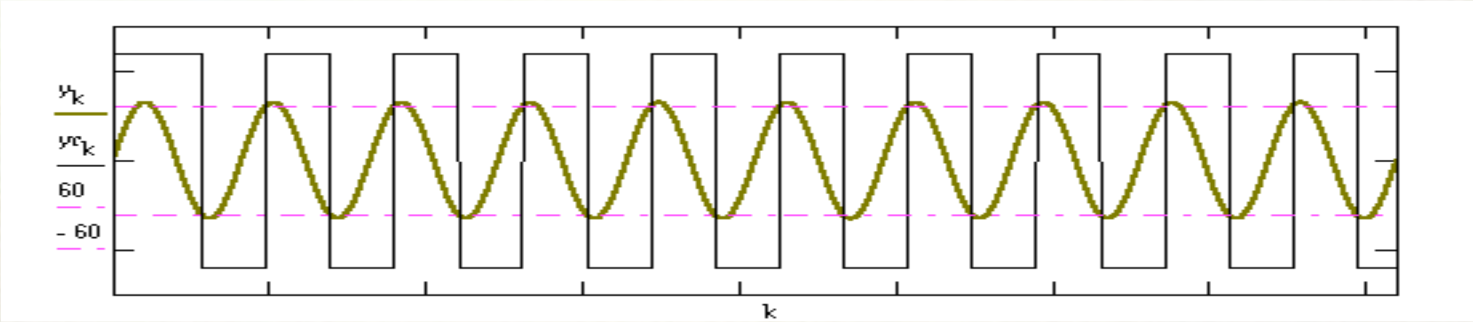
The RESONANT TRAPPING effect:

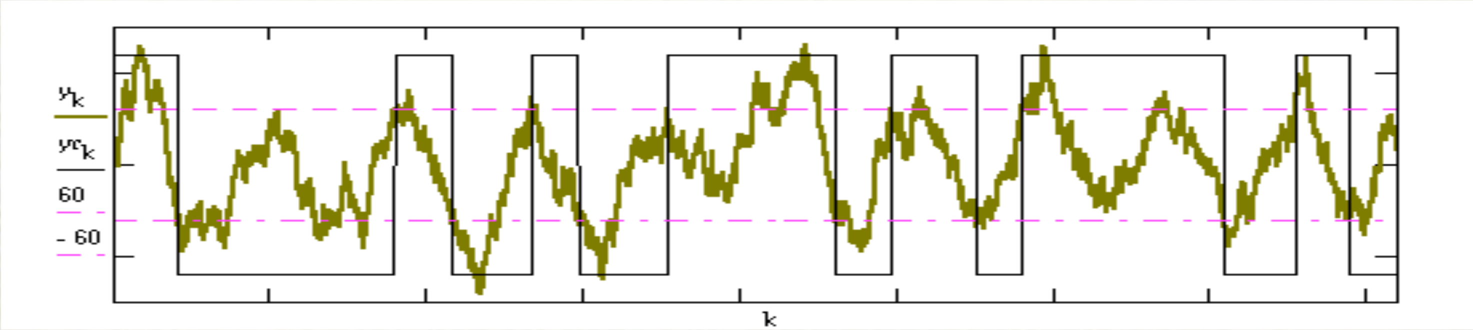
The trigger switches are tightly driven by the input periodic modulation, random failure events occurring sparsely in time due to the noise input component.

Stochastic Resonance

http://www.pg.infn.it/sr (in Italy)
http://www.umbrars.com/sr (in USA)

SCHMIDT TRIGGER in the SUPRA-THRESHOLD regime



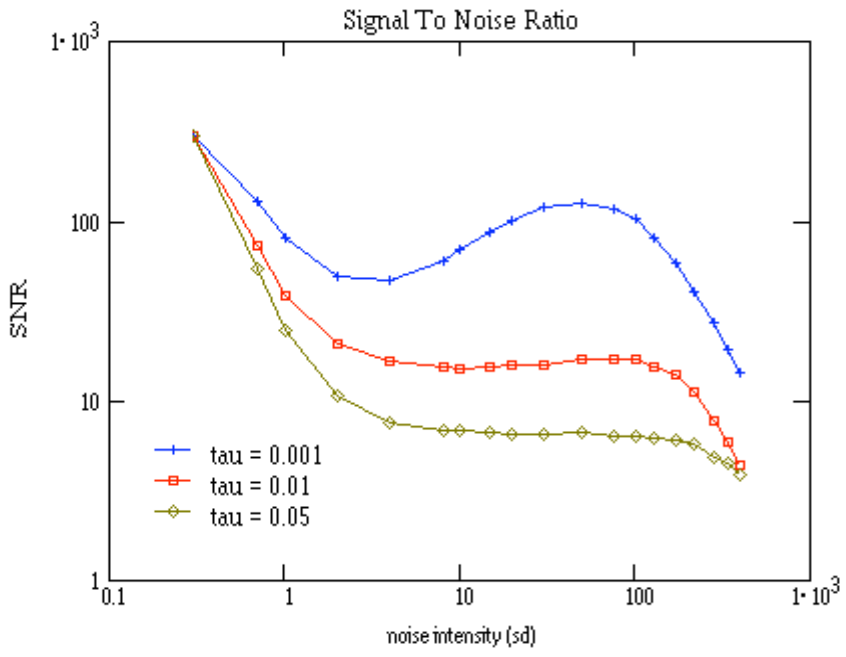


Resonant Trapping: A Failure Mechanism in Switch Transitions

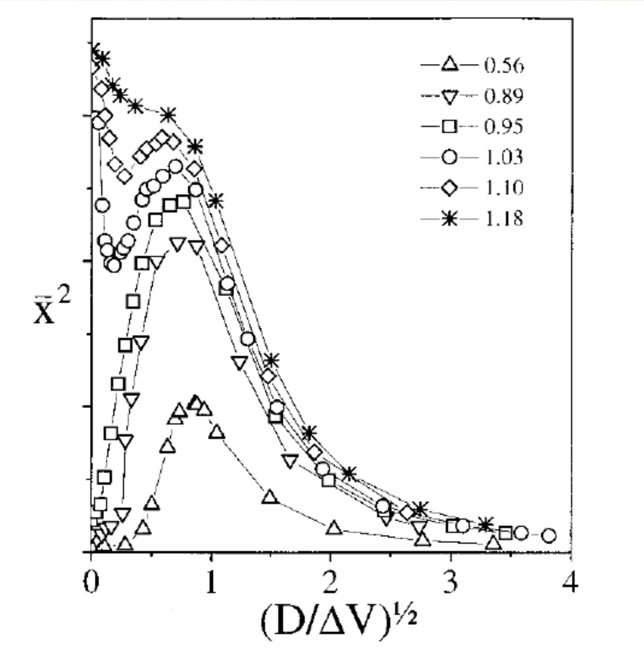
F. Apostolico, L. Gammaitoni, F. Marchesoni, S. Santucci

Phys. Rev. E 55, 36 (1997)

Resonant Trapping in a Schmidt Trigger



Resonant Trapping in a double well



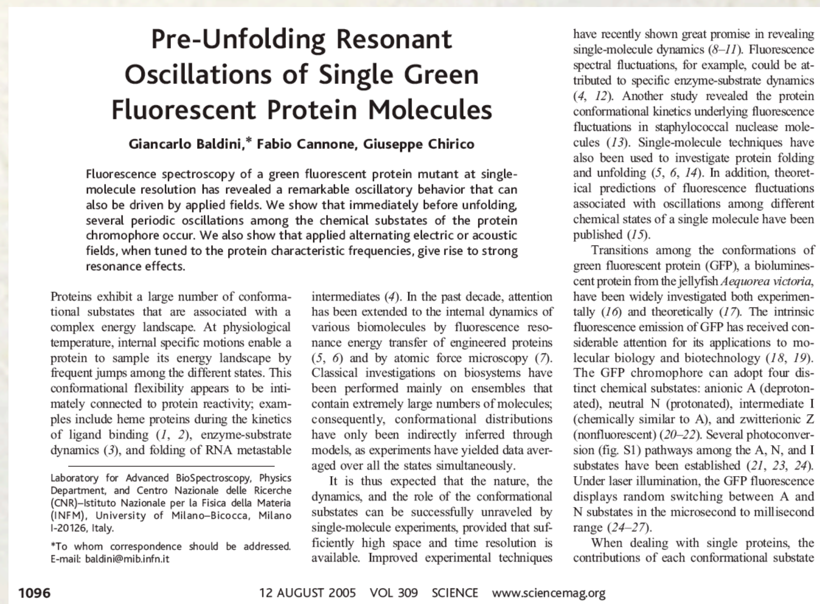
Where are we !?

» **list of contents**

Stochastic nonlinear Dynamics at the nanoscale: modelling protein dynamics

An example from the neighbors:

Pre-Unfolding Resonant Oscillations of Single Green Fluorescent Protein Molecules
Giancarlo Baldini, Fabio Cannone, Giuseppe Chirico
Science 309, 1096 (2005);



Pre-Unfolding Resonant Oscillations of Single Green Fluorescent Protein Molecules

Giancarlo Baldini,* Fabio Cannone, Giuseppe Chirico

Fluorescence spectroscopy of a green fluorescent protein mutant at single-molecule resolution has revealed a remarkable oscillatory behavior that can also be driven by applied fields. We show that immediately before unfolding, several periodic oscillations among the chemical substates of the protein chromophore occur. We also show that applied alternating electric or acoustic fields, when tuned to the protein characteristic frequencies, give rise to strong resonance effects.

Proteins exhibit a large number of conformational substates that are associated with a complex energy landscape. At physiological temperature, internal specific motions enable a protein to sample its energy landscape by frequent jumps among the different states. This conformational flexibility appears to be intimately connected to protein reactivity; examples include heme proteins during the kinetics of ligand binding (*1*, *2*), enzyme-substrate dynamics (*3*), and folding of RNA metastable intermediates (*4*). In the past decade, attention has been extended to the internal dynamics of various biomolecules by fluorescence resonance energy transfer of engineered proteins (*5*, *6*) and by atomic force microscopy (*7*). Classical investigations on biosystems have been performed mainly on ensembles that contain extremely large numbers of molecules; consequently, conformational distributions have only been indirectly inferred through models, as experiments have yielded data averaged over all the states simultaneously.

It is thus expected that the nature, the dynamics, and the role of the conformational substates can be successfully unraveled by single-molecule experiments, provided that sufficiently high space and time resolution is available. Improved experimental techniques have recently shown great promise in revealing single-molecule dynamics (*8–11*). Fluorescence spectral fluctuations, for example, could be attributed to specific enzyme-substrate dynamics (*4*, *12*). Another study revealed the protein conformational kinetics underlying fluorescence fluctuations in staphylococcal nuclease molecules (*13*). Single-molecule techniques have also been used to investigate protein folding and unfolding (*5*, *6*, *14*). In addition, theoretical predictions of fluorescence fluctuations associated with oscillations among different chemical states of a single molecule have been published (*15*).

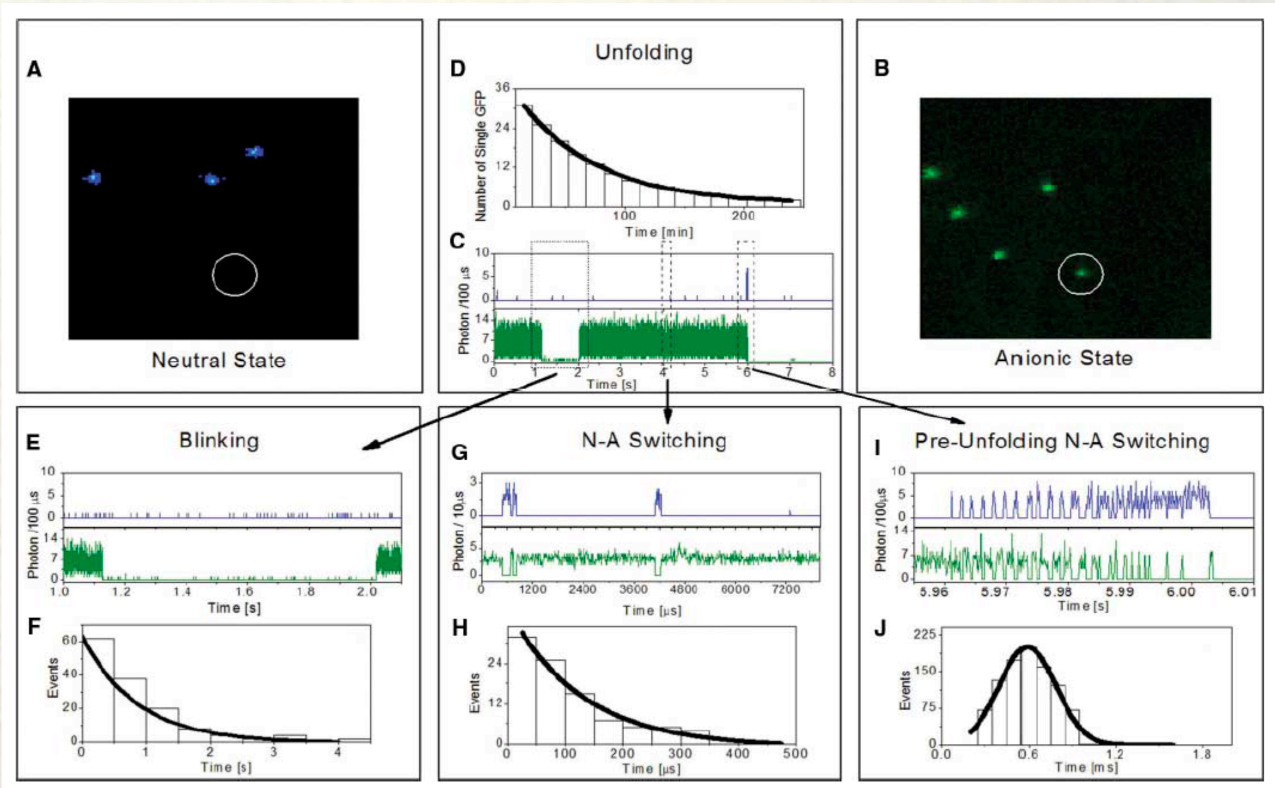
Transitions among the conformations of green fluorescent protein (GFP), a bioluminescent protein from the jellyfish *Aequorea victoria*, have been widely investigated both experimentally (*16*) and theoretically (*17*). The intrinsic fluorescence emission of GFP has received considerable attention for its applications to molecular biology and biotechnology (*18*, *19*). The GFP chromophore can adopt four distinct chemical substates: anionic A (deprotonated), neutral N (protonated), intermediate I (chemically similar to A), and zwitterionic Z (nonfluorescent) (*20–22*). Several photoconversion (fig. S1) pathways among the A, N, and I substates have been established (*21*, *23*, *24*). Under laser illumination, the GFP fluorescence displays random switching between A and N substates in the microsecond to millisecond range (*24–27*).

When dealing with single proteins, the contributions of each conformational substate

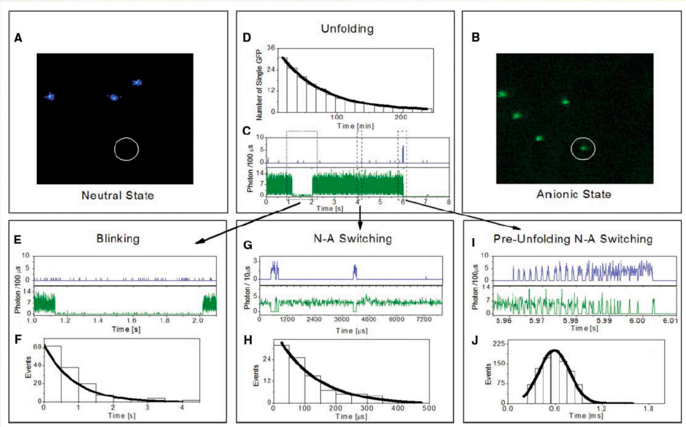
Laboratory for Advanced BioSpectroscopy, Physics Department, and Centro Nazionale delle Ricerche (CNR)–Istituto Nazionale per la Fisica della Materia (INFM), University of Milano–Bicocca, Milano I-20126, Italy.

*To whom correspondence should be addressed. E-mail: baldini@mib.infn.it

Two-photon fluorescence images of eight single GFPs in the 8 mm by 8 mm field of view.
Blue spots are molecules in the neutral state N; green spots are molecules in the anionic state A.



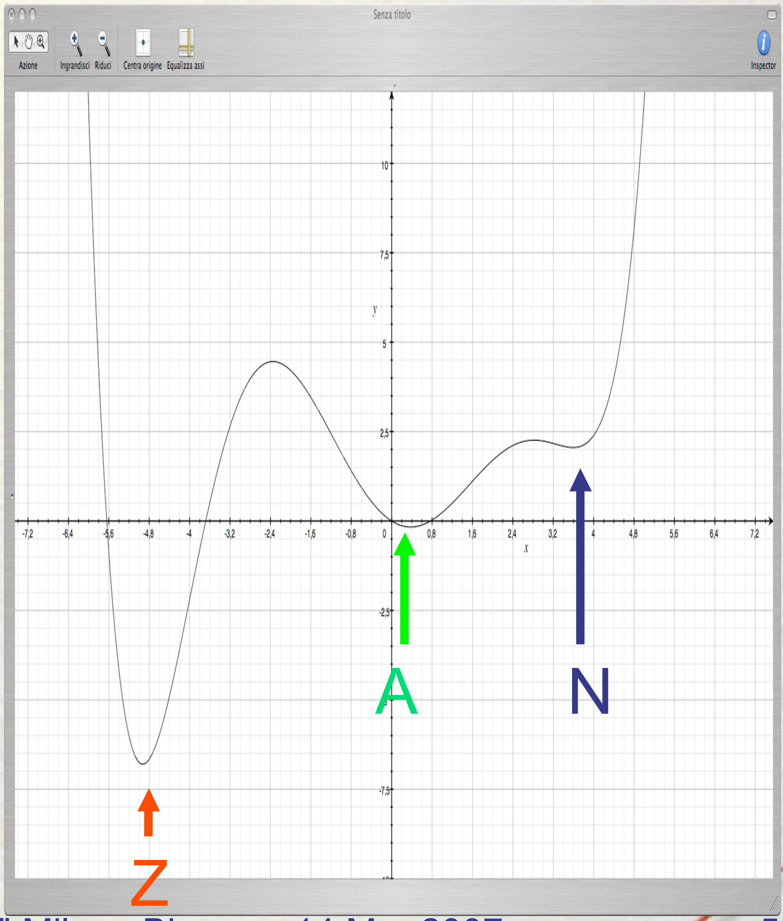
Phenomenological approach



Nonlinear stochastic
Dynamical model

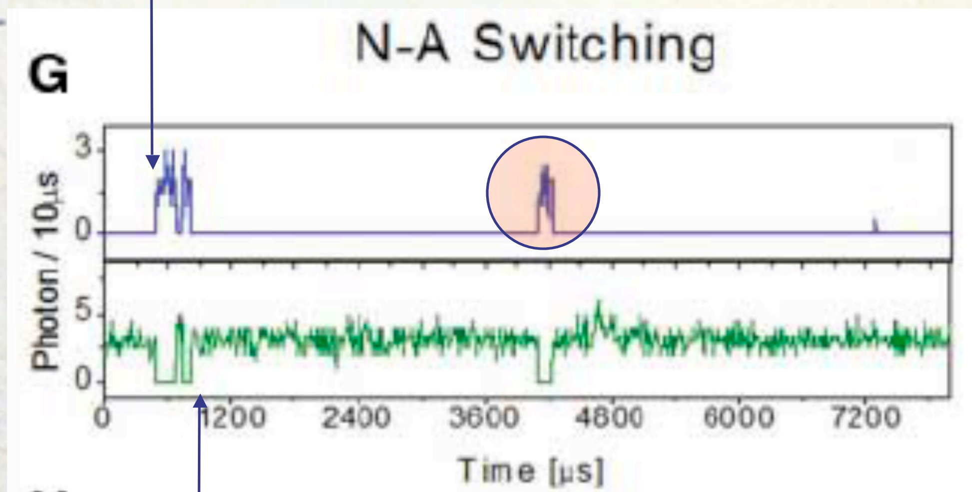
$$dx/dt = -dV(x)/dx + \xi(t)$$

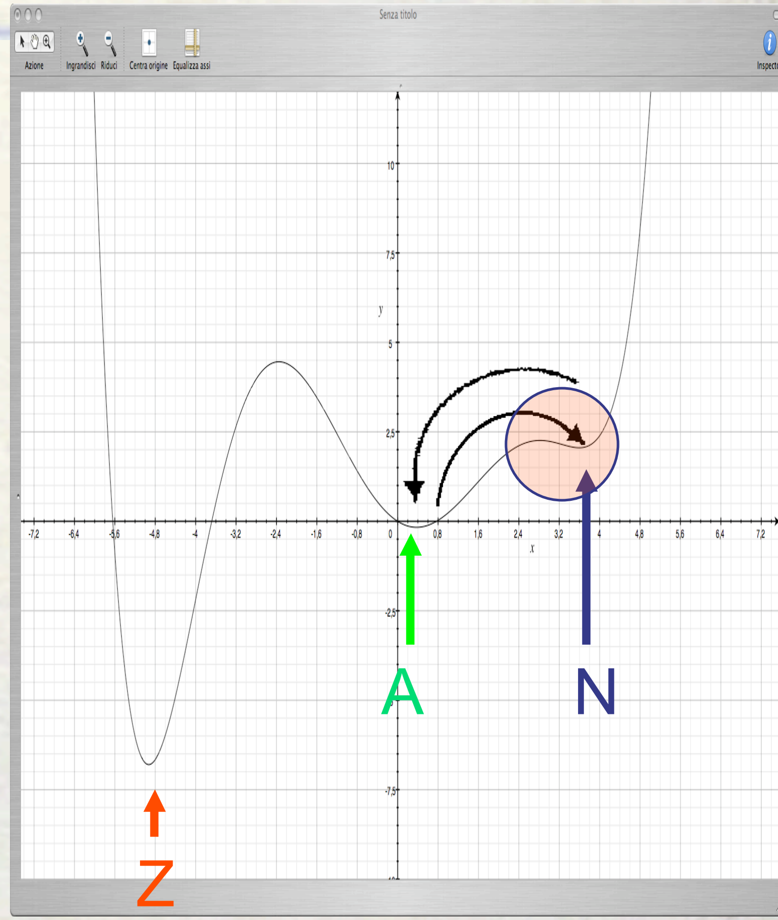
Noise !!!



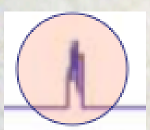
Phenomenon: N-A switching

Transition A-N

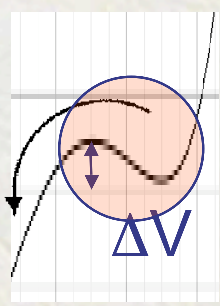




Transition N-A

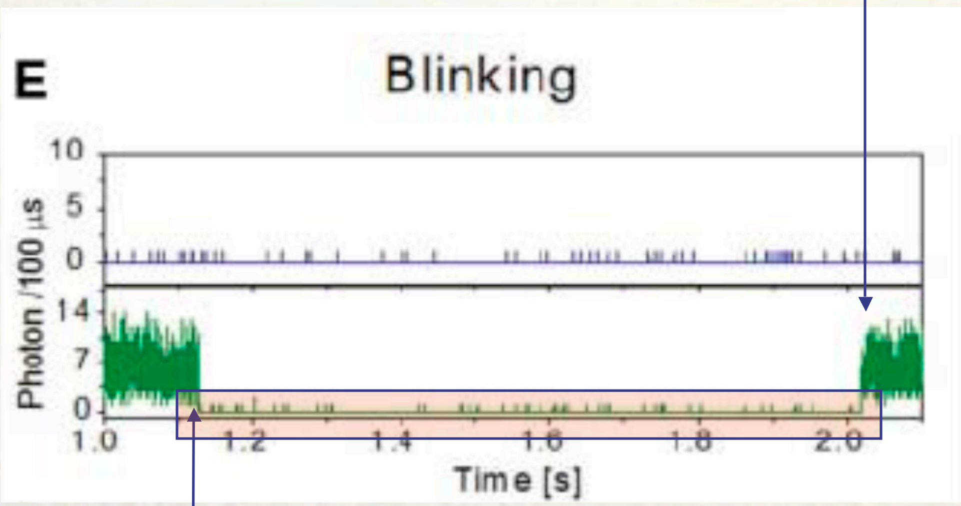


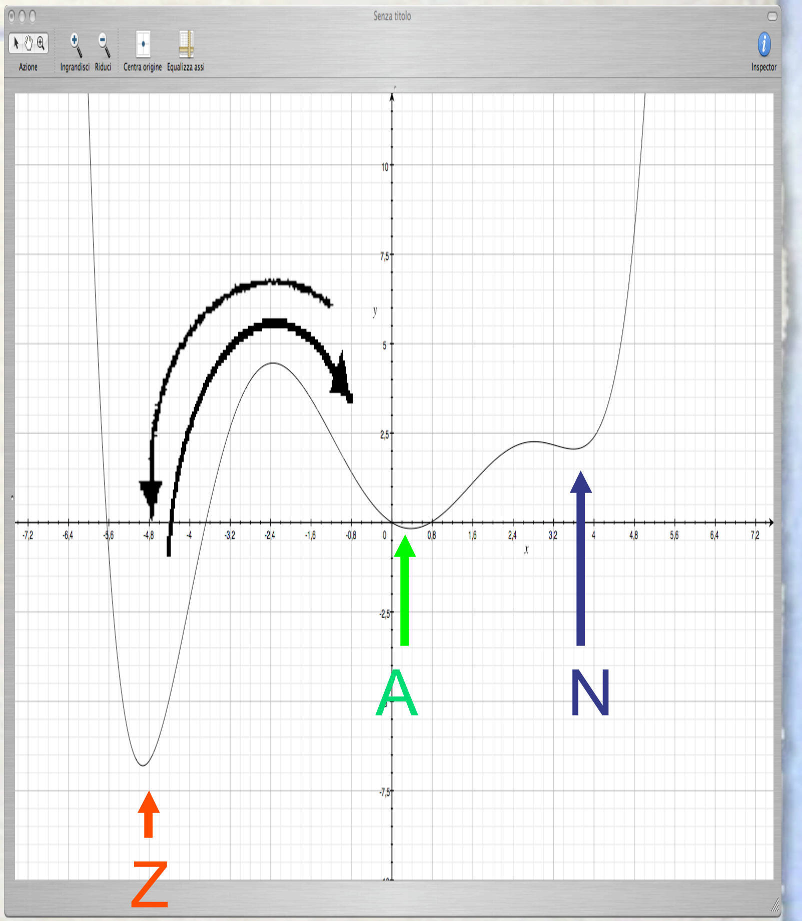
The average width is related to the height of the potential barrier



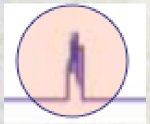
Phenomenon: A-Z Blinking

Transition Z-A

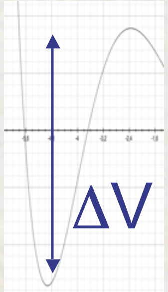




Transition A-Z

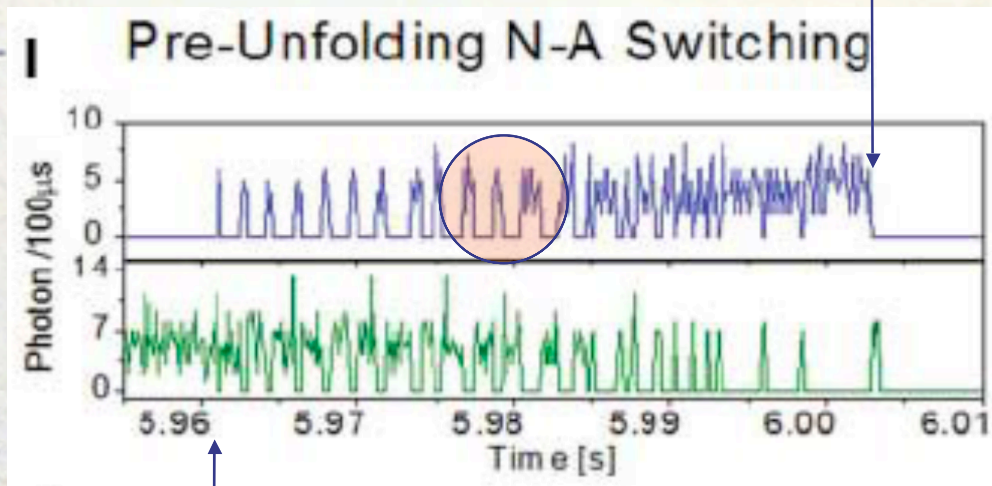


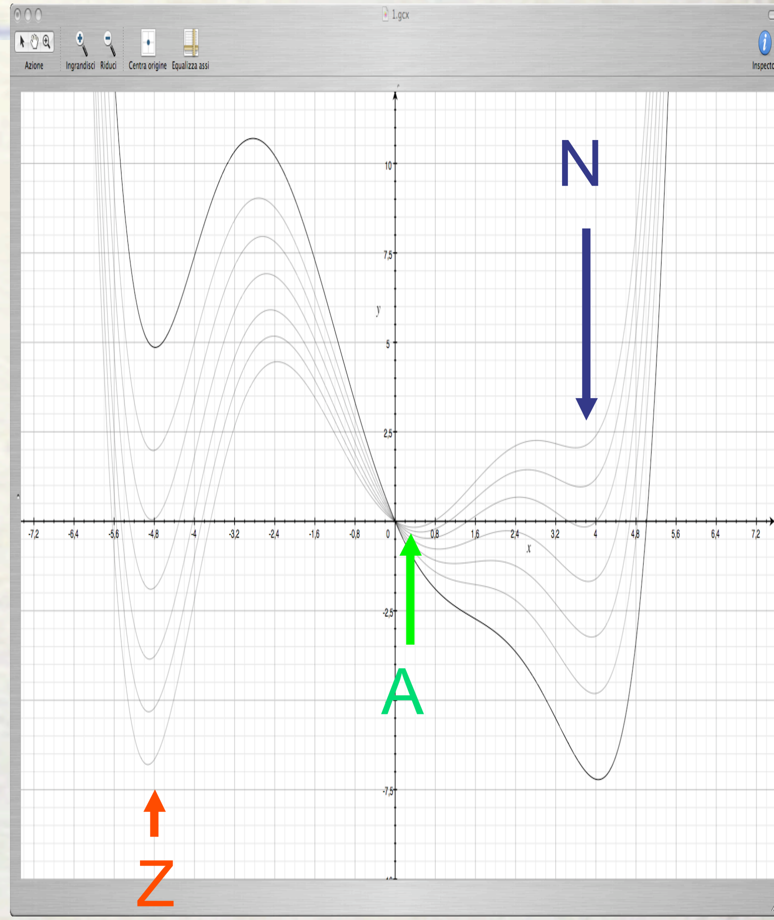
The average width is related to the height of the potential barrier



Pre-Unfolding: N-A Switching

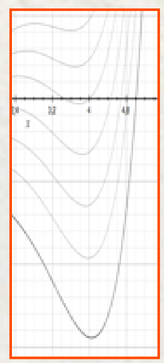
End unfolding N prevalence





beginning unfolding A prevalence

The width (res. Time) changes as
the unfonding proceeds.



Conclusions…

Noise and Nonlinearity: an interesting mix!!!

There are more things in heaven and earth, Horatio, than are dreamt of in our philosophy.

W.Shakespeare, Hamlet