Statistical Mechanics
E0415

Fall 2020,
Overview of the course

Main facts (2020 pandemic version)

Lecturer Mikko Alava

Assistant Henri Salmenjoki

Pass the course: do the homework, present a research paper. Read the material, do the Take-home assignments. Computational home project and paper: done in groups.

50 (home work) + 10 (presentation) + 10 (computational project) + 12 (pre-exam) + 20 (take-home)+18 (exam) points: 120 max.

Pre-requisites for the courses

BSc level (EP major in the BSc @SCI):

PHYS-C0220 - Termodynamiikka ja statistinen fysiikka

Alternatively, basic thermodynamics. We have a take-home test for this purpose.

Material:

Statistical Mechanics

Entropy, Order Parameters, and Complexity

James P. Sethna
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853-2501

Book is available on-line. Additional lecture notes….

How this works…

- On Tuesdays, the teaching assistant provides additional help. On Fridays, we have a short summary of the material to be studied, a student research paper presentation, and a brief introduction to the next topic in the programme (take-home material, important points).
- Each week a set of exercises is published, out of which one problem is to be returned via MyCourses. The exercises will be based on the lecture notes. Also, the students are to do a take-home task (study the material for the week, reply to a question or two). On Friday, you get the take-home for next week and the home and demonstration problems. On Tuesday, you get hints and the demo problems are discussed. The answers are then expected by next Tuesday (so you have 1.5 weeks to do them). The take-home tasks have deadline on Thursday noon, so that we are able to collect your best solutions for discussion for the lecture on Friday. (First ones 17.9)

Organization of the course

The exercise slot is on Tuesdays at 14.15

The lecture slot is on Fridays 12.15-15. There are some changes as to the starting time (11.9 @14.30) due to other constraints (remote work by prof. Alava). MyCourses will follow this. 18.9 is at 12.15.

Lecture times preliminary scheme: 11.9, 18.9, 25.9, 2.10, 9.10, 16.10, 30.10 (note!), 6.11, 13.11, 20.11, 27.11 (10 times) and 4.12 a summary.

Computational projects presentation TBD, so for the presentations (after we divide you into groups).

Exercises 22.9, 29.9, 6.10, 13.10, 27.10 (note!), 3.11, 10.11, 17.11, 24.11, 1.12.

…. More on that…

The students are formed into groups to prepare the article presentations and the computational projects. The presentation and project topics are announced during the first lecture on Friday, September 11. You are expected to provide us your preferences from the topics (and eventual group partners) by email to TA Henri Salmenjoki by September 17 noon so that we are able to form the groups. The presentations are scheduled once we have assigned them to groups. The computational projects are returned towards the end of the course. We will dedicate one session to discuss these.

Questions?

- Homework, pre-test, computational projects, groups for them and presentations: Henri
- Presentations, lecture materials, general ones, Take-home sets: Mikko

Either check with us at Tuesdays/Fridays or send an email. The Zoom channel can be used for a remote meeting “at any time”.

Warning

We believe the work needed to learn and pass is reasonable.

However due to the changes in the organization we are not sure.

So at 1/3 we’ll give you a questionnaire.

Computational projects

1. Calculation of the Lyapunov spectrum
2. A spinning magnet
3. Models of opinion formation
4. The minority game
5. Nucleation and the Ising model
6. Domain growth kinetics
7. The classical Heisenberg model in two dimensions
8. Machine learning the phase transition of Ising model*

Student presentations

1) Nature Phys. **10**, 67 (2014), Negative temperatures I
2) Am. J. Phys. **83**, 163 (2015), Negative temperatures II
3) Science **296**, 1832 (2002), Jarzynski inequality
4) Science **324**, 1165 (2009), Entropy & information
5) Nature Phys. **16**, 186 (2020), Negative Representation and Instability in Democratic Elections
6) Phys. Rev. Lett. **95**, 105701 (2005), Quantum phase transition
7) Nature Phys. **9**, 644 (2013), Entropy production
8) Nature Comm. **4**, 2927 (2013) , Avalanches and their shape

Overview (additional comments)

- The first part concerns **equilibrium statistical mechanics**. The students are expected to have a basic understanding of traditional thermodynamics on the 2nd year undergraduate level (free energy, ensembles, and quantum gases) of non-interacting systems. This is tested at the first exercise session (compulsory attendance, please contact the lecturer if you can not make it) at the beginning of the course.
- We discuss fluctuations and scale-invariance in terms of **random walks**. Then second order **phase transitions** are studied in the framework of the Ising model and in the context of percolation. The question of how a phase transition looks like when abrupt (first order) is discussed, as well as the role of entropy, disorder, and quantum effects all of which are fundamental in **correlated systems**.
- In the second part we turn to **nonequilibrium** statistical mechanics. We go through the fundaments of how physical systems behave slightly out of usual equilibrium: how the fluctuations in thermodynamic quantities reflect this and how does the relaxation take place. We then move over to truly nonequilibrium systems. The fundamental ideas relevant to common examples are overviewed (the theory of absorbing state phase transitions among others) as well as concrete examples.

Student paper presentations

Research articles:

We discuss a research article related to current topics in statistical mechanics. Students will be designated (or volunteer) to give a brief presentation of the paper. All students are strongly encouraged to read the article at least once or twice. While reading, think about the following five questions (and try not to get caught up in the details):

- 1. What is the main idea of the paper? (What do the authors actually do?)
- 2. What is the key message of the paper?
- 3. How do the authors reach that conclusion?
- 4. What is the most interesting aspect of the paper?
- 5. In what way could the research be improved or extended? What are the open questions?

The presentations:

We will have a 15 minutes presentation of the paper given by the designated students. The presentation is short, so spend the time wisely, keeping the questions above in mind. Try to present the main ideas of the paper without dwelling too much on details. After the presentation, we will have about 10 minutes for discussions to wrap up the session. All students/groups are encouraged to share their views during the discussions.

Additional material: Topics I

- Properties of typical random walks as examples of coarse-graining, and fluctuations. Diffusion equation, Fokker-Planck and Langevin equations.
- Response and correlation functions.
- Second order phase transitions: order parameter, scaling.
- Examples: the Ising (and Potts) models, percolation, applications.
- First order transitions.

Topics II

- Entropy in correlated systems and applications (information), the role of disorder and quantum effects (quantum phase transitions).
- Jarzynski and Crooks relations for systems pushed out of equilibrium, relaxation processes.
- Fluctuations and scaling in out of equilibrium systems and their phase transitions.
- Branching processes as a theory, and applications.

“What is statistical mechanics?”

- Ensembles
- Entropy
- Quantum statistical mechanics
- Monte Carlo
- Phases
- Fluctuations and correlations
- Abrupt phase transitions
- Criticality

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Entropy

“Thermodynamic property” (Free energy: $F = U - TS$)

Now: a measure of disorder and information – “how many bytes do I need to represent some data?” “how complicated is this empirical data?”

Uses in computer science and algorithms (Shannon)

Fluctuations and correlations

- Systems are not uniform, and nor random – they are correlated. They can be VERY correlated (close to phase transitions). We need measures.
- Physical systems fluctuate in time and space. We need measures for this and we need to understand how these scale with time and lengthscale(s) – Random walks and diffusion.
- Systems are "dissipative"- there is friction. Thus the response, and the correlations, and the fluctuations, are connected. Why? They all are dependent on the dissipation.

Phases

- Gases and liquids and solids tell us that the same stuff can be in different phases. All these are characterized by an order parameter, a quantity which tells that (if measured) the system is just in this phase and not in another.
- Order parameter means the presence of some kind of symmetry which distinguishes the phase (think of crystal lattices, or magnets with a finite permanent magnetization).
- The order parameter is a field, it varies in time and space (line, plane, sphere, 3D space). The field can have “typical defects”, or topological defects (the symmetry goes missing).

Criticality

- Many phase transitions are such that the time and space need to be re-defined close to the transition point (eg. critical temperature, force driving the system): they become scale-free below a time scale (correlation time) or spatial scale (correlation length). This diverges approaching the transition.
- Such systems exhibit often universality: minor details may be forgotten due to the divergent scales. The concept of universality classes ensues (what are the typical symmetries / properties?).
- Technical terms: scaling, renormalization – to grasp the critical exponents such as describe the correlation length.

Abrupt phase transitions

- Most systems do NOT have continuous transitions – gas to liquid: an energy cost to heat to liquid to gas exists and is important.
- Such systems show metastability – one can push a system into another phase, where it will exhibit a “lifetime”, before equilibrium takes over.
- Since correlation lengths are not “large” another characteristics are needed to describe the phases separated the phase transition (liquid-gas, gas-solid for two examples).

Monte Carlo

- Markov chains: basic mathematical tool (to understand convergence) to simulate the properties of systems at finite temperatures.
- Many systems of interest not amenable to analytical treatments: MC the way to compute statistical quantities numerically.
- Phase diagrams (order parameter at a temperature), response to external perturbations (temperature, magnetic field…), relaxation from out of equilibrium and nucleation phenomena, truly non-equilibrium systems.