UAB
Universitat Autònoma de Barcelona

Thermodynamics and Statistical Mechanics

Code: 100157
ECTS Credits: 9

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Degree	Type	Year
2500097 Physics	OB	3

Contact

Name: Vicente Mendez Lopez

Email: vicenc.mendez@uab.cat

Teachers

Juan Camacho Castro

Daniel Campos Moreno

Teaching groups languages

You can view this information at the end of this document.

Prerequisites

Some course of introduction to thermodynamics is preferred

Objectives and Contextualisation

1. To understand the conditions of a thermodynamical systems

2. To identify system and environment

3. Distinguish between state variables and process variables

4. To interpret the different kinds of thermal processes

5. To understand the concept of the thermodynamical limit

6. To derive the partition function of a system and find the state equations from it

7. To apply the energy equipartition theorem

8. To distinguish between reversible and irreversible processes

9. To change the fundamental equation of representation

10.To understand the microscopic concept of pressure of a gas

11. Interpret the stability criteria and relate them with the onset of phase ransitions

12. To analyze the first and second order phase transitions. Understand the Landau theory for phase transitions

13. To construct the Ising model. Apply the mean field approximation, the interactions between nearest neighbours and the method of transfer matrix

14. To distinguish between ideal and real gases. Connect the intermolecular potential with the virial expansion

15. To understand the processes of cooling gases

16. To interpret the electromagnetic radiation as a gas of bosons and obtain the equations of state

17. Make use of the grancanonical ensable to study the fluctuations in the number of particles and the phase equilibrium

Competences

- Develop strategies for analysis, synthesis and communication that allow the concepts of physics to be transmitted in educational and dissemination-based contexts
- Formulate and address physical problems identifying the most relevant principles and using approximations, if necessary, to reach a solution that must be presented, specifying assumptions and approximations
- Know the fundamentals of the main areas of physics and understand them
- Take account of social, economic and environmental impacts when operating within one's own area of knowledge.
- Use critical reasoning, show analytical skills, correctly use technical language and develop logical arguments
- Use mathematics to describe the physical world, selecting appropriate tools, building appropriate models, interpreting and comparing results critically with experimentation and observation

Learning Outcomes

1. Analyse limits at low and high temperature for any given system.
2. Analyse the information contained in the distinct phase diagrams in equilibrium.
3. Calculate the number of microstates for classic and discrete systems.
4. Calculate the partition function of a system in any group.
5. Calculate the second virial coefficient from the interaction potential.
6. Clarify the need for a classic or quantum statistical description for an ideal gas.
7. Deduce the equations of state within a system from the partition function.
8. Deduce the fundamental equation in different representations.
9. Describe the information contained in the different equations of state within a system.
10. Describe the physical information contained in virial coefficients.
11. Describe the properties that differentiate real behaviour from ideal in a gas.
12. Distinguish between the domains of action in thermodynamics and statistical mechanics.
13. Establish the thermodynamic variables describing equilibrium states for different systems and propose the corresponding Gibbs' equation.
14. Identify the social, economic and environmental implications of academic and professional activities within one's own area of knowledge.
15. Physically interpret the partial derivatives of the distinct thermodynamic quantities.
16. Relate stability criteria to the principles of thermodynamics and verify the stability of a thermodynamic system.
17. Transmit, orally and in written format, physical concepts of a certain complexity, making them understandable to non-specialist settings.

18. Use critical reasoning, show analytical skills, correctly use technical language and develop logical arguments

Content

1. Formal structure of thermodynamics

1.0. Review of the laws of thermodynamics

1.1. The fundamental equation

1.2. Euler's form of internal energy. Gibbs-Duhem equation

1.3. Transformed by Legendre. Thermodynamic potentials

1.4. Maxwell relations for a fluid

1.5. Stability conditions

2. Microscopic description of macroscopic systems

2.1. Microstats and Macrostats. Phase space

2.2. Ensembles

2.3. Microcanonical ensemble

2.4 Thermodynamic-Statistical Mechanical Connection

2.5. Application to the ideal monoatomic gas

2.6. Discrete systems

2.7. Statistical entropy

2.8. Maxwell-Boltzmann distribution

2.9. Pressure

2.10. Effusion

3. Canonical ensemble

3.1. Partition function.

3.2. Ideal systems

3.3. Energy degeneration

3.4. The ideal monoatomic gas in a potential

3.5. Equipartition of energy theorem

3.6. Discrete systems

4. Magnetic systems

4.1. Thermodynamics of magnetic systems

4.2. Classical paramagnetism

4.3. Spin Paramagnetism 1/2. Microcanonical and canonical treatments

4.4. Adiabatic demagnetization

5. Phase transitions

5.1. Classification. P-V, P-μ and P-T diagrams. Clapeyron equation

5.2. Vapor-condensed phase equilibrium

5.3. The critical point

5.4. Ehrenfest classification of phase transitions

5.5. Second order phase transitions.

6. Ising model

6.1. One-dimensional chain

6.2. One-dimensional open chain

6.3. Meanfield approximation

7. Real gases

7.1. Compressibility factor. Virial expansion

7.2. Interaction potential. Configuration partition function

7.3. Second coefficient of the virial. Van der Waals equation

7.4. Reticular gas

7.5. Corresponding State Law

7.6. Joule and Joule-Kelvin expansions

8. Photons

8.1. Statistics of bosons and fermions

8.2 Energy density. Degeneration of states

8.3. Planck distribution

8.4. Equations of state of a photon gas

9. Macrocanonical collectivity

9.1. Partition function

9.2. Connection with thermodynamics

9.3. Discrete systems

9.4. Fluctuations

9.5. Ideal systems. The ideal monoatomic gas

9.6. Solid-vapor equilibrium

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problems	30	1.2	
Teaching lectures	45	1.8	
Type: Autonomous			
Problems solving	49	1.96	
Study	92	3.68	

METHODOLOGY

Classroom activities

1 Teaching lectures

The lectures will be taught by the theory teacher where the concepts, developments and basic principles of the subject will be presented.

2 Teaching Problems

The problem's teacher will solve in class some of the problems of the collection that previously the student will have had to try to solve. We will try to make use of dynamical discussions of alternative results.

3 Tutorial activities

In case of virtual teaching along the seasons of tutorial activites questions of theory and practical will be solved in class

Authonomous activities

1 Troubleshooting

The teacher of problems will deliver (will also be posted on the virtual campus) a list of problems and computer practices that each student must solve individually and deliver it on the established date

2 Study

We have counted that the student must dedicate 2 hours of study for each hour of master class.

SURVEYS

It is planned to leave 15 minutes at the end of class when the institutional surveys need to be answered

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Final exam	70%	3	0.12	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17, 18
First part exam	35%	3	0.12	3, 4, 6, 7, 8, 9, 11, 12, 13, 15, 16
Homework	30%	0	0	14, 18
Second part exam	35%	3	0.12	1, 2, 5, 10, 11

Partial exams and final exam
There will be two partial exams. The first one will evaluate the first part of the course while the second will evaluate the rest. in case the mean of the qualifications is less than 4 the student must do the final exam. To be examined in the final exam is compulsery to be examend in the first and second partial exams.

Remedial exam

Those who have been evaluated in the partial exams obtaining a qualification lower than 4 (compulsory) or those who want to improve their marks (optional) may do the remedial exam. In the latter case, the final mark will be the best of the marks obtained from the remidial and partials examams

Homework

The homowork problems will be evaluated and their solutions will be published at the virtual campus. This part cannot be remedied

Final mark

The finals mark will be calculated from the specific weights only if the student has passed the partials or the final exam. The final mark will be the 70% of the fianl exam/mean of partials plus the 30% of the homework if the final exam mark is equal or higher than 4. Otherwise, the studend does not pass

Unique assessment

Students who have accepted the single assessment modality will have to take a final test which will consist of a problem-based exam. When the student has finished, he/she will hand in the assignments corresponding to the first semester and the simulation work of the second semester which will be published on the virtual campus and which will be the same as for the rest of the students.

These tests will take place on the same day, time and place as the tests of the second part of the continuous assessment modality.

The final grade will be 70% of the test plus 30% of the delivered problems including the simulation work if the final exam grade is greater than or equal to 4.0. If the grade of the test is lower than 4.0 or if the final grade previously calculated does not reach 5, the student has another opportunity to pass the subject through the make-up exam that will be held on the date set by the coordination of the degree. The final grade will be calculated again as before, i.e. if the retake exam grade is greater than or equal to 4.0 then the final grade will be 70% of the test plus 30% of the delivered problems including the work of simulation

The 30% of the delivered work is distributed in the following way: 15% for the delivered problems and 15%f or the simulation work

Bibliography

Modern texts

- Robert H Swendsen, An Introduction to Statistical Mechanics and Thermodynamics (Oxford Univ. Press, 2012)
- S. K. Roy, Thermal Physics And Statistical Mechanics (New Age International Publishers, 2001)

- K. Huang, *Introduction to Statistical Physics*, CRC, 2001
- D. V. Schroeder, *An Introduction to Thermal Physics*, Addison Wesley, 2000
- S. J. Blundell and K. M. Blundell, *Concepts in Thermal Physics*, Oxford UP, 2006
- M. Criado-Sancho y J. Casas-Vázquez, *Termodinámica química y de los procesos irreversibles*, Pearson/Addison Wesley, Madrid, segona edició, 2004.
- Yi-Chen Cheng, Macroscopic and Statistical Thermodynamics (World Scientific, 2006)

Classical texts

- J. J. Brey, J. de la Rubia, J. de la Rubia, *Mecánica Estadística*, UNED, 2001
- R. Kubo, *Thermodynamics*, North Holland, Amsterdam, 1968.
- F. Reif, *Fundamentals of Statistical Physics and Thermal Physics*, McGraw-Hill, 1985
- D. A. McQuarrie, *Statistical Mechanics*, Harper Collins, 1976
- M.W. Zemansky y R.H. Dittman, *Calor y Termodinámica*, McGraw-Hill, Madrid, 1990.
- C.J. Adkins, *Termodinámica del equilibrio*, Reverté, Barcelona, 1977.
- P.W. Atkins, *La Segunda ley*, Prensa científica, Barcelona 1992.

Software

We shall make use of Python for the simulations activities along the second semester

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	annual	morning-mixed
(PAUL) Classroom practices	2	Catalan	annual	morning-mixed
(TE) Theory	1	Catalan	annual	morning-mixed
(TE) Theory	2	Catalan	annual	morning-mixed