Syllabus

«Statistical Mechanics: Algorithms and Computations»

for educational program “Materials. Devices. Nanotechnologies”

Approved by

The Academic Council

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Credits	3
Contact work (hours)	0
Individual work (hours)	114
Course	1
The format of the discipline	on-line

I. Purpose, Learning Outcomes and Prerequisites

Purpose

Objectives of mastering the discipline "Statistical Mechanics: Algorithms and Computations":

- give students an idea of modern physics (classical and quantum) from basic computer programs that you will download, generalize, or write from scratch, discuss, and then hand in;
- give students an understanding of the essential concepts of Monte Carlo techniques (detailed balance, irreducibility, and a-periodicity), and Metropolis algorithm.

Learning Input

The study of this discipline is based on the following disciplines:

- classical statistical mechanics
- quantum mechanics

To master the discipline, students must possess the following knowledge and competencies:

- Python programming
- quantum statistical mechanics

Learning Outcomes

On completion of the course, the student should:

- understand the sampling, and its connection with integration
- understand the density matrices and path integrals

- understand the matrix-squaring technique

II. Topic-wise Course Content

Topic 1. Monte Carlo algorithms (Direct sampling, Markov-chain sampling).

This lecture covers Monte Carlo algorithms. In the tutorial we will use the 3x3 pebble game to understand the essential concepts of Monte Carlo techniques (detailed balance, irreducibility, and a-periodicity), and meet the celebrated Metropolis algorithm.

Topic 2. Hard disks: From Classical Mechanics to Statistical Mechanics

This lecture covers the hard-disk model, which was first simulated by Molecular Dynamics in the 1950's. The tutorial includes the difference between direct sampling and Markov-chain sampling, and the connection of Monte Carlo and Molecular Dynamics algorithms, that is, the interface between Newtonian mechanics and statistical mechanics. The tutorial also includes classical concepts from statistical physics (partition function, virial expansion et. al.).

Topic 3. Entropic interactions and phase transitions

This lecture covers the entropic interactions, coming only from statistical-mechanics considerations.

Topic 4. Sampling and integration

This lecture covers the sampling, and its connection with integration, the Maxwell and Boltzmann distributions of velocities and energies.

Topic 5. Density matrices and Path integrals (Quantum Statistical mechanics 1/3)

This lecture covers quantum statistical mechanics. The lecture starts from learning about density matrices and path integrals, fascinating tools to study quantum systems. In many cases, the Trotter approximation will be useful to consider non-trivial systems, and also to follow the time evolution of a system.

Topic 6. Lévy Quantum Paths (Quantum Statistical mechanics 2/3)

This lecture covers the properties of bosons, indistinguishable particles with peculiar statistics. At the same time, it will also go further by learning a powerful sampling algorithm, the Lévy construction.

Topic 7. Bose-Einstein condensation (Quantum Statistical mechanics 3/3)

This lecture covers the Bose-Einstein condensation phenomenon, theoretically predicted in the 1920's and observed in the 1990's in experiments with ultracold atoms.

Topic 8. Ising model - Enumerations and Monte Carlo algorithms

This lecture covers the Ising model, which captures the essential physics of a set of magnetic spins. This is also a fundamental model for the development of sampling algorithms.

Topic 9. Dynamic Monte Carlo, simulated annealing

This lecture covers dynamic Monte Carlo algorithm which runs faster than the clock. This is easily devised for a single-spin system, and can also be generalized to the full Ising model. In the tutorial we move towards the simulated-annealing technique, a physics-inspired optimization method with a very broad applicability.

Topic 10. The Alpha and the Omega of Monte Carlo, Review, Party

This lecture includes the experiment of Buffon's needle, already performed in the 18th century and its connection with the central limit theorem.

III. Assessment

An exam at the end of the course involves practical work for all students enrolled in the course. Topics covered by the test embraces all course material. If a student misses the exam because of some valid reason, s/he receives «absence» grade. The exam is assessed on usual 10-point scale. Formula for the final grade G is the following:

$$G=0.6Ex+0.4C,$$

where Ex is the grade for the exam, C is the cumulated grade for the course. If the cumulated grade for the course is bigger (or equal) than 40%, then the exam is cancelled and Ex is set equal to C.

100% scale	10-point scale
80-100 %	10
76-80 %	9
71-75 %	8
60-70 %	7
51-59 %	6
45-50 %	5
40-45 %	4
20-39 %	3
5-19 %	2
0-4 %	1

IV. Evaluation tools for student certification assessment

Current control of knowledge is not provided.

The knowledge gained in the course is evaluated on the exam.

V. Reading list

5.1 Optional

1. Reif, Frederick (1965). Fundamentals of Statistical and Thermal Physics. McGraw-Hill ISBN 0-07-051800-9.

2. Kittel, Charles (1969) Thermal Physics. Chichester: Wiley. ISBN 0-471-49030-X.2e Kittel, Charles; and Kroemer, Herbert (1980) New York: W.H. Freeman ISBN 0-7167-1088-9.

3. Mandl, Franz (1971). Statistical physics. Chichester: Wiley. ISBN 0-471-56658-6.2e (1988) Chichester: Wiley ISBN 0-471-91532-7, ISBN 0-471-91533-5.

5.2 Software

№ п/п	Title	Access conditions
1.	Python	From the university's internal network (contract)

5.3. Professional databases, information reference systems, Internet resources (electronic educational resources)

not required

5.4. Material and technical support of the discipline

not required