Statistical Mechanics
E0415

Fall 2020, lecture 10
Out-of-equilibrium

… previous take home

Fluctuation relations and strong inequalities for thermally isolated systems:

"I chose the Fluctuation relation article because I hadn’t heard about the second law of thermodynamics having two lower bounds on the amount of work performed on the system, so that caught my attention and I wanted to learn more about that. Also, I wanted more insight on how the results were derived both in the classical and quantum realms."

"I am not that interested in biology."

Recovery of Equilibrium Free Energy from Nonequilibrium Thermodynamics with Mechanosensitive Ion Channels in E. Coli:

"I chose the article “Recovery of Equilibrium Free Energy from Nonequilibrium Thermodynamics with Mechanosensitive Ion Channels in E. Coli”mostly because I was interested in the application of non-equilibrium thermodynamics to the other fields. Also, this paper introduced several new concepts and techniques used in biology that were new to me."

"The reason why I chose this paper was because it is interesting to see the elements of statistical mechanics applied to fields that are very different from my own."

"This time, I picked the paper focused on applications, as the protein-folding example in Fourcade's lecture notes seemed interesting and this paper on biological systems is from the same field."

… examples…

"The paper introduces how fluctuation relations can be used as a route both for deriving the bounds/inequalities of the 2nd law, and how the law applies to microscopic systems. For example, the non-equilibrium work relation is valid as a fluctuation relation for both adiabatic and isothermal processes, and implies the validity of the weak bound.

In particular, the strong bound for adiabatic processes is explored via the derivation of an integral fluctuation relation and is satisfied on average for an example of an adiabatic system.

For a quantum system with a non-degenerate energy spectrum undergoing an adiabatic process, it is suggested that the final quantum number is on average greater than the initial quantum number. This implies an inequality between the two numbers and thus a work inequality for the given system.

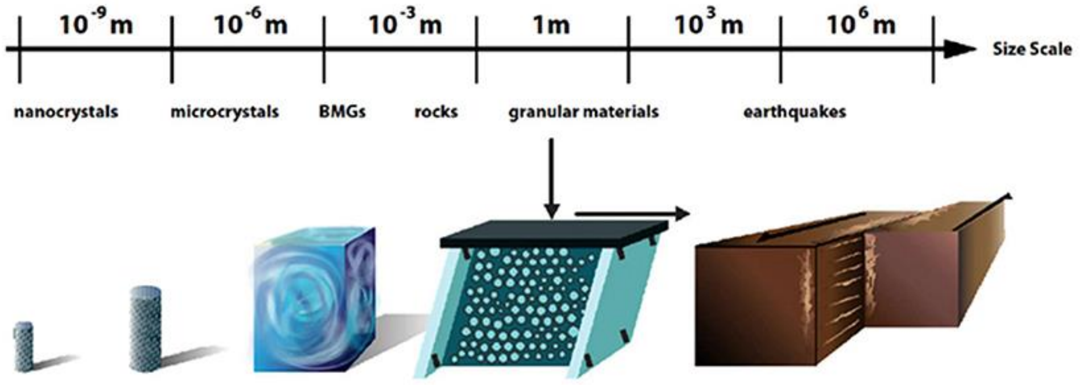
Overall, the paper shows that the probability to observe violations of the strong bound decays exponentially in the near tail of the work distribution, and can be neglected in the fair tail. They also note the consistency with empirical observations where macroscopic violations of the strong bound are never observed."

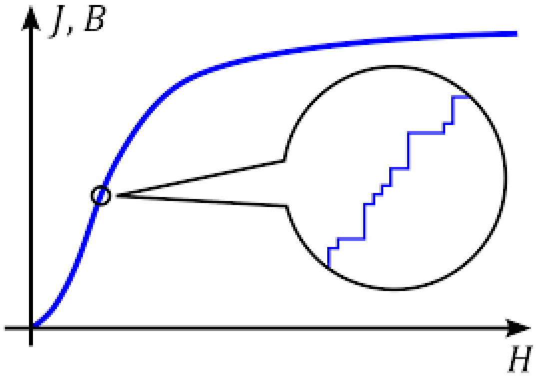
Biology:

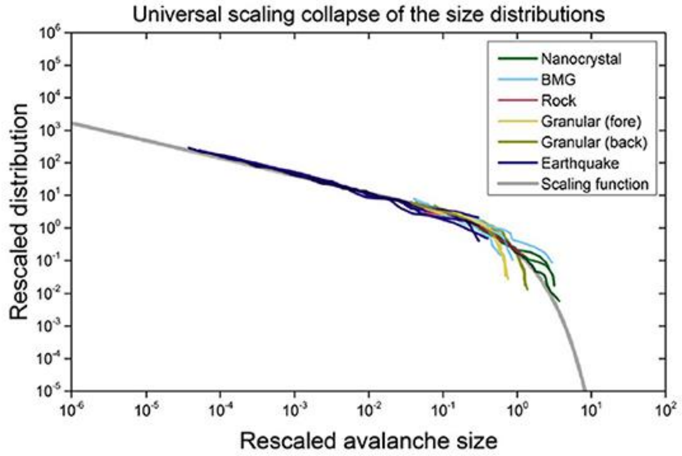
"The paper is about measuring the free energy difference between the states of open and closed ion channels on a cell membrane. A cell uses ion channels on its membrane to regulate the pressure of water inside the cell. For example, during a rainstorm a bacterium might face high osmotic pressures on its cell membrane (lots of water molecules suddenly coming in), at which point it opens ion channels on the membrane to release some of this water to avoid mechanical collapse. Now, this opening of ion channels can be experimentally realized by applying tension to the membrane. The authors propose to measure the work done on the system as the ion channels are opening, and again measure the work released when the tension is removed and the channels close, and then use Jarzynski's equality and similar statistical mechanics estimators to obtain a value for the free energy difference between the two states. Previously, equilibrium-based methods have been used to obtain varying values for the free energy difference, but this is not an equilibrium system. From the experimental data gained from bacteria, the authors use multiple different estimators and get much smaller variability in the obtained values than before. Finally, the authors point out that this methodology is quite general and could be applied to many other non-equilibrium biological systems as well."

Statistical mechanics for complex systems

Here are a few examples of "avalanching" systems: deformation up to earthquakes , Barkhausen noise (magnets), a real snow avalanche. How to understand such statistics?







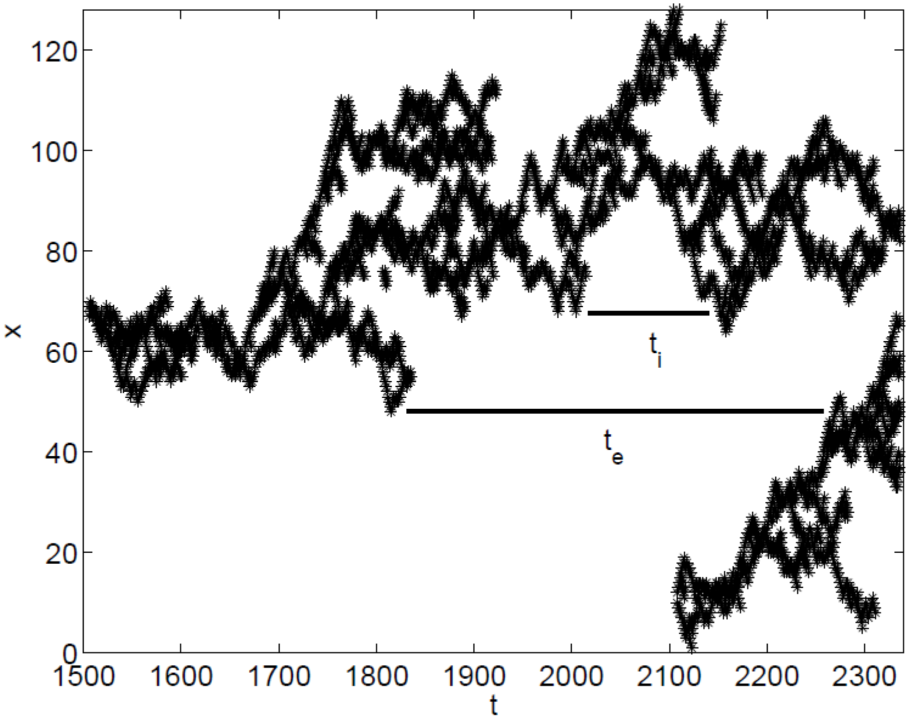
Activity map

A 1D model of activated random walkers.

Plot the locations where there is activity.

The pattern is (here) a self-affine fractal, since the system is in a (self-organized) critical state.

Correlation functions….
Avalanche distributions.

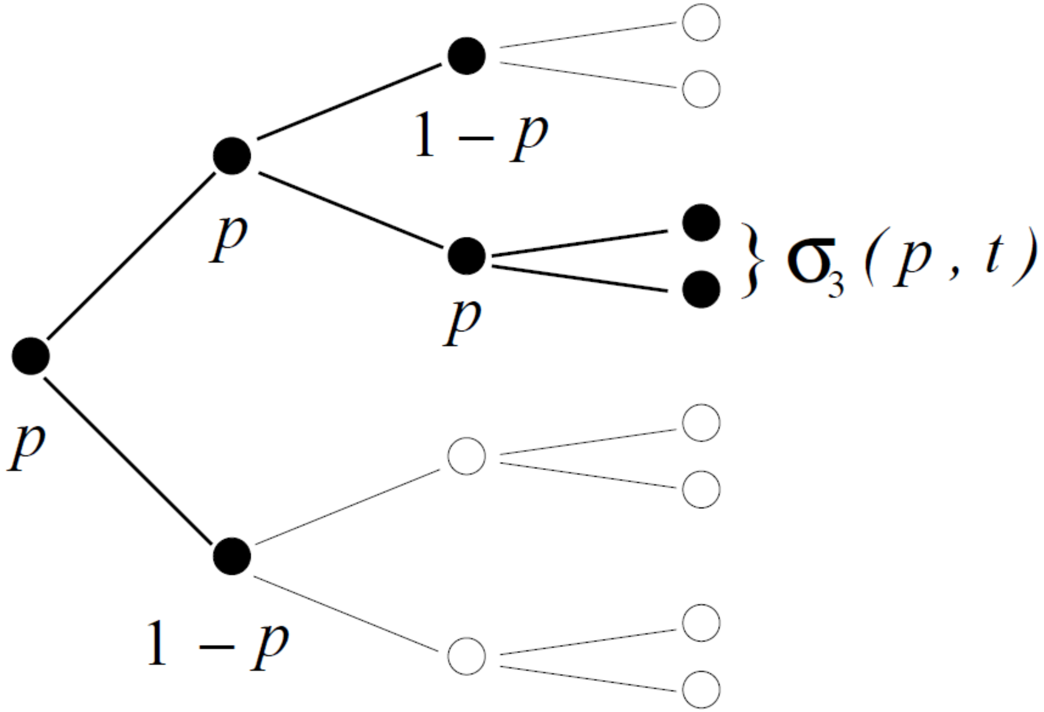


Branching process on a tree

Size of the avalanche? ”7”

Number of generations? 4 (0…3 counting also the seed).

Limit of infinite dimensions: the avalanche never re-visits the same location.

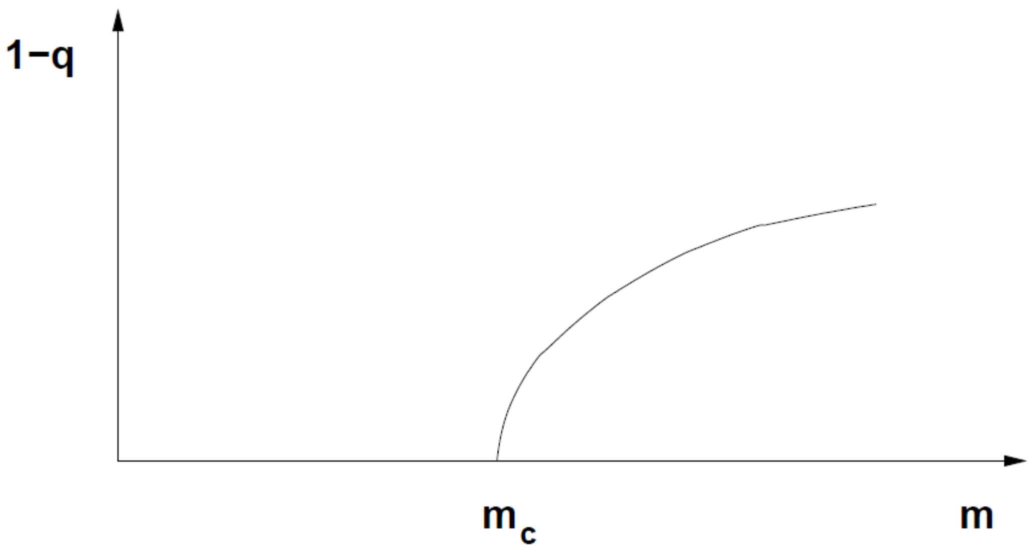


Critical properties

$$\text{Prob(survival)} = \begin{cases} 0, & m \leq m_c \\ (m - m_c)^{\beta}, & m > m_c. \end{cases}$$

Order parameter: survival probability.

Critical point value, order parameter exponent β.



Properties of critical branching processes

The statistics can be solved with the aid of the generating functions of the stochastic process as a function of generation n, and looking at the scale-free, Fixed-Point solution.

This shows that indeed, the avalanches are scale-free apart from a cut-off function.

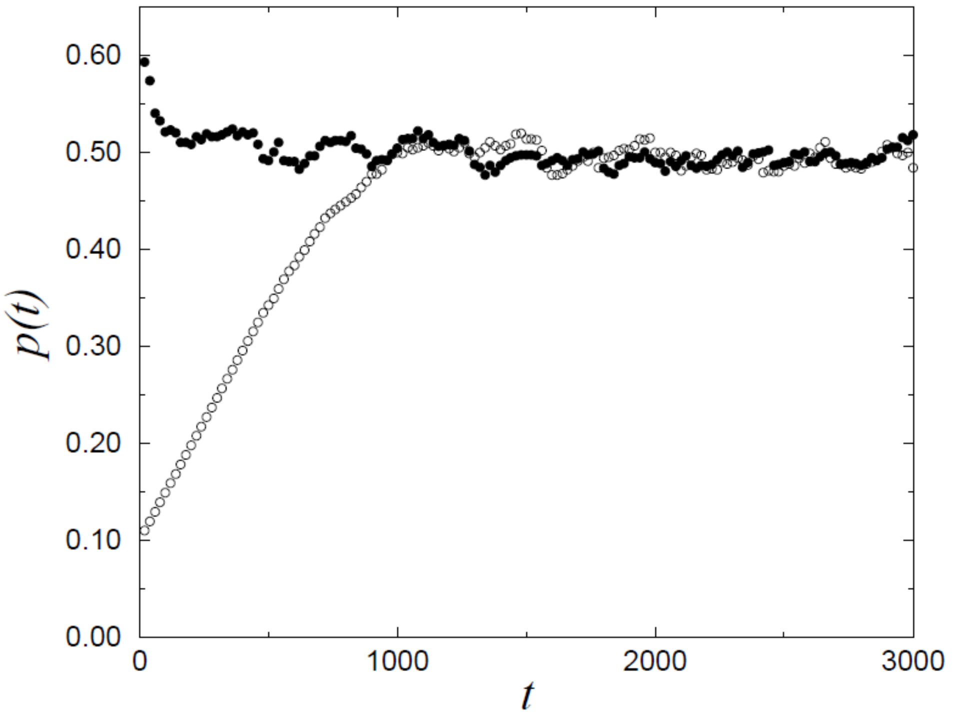
$$f(x,p) = \frac{1 - \sqrt{1 - 4x^2p(1-p)}}{2xp}.$$

$$P_n(s,p) = \frac{\sqrt{2(1-p)/\pi p}}{s^{3/2}} \exp\left(-s/s_c(p)\right).$$

Self-organized Branching Process

At a fixed n, we study the effect of the initial condition on the time-dependent branching probability p(t) (above and below the critical value).

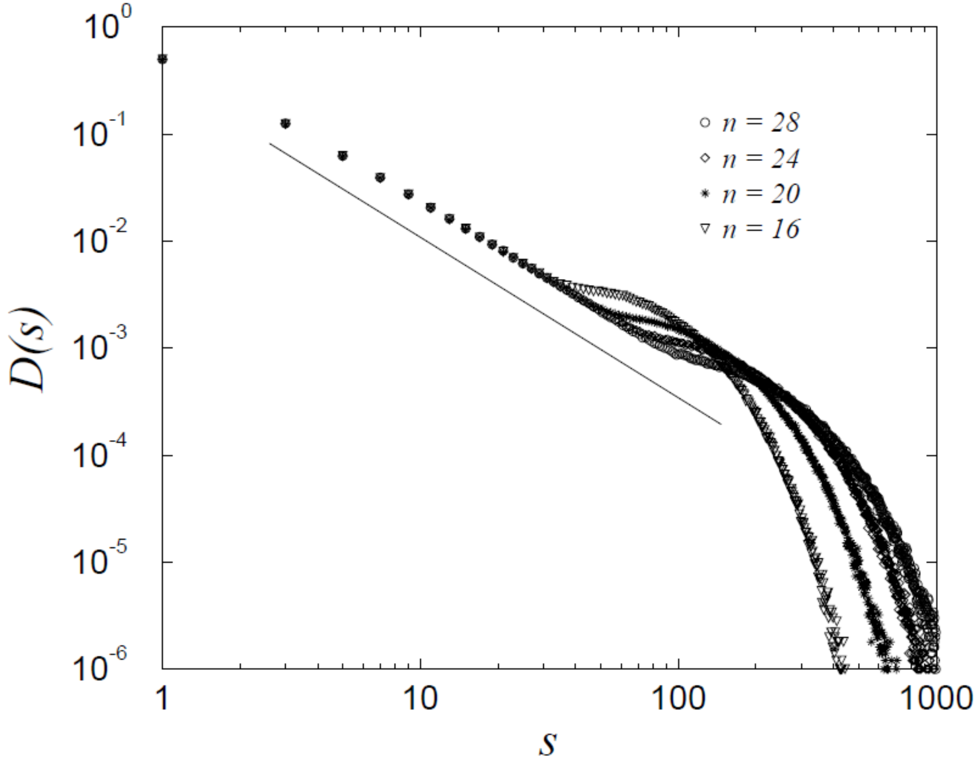
After transient periods, a fluctuating steady-state is reached.



SOBP: avalanches

At finite n, the avalanches follow the theoretical prediction (exponent -3/2, exponential cut-off).

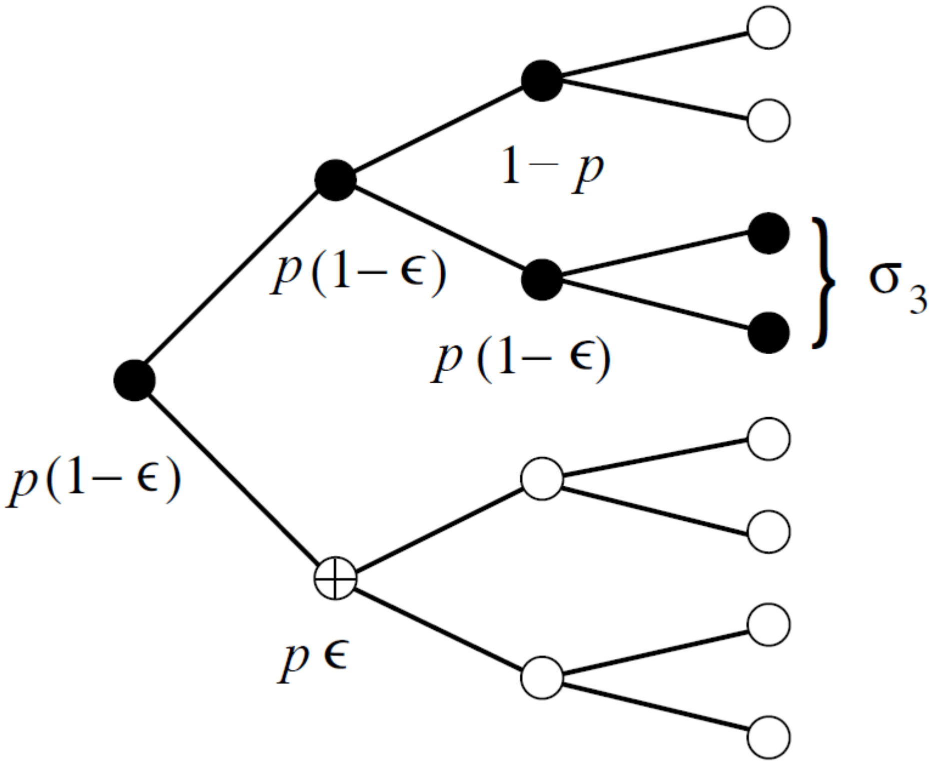
Similar results for durations T.



SOBP with dissipation

How does dissipation (of particles, energy…) influence the critical properties.

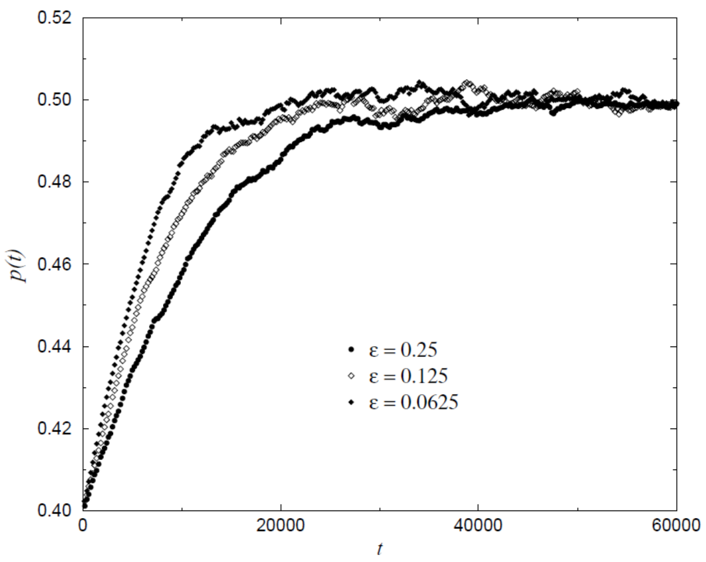
In the tree/mean-field picture this, “ε”, is easy to add to the process dynamics.

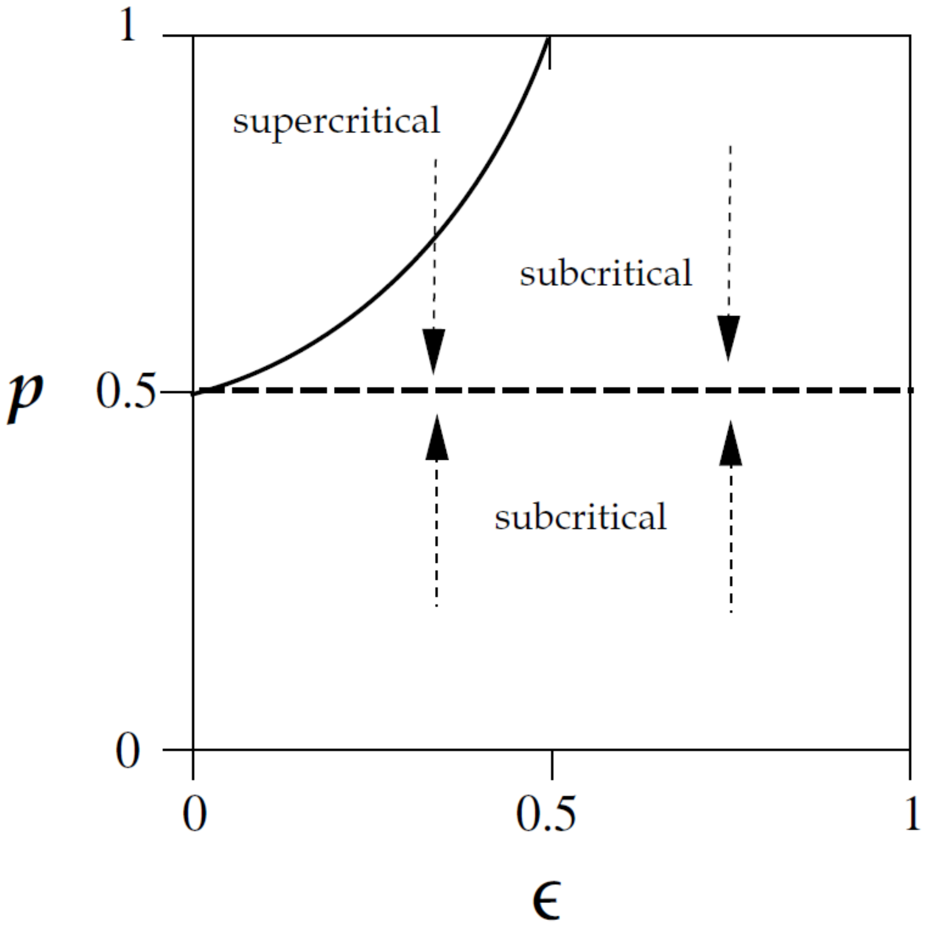


Phase diagram in the presence of dissipation

Dynamical equation for p(t):
steady-state.

Resulting phase diagram.

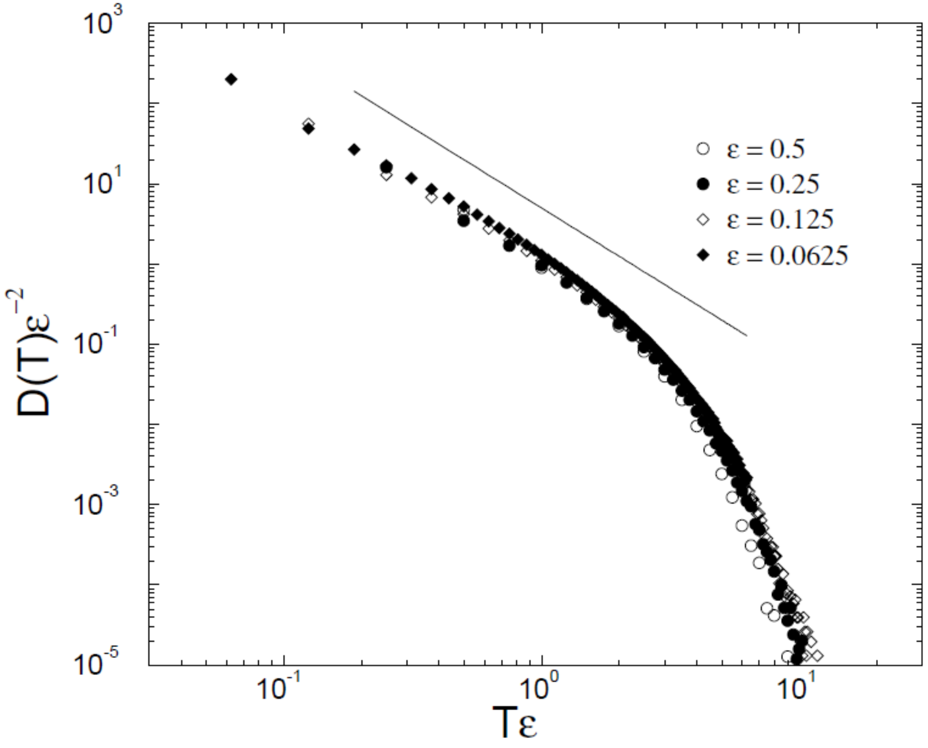


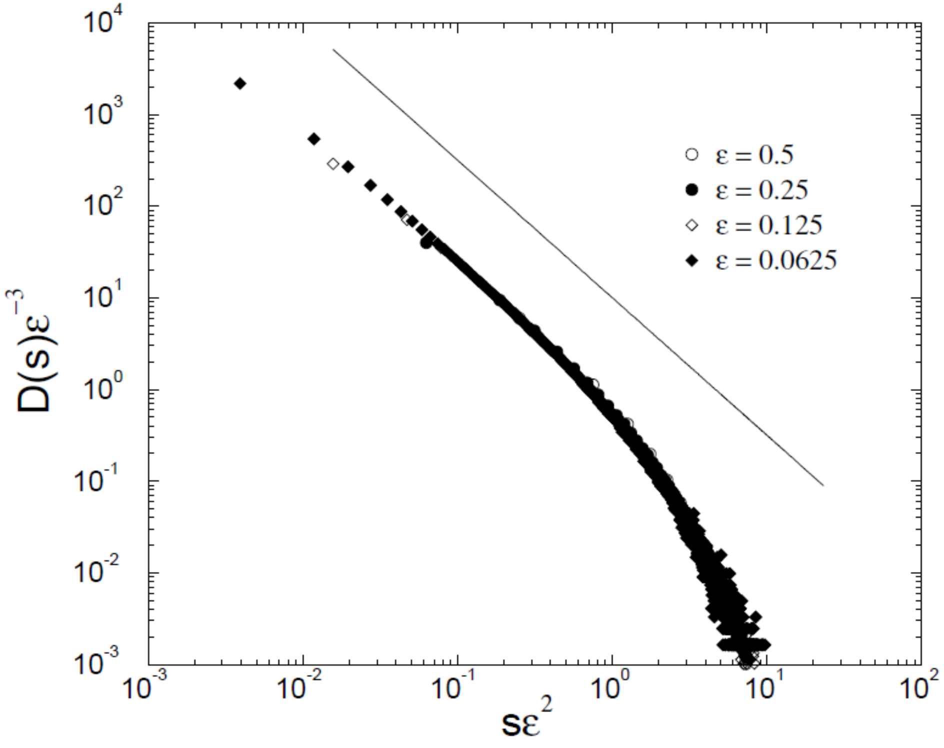


Avalanche distributions with dissipation

Distributions of durations, sizes with varying dissipation.

Rescaling/collapse of statistics (cf. x/y-axis).





Last take home

This time we study out-of-equilibrium systems that exhibit what is called crackling noise or bursts of activity. Such phenomena arise in many contexts (materials, astrophysics, geophysics - earthquakes, neuroscience, biology)…. and so forth. The material for this lecture is a set of lecture notes.

The key points are: understand some mechanisms (there are more) by which systems in nature produce such behavior. If you are really interested and want more depth you may have a look at the very recent review article in https://www.frontiersin.org/articles/10.3389/fphy.2020.00333/full

To finish off the take homes, we have again then a pick of THREE recent papers for you. These illustrate (all from 2020) the applications of such ideas to various fields.

We start from neuroscience

https://arxiv.org/abs/2011.03263

... move over to the deformation of materials....

https://advances.sciencemag.org/content/6/41/eabc7350

... and finish with earthquake (prediction) in a laboratory.

https://arxiv.org/abs/2011.06669

And your task is like the previous time "2+8" sentences on the selection and main points.

… end of the course…

On the 4th of December presentations of the computational projects.

We will that week let you know of your projected total score for the course.

Enjoy!