

## **Theoretical Physics (Statistical Physics)**

### **Course contents:**

**Statistical Physics** is quantitative study of systems consisting of a large number of interacting elements, such as the atoms or molecules of a solid, liquid, or gas, or the individual quanta of light (see photon) making up electromagnetic radiation. Although the nature of each individual element of a system and the interactions between any pair of elements may both be well understood, the large number of elements and possible interactions can present an almost overwhelming challenge to the investigator who seeks to understand the behavior of the system.

The purpose of the course is to give the descriptions of macroscopic and microscopic features of the systems by taking advantage of these systems to examine the properties and methods of calculations. This course provides a comprehensive presentation of the basics of statistical physics. The first part explains the essence of statistical physics and how it provides a bridge between microscopic and macroscopic phenomena, allowing one to derive quantities such as entropy. In the second part, statistical mechanics is applied to various systems which, although they look different, share the same mathematical structure. In this way listener can deepen their understanding of statistical physics. The course also features applications to quantum dynamics, thermodynamics, the Ising model and the statistical dynamics of free spins.

### **Subjects covered by the lectures are**

- Statistical Physics: Is More than Statistical Mechanics. Modeling of Statistical Systems
- Random Variables: Fundamentals of Probability Theory and Statistics
- Random Variables in State Space: Classical Statistical Mechanics of Fluids
- Random Fields: Textures and Classical Statistical Mechanics of Spin Systems
- Time-Dependent Random Variables: Classical Stochastic Processes
- Quantum Random Systems
- Changes of External Conditions
- Analysis of Statistical Systems. Estimation of Parameters. Signal Analysis: Estimation of Spectra
- Estimators Based on a Probability Distribution for the Parameters
- Estimating the Parameters of a Hidden Stochastic Model
- Statistical Tests and Classification Methods

### **Learning outcomes of the course :**

Through a deep understanding of the theory and the realization of a project, the student will be know fundamentals of statistical physics and applications of statistical physics to various systems. In particular:

- He will have a deep understanding of notions, concepts of statistical physics and will be able to summary, compare and explain them (substances pressure, the macroscopic properties such as temperature, due to the microscopic level).
- He will have a more penetrating insight into models of materials (the ideal gas, Van der Waals fluids).
- He will have a more penetrating insight into statistical mechanics and its basic notions (Macroscopic System, Statistics Meaning of Particle Systems, Temperature Interactions, Macroscopic Theory and macroscopic measurements, Gibbs Statistical Mechanics, Ensemble of Systems, Phase Space, Ensemble Averages, Thermodynamics of Ensemble).
- He will have a deep understanding of the resolution methods of statistical physics, and will be able to summary, compare and explain them (calculate the macroscopic properties of matter by making microscopic scale accounts). He will also know their application range.
- He will be able to describe modern and advanced approaches of statistical physics.

- He will be able to analyze and to evaluate (justify and criticise) these methods.
- He will be able to analyze new problems.

**Prerequisites and co-requisites/ Recommended optional programme components :**

Basic knowledge in

- Basic Concepts of Probability
- Differential Equations
- Differential and Integral Calculations
- Elasticity Theory
- Fluid Mechanics
- Solid Mechanics

**Planned learning activities and teaching methods :**

Exercises with professor assistance and personal project.

**Mode of delivery (face-to-face ; distance-learning) :**

Face-to-Face

**Required readings :**

- Honerkamp J. Statistical Physics. An Advanced Approach with Applications. Springer, 2012. 553.
- Joshioka D. Statistical Physics. An introduction. Springer, 2007. 208 p.
- Helrich C.S. Modern Thermodynamics with Statistical Mechanics. Springer, 2009.
- Reif F. Statistical Physics. Berkeley Physics Series. Volume V.
- Sears Salinger Thermodynamics Kinetic Theory and Statistical Thermodynamics.
- Kondepudi D., Prigogine I. Modern Thermodynamics. Chichester: John Wiley & Sons. 1999.

**Assessment methods and criteria :**

Evaluation is based on the realization of a project related to the use / development of methods specific to statistical physics and on an examination.

The examination is based on the whole content of the class. Problems similar to the ones studied during the classes, and new problems will be part of the questions. Justification using the theoretical content is also asked.

Participation to the examination and achievement of the project are mandatory.

**Detailed Syllabus**

week	SUBJECTS		
	Theoretical Subjects	Theoretical	Laboratory (Seminar) Work
1	Fluctuations in case of equilibrium, irreversibility and steady state approach		
2	Determining the properties of equilibrium, heat and temperature, analog indicator, problem solutions		

3	Communities of statistics, probability relations between simple, binomial distribution		
4	Average values, average values for a spin system account		
5	Status of a system to be specified, statistics community		
6	Predictions statistics, probability calculations		
7	Number of status of a macroscopic system Girileilir, equilibrium bond terms and irreversibility		
8	Colloquium		
9	Interactions between systems, the solution of the problems		
10	Distribution of energy between macroscopic systems, interact approach temperature		
11	Small heat transport, heat reservoir that touch the system, paramagnetism, the ideal gas in the average energy and pressure		
12	Determination of the absolute temperature, high and low absolute temperatures, work, internal energy, entropy		
13	Classical approximation, Maxwell's velocity distribution, perfusion and molecular bundles		
14	The equipartition theorem and its applications		
15	Heat of solids self, solving problem		
16	Final Exam		

**Socratic Teaching Method:** Class participation is mandatory. Everyone is expected to participate in discussions relating to reading materials, homework, exams and lectures.

**Guaranteed Recipe for Success:**

- 1) Take notes during lecture and sections.
- 2) After each lecture but before the next lecture review your notes. Identify the parts you do not understand.
- 3) Come to each lecture and discussion section with specific questions.
- 4) Keep up with the reading so that you have some familiarity with each topic prior to hearing about it in the lecture.
- 5) Find at least one "partner" in the class with whom you can meet at least once or twice a week to discuss materials from the lectures, the reading assignments and the homework.
- 6) Take the homework assignment seriously. Do not try to do the whole assignment the night before it is due. Some version of the homework questions will appear on the exams.

**Course Contents**

**Theoretical Physics (Statistical Physics)**

# **1 Statistical Physics: Is More than Statistical Mechanics. Part I Modeling of Statistical Systems**

## **2 Random Variables: Fundamentals of Probability Theory and Statistics**

### 2.1 Probability and Random Variables

#### 2.1.1 The Space of Events

#### 2.1.2 Introduction of Probability

#### 2.1.3 Random Variables

### 2.2 Multivariate Random Variables and Conditional Probabilities

#### 2.2.1 Multidimensional Random Variables

#### 2.2.2 Marginal Densities

#### 2.2.3 Conditional Probabilities and Bayes' Theorem

### 2.3 Moments and Quantiles

#### 2.3.1 Moments

#### 2.3.2 Quantiles

### 2.4 The Entropy

#### 2.4.1 Entropy for a Discrete Set of Events

#### 2.4.2 Entropy for a Continuous Space of Events

#### 2.4.3 Relative Entropy

### 2.5 Computations with Random Variables

#### 2.5.1 Addition and Multiplication of Random Variables

#### 2.5.2 Further Important Random Variables

#### 2.5.3 Limit Theorems

### 2.6 Stable Random Variables and Renormalization

#### Transformations

#### 2.6.1 Stable Random Variables

#### 2.6.2 The Renormalization Transformation

#### 2.6.3 Stability Analysis

#### 2.6.4 Scaling Behavior

### 2.7 The Large Deviation Property for Sums of Random Variables

## **3 Random Variables in State Space: Classical Statistical Mechanics of Fluids**

### 3.1 The Microcanonical System

### 3.2 Systems in Contact

#### 3.2.1 Thermal Contact

#### 3.2.2 Systems with Exchange of Volume and Energy

#### 3.2.3 Systems with Exchange of Particles and Energy

### 3.3 Thermodynamic Potentials

### 3.4 Susceptibilities

#### 3.4.1 Heat Capacities

#### 3.4.2 Isothermal Compressibility

#### 3.4.3 Isobaric Expansivity

#### 3.4.4 Isochoric Tension Coefficient and Adiabatic

#### Compressibility

#### 3.4.5 A General Relation Between Response Functions

### 3.5 The Equipartition Theorem

### 3.6 The Radial Distribution Function

### 3.7 Approximation Methods

#### 3.7.1 The Virial Expansion

#### 3.7.2 Integral Equations for the Radial Distribution

#### Function

#### 3.7.3 Perturbation Theory

### 3.8 The van der Waals Equation

#### 3.8.1 The Isotherms

#### 3.8.2 The Maxwell Construction

#### 3.8.3 Corresponding States

3.8.4 Critical Exponents

3.9 Some General Remarks about Phase Transitions  
and Phase Diagrams

## **4 Random Fields: Textures and Classical Statistical Mechanics of Spin Systems**

4.1 Discrete Stochastic Fields

4.1.1 Markov Fields

4.1.2 Gibbs Fields

4.1.3 Equivalence of Gibbs and Markov Fields

4.2 Examples of Markov Random Fields

4.2.1 Model with Independent Random Variables

4.2.2 Auto Model

4.2.3 Multilevel Logistic Model

4.2.4 Gauss Model

4.3 Characteristic Quantities of Densities for Random Fields

4.4 Simple Random Fields

4.4.1 The White Random Field or the Ideal  
Paramagnetic System

4.4.2 The One-Dimensional Ising Model

4.5 Random Fields with Phase Transitions

4.5.1 The Curie–Weiss Model

4.5.2 The Mean Field Approximation

4.5.3 The Two-Dimensional Ising Model

4.6 The Landau Free Energy

4.7 The Renormalization Group Method for Random  
Fields and Scaling Laws

4.7.1 The Renormalization Transformation

4.7.2 Scaling Laws

## **5 Time-Dependent Random Variables: Classical Stochastic Processes**

5.1 Markov Processes

5.2 The Master Equation

5.3 Examples of Master Equations

5.3.1 One-Step Processes

5.3.2 Chemical Reactions

5.3.3 Reaction–Diffusion Systems

5.3.4 Scattering Processes

5.4 Analytic Solutions of Master Equations

5.4.1 Equations for the Moments

5.4.2 The Equation for the Characteristic Function

5.4.3 Examples

5.5 Simulation of Stochastic Processes and Fields

5.6 The Fokker–Planck Equation

5.6.1 Fokker–Planck Equation with Linear Drift  
Term and Additive Noise

5.7 The Linear Response Function and the Fluctuation–  
Dissipation Theorem

5.8 Approximation Methods

5.8.1 The  $\Omega$  Expansion

5.8.2 The One-Particle Picture

5.9 More General Stochastic Processes

5.9.1 Self-Similar Processes

5.9.2 Fractal Brownian Motion

5.9.3 Stable Levy Processes

5.9.4 Autoregressive Processes

## **6 Quantum Random Systems**

## 6.1 Quantum-Mechanical Description of Statistical Systems

### 6.2 Ideal Quantum Systems: General Considerations

#### 6.2.1 Expansion in the Classical Regime

#### 6.2.2 First Quantum-Mechanical Correction Term

#### 6.2.3 Relations Between the Thermodynamic Potential and Other System Variables

### 6.3 The Ideal Fermi Gas

#### 6.3.1 The Fermi–Dirac Distribution

#### 6.3.2 Determination of the System Variables at Low Temperatures

#### 6.3.3 Applications of the Fermi–Dirac Distribution

### 6.4 The Ideal Bose Gas

#### 6.4.1 Particle Number and the Bose–Einstein Distribution

#### 6.4.2 Bose–Einstein Condensation

#### 6.4.3 Pressure

#### 6.4.4 Energy and Specific Heat

#### 6.4.5 Entropy

#### 6.4.6 Applications of Bose Statistics

### 6.5 The Photon Gas and Black Body Radiation

#### 6.5.1 The Kirchhoff Law

#### 6.5.2 The Stefan–Boltzmann Law

#### 6.5.3 The Pressure of Light

#### 6.5.4 The Total Radiative Power of the Sun

#### 6.5.5 The Cosmic Background Radiation

### 6.6 Lattice Vibrations in Solids: The Phonon Gas

### 6.7 Systems with Internal Degrees of Freedom: Ideal Gases of Molecules

### 6.8 Magnetic Properties of Fermi Systems

#### 6.8.1 Diamagnetism

#### 6.8.2 Paramagnetism

### 6.9 Quasi-Particles

#### 6.9.1 Models for the Magnetic Properties of Solids

#### 6.9.2 Superfluidity

## **7 Changes of External Conditions**

### 7.1 Reversible State Transformations, Heat, and Work

#### 7.1.1 Finite Transformations of State

### 7.2 Cyclic Processes

### 7.3 Energy and Relative Entropy

### 7.4 Time Dependence of Statistical Systems

## **Analysis of Statistical Systems**

## **8 Estimation of Parameters**

### 8.1 Samples and Estimators

#### 8.1.1 Monte Carlo Integration

### 8.2 Confidence Intervals

### 8.3 Propagation of Errors

#### 8.3.1 Application

### 8.4 The Maximum Likelihood Estimator

### 8.5 The Least-Squares Estimator

## **9 Signal Analysis: Estimation of Spectra**

### 9.1 The Spectrum of a Stochastic Process

### 9.2 The Fourier Transform of a Time Series and the Periodogram

### 9.3 Filters

#### 9.3.1 Filters and Transfer Functions

#### 9.3.2 Filter Design

- 9.4 Consistent Estimation of Spectra
- 9.5 Cross-Spectral Analysis
- 9.6 Frequency Distributions for Nonstationary Time Series
- 9.7 Filter Banks and Discrete Wavelet Transformations
  - 9.7.1 Examples of Filter Banks
- 9.8 Wavelets
  - 9.8.1 Wavelets as Base Functions in Function Spaces
  - 9.8.2 Wavelets and Filter Banks
  - 9.8.3 Solutions of the Dilation Equation
- 10 Estimators Based on a Probability Distribution for the Parameters**
  - 10.1 Bayesian Estimator and Maximum a Posteriori Estimator
  - 10.2 Marginalization of Nuisance Parameters
  - 10.3 Numerical Methods for Bayesian Estimators
- 11 Identification of Stochastic Models from Observations**
  - 11.1 Parameter Identification for Autoregressive Processes
  - 11.2 Granger Causality
    - 11.2.1 Granger Causality in the Time Domain
    - 11.2.2 Granger-Causality in the Frequency Domain
  - 11.3 Hidden Systems
  - 11.4 The Maximum a Posteriori Estimator for the Inverse Problem
    - 11.4.1 The Least Squares Estimator as a Special MAP Estimator
    - 11.4.2 Strategies for Choosing the Regularization Parameter
    - 11.4.3 The Regularization Method
    - 11.4.4 Examples of the Estimation of a Distribution Function by a Regularization Method
  - 11.5 Estimating the Realization of a Hidden Process
    - 11.5.1 The Viterbi Algorithm
    - 11.5.2 The Kalman Filter
    - 11.5.3 The Unscented Kalman Filter
    - 11.5.4 The Dual Kalman Filter
- 12 Estimating the Parameters of a Hidden Stochastic Model**
  - 12.1 The Expectation Maximization Method (EM Method)
  - 12.2 Estimating the Parameters of a Hidden Markov Model
    - 12.2.1 The Forward Algorithm
    - 12.2.2 The Backward Algorithm
    - 12.2.3 The Estimation Formulas
  - 12.3 Estimating the Parameters in a State Space Model
- 13 Statistical Tests and Classification Methods**
  - 13.1 General Comments Concerning Statistical Tests
    - 13.1.1 Test Quantity and Significance Level
    - 13.1.2 Empirical Moments for a Test Quantity: The Bootstrap Method
    - 13.1.3 The Power of a Test
  - 13.2 Some Useful Tests
    - 13.2.1 The z- and the t-Test
    - 13.2.2 Test for the Equality of the Variances of Two Sets of Measurements, the F -Test
    - 13.2.3 The  $\chi^2$ -Test
    - 13.2.4 The Kolmogorov–Smirnov Test
    - 13.2.5 The F-Test for Least-Squares Estimators
    - 13.2.6 The Likelihood-Ratio Test
  - 13.3 Classification Methods
    - 13.3.1 Classifiers
    - 13.3.2 Estimation of Parameters that Arise in Classifiers
    - 13.3.3 Automatic Classification (Cluster Analysis)

## Further Reading

1. Landau L. D., Lifshitz E. M. (1980) [1976]. Statistical Physics. **5** (3 ed.). Oxford: Pergamon Press. ISBN 0-7506-3372-7. Translated by J.B. Sykes and M.J. Kearsley
2. Ebeling W.; Sokolov I. M. (2005). Statistical Thermodynamics and Stochastic Theory of Nonequilibrium Systems. World Scientific Publishing Co. Pte. Ltd.. pp.3–12. ISBN 978-90-277-1674-3. (section 1.2)
3. Mahon Basil (2003). The Man Who Changed Everything – the Life of James Clerk Maxwell. Hoboken, NJ: Wiley. ISBN 0-470-86171-1.
4. Dill, Ken; Bromberg, Sarina (2003). Molecular Driving Forces. Garland Science. ISBN 0-8153-2051-5.
5. Entropy, Order Parameters, and Complexity: A Broad View of Statistical Physics, J. P. Sethna, Cornell University, 2004.
6. Schrodinger, Erwin (1946). Statistical Thermodynamics. Dover Publications, Inc.. ISBN 0-486-66101-6.
7. Ben-Naim, Arieh (2007). Statistical Thermodynamics Based on Information. ISBN 978-981-270-707-9.

## Statistical Physics of Fields Problems

1. The binary alloy: A binary alloy consists of  $N_A$  atoms of atom A and  $N_B$  atoms of type B. The atoms form a simple cubic lattice, each interacting only with its six nearest neighbors. Assume an interactive energy of  $-J$  ( $J > 0$ ) between like neighbors A-A and B-B, but a repulsive energy of  $+J$  for an A-B pair.
  - a) What is the minimum energy configuration, or the state of the system at zero temperature?
  - b) Estimate the total interaction energy assuming that the atoms are randomly distributed among the  $N$  sites; i.e. each site is occupied independently with probabilities  $p_A = N_A / N$  and  $p_B = N_B / N$ .
  - c) Estimate the mixing entropy of the alloy with the same approximation. Assume  $N_A, N_B \gg 1$ .
  - d) Using the above, obtain a free energy function  $F(x)$ , where  $x = (N_A - N_B) / N$ . Expand  $F(x)$  to the fourth order in  $x$  and show that the requirement of convexity of  $F(x)$  breaks down below a critical temperature  $T_c$ . For the remainder of this problem use the expansion obtained in d) in place of the full function  $F(x)$ .
  - e) Sketch  $F(x)$  for  $T > T_c$ ,  $T = T_c$  and for  $T < T_c$ . For  $T < T_c$  there is a range of compositions  $x < |x_{sp}(T)|$  where  $F(x)$  is not convex and hence the composition is locally unstable. Find  $x_{sp}(T)$ .
  - f) The alloy globally minimizes its free energy by separating into A rich and B rich phases of compositions  $\pm x_{eq}(T)$ , where  $x_{eq}(T)$  minimizes the function  $F(x)$ . Find  $x_{eq}(T)$ .
  - g) In the  $(T, x)$  plane sketch the phase separation boundary  $\pm x_{eq}(T)$ ; and the so called spinoidal line  $\pm x_{sp}(T)$ . (The spinoidal line indicates onset of metastability and hysteresis effects).
2. The Ising model of magnetism: The local environment of a an electron in a crystal sometimes forces its spin to stay parallel or anti-parallel to a given lattice direction. As a model of magnetism in such materials we denote the direction of the spin by a single variable  $\sigma_i = \pm 1$  (an Ising spin)/ The energy of a configuration  $\{\sigma_i\}$  of spin is then given by



$$H = \frac{1}{2} \sum_{i,j=1}^N J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i$$

where  $h$  is an external magnetic field and  $J_{ij}$  is the interaction energy between spins at sites  $i$  and  $j$ .

- a) For  $N$  spins we make the drastic approximation that the interaction between all spins is the same, and  $J_{ij} = -J/N$  (the equivalent neighbor model)/ Show that the energy can be

written as  $E(M, h) = -N \left[ \frac{Jm^2}{2} + hm \right]$  with a magnetization

$$m = \sum_{i=1}^N \sigma_i / N = M / N.$$

- b) B) Show that the partition function  $Z(h, T) = \sum_{\{\sigma_i\}} \exp(-\beta H)$  can be rewritten as

$Z = \sum_M \exp[-\beta F(m, h)]$  with  $F(m, h)$  easily calculated by analogy to problem

(1). For the remainder of the problem work only with  $F(m, h)$  expanded to 4<sup>th</sup> order in  $m$ .