

COURSE OUTLINE

1. Course: PHYS 449, Statistical Mechanics I - Fall 2023

Lecture 01: TR 11:00 - 12:15 in MFH 160

Instructor Email Phone Office Hours

Dr Javier Orlandi javier.orlandi@ucalgary.ca 403 210-6548 SB 505 Wed 3:00PM - 4:30 PM

To account for any necessary transition to remote learning for the current semester, courses with in-person lectures, labs, or tutorials may be shifted to remote delivery for a certain period of time. In addition, adjustments may be made to the modality and format of assessments and deadlines, as well as to other course components and/or requirements, so that all coursework tasks are in line with the necessary and evolving health precautions for all involved (students and staff).

In Person Delivery Details:

Both lectures and tutorials will be delivered in-person in a classroom setting. Class notes and other learning materials, including review questions from our in-class group discussions, will be posted on D2L for self-study. Worksheets with solutions will be uploaded to D2L after each tutorial. While attendance of both the lectures and tutorials is not mandatory, it is an important learning opportunity, and it provides direct feedback on the individual learning progression.

Course Site:

D2L: PHYS 449 L01-(Fall 2023)-Statistical Mechanics I

Note: Students must use their U of C account for all course correspondence.

Equity Diversity & Inclusion:

The University of Calgary is committed to creating an equitable, diverse and inclusive campus, and condemns harm and discrimination of any form. We value all persons regardless of their race, gender, ethnicity, age, LGBTQIA2S+ identity and expression, disability, religion, spirituality, and socioeconomic status. The Faculty of Science strives to extend these values in every aspect of our courses, research, and teachings to better promote academic excellence and foster belonging for all.

The Physics and Astronomy EDI Committee acknowledges there are persistent barriers that prevent such accessibility and hinder our progress towards EDI. Our representatives (faculty, postdocs, graduate and undergraduate students) are committed to addressing any concerns and work towards proactive solutions that enact necessary change within the department. To submit anonymous questions, comments or concerns regarding EDI related issues, please reach out to our Associate Head EDI, Claudia Gomes da Rocha (claudia.gomesdarocha@ucalgary.ca)

2. Requisites:

See section 3.5.C in the Faculty of Science section of the online Calendar.

Prerequisite(s):

Physics 229 or 325; and Mathematics 375 or 376; and either Physics 343 and Mathematics 367 or Physics Engineering 383.

3. Grading:

The University policy on grading and related matters is described in <u>F.1</u> and <u>F.2</u> of the online University Calendar.

In determining the overall grade in the course the following weights will be used:

2023-08-25 1 of 7

Course Component	Weight	Due Date (duration for exams)	Modality for exams	Location for exams				
Assignments (8 - 9)	45%	Ongoing						
Midterm ¹	15%	Oct 31 2023 at 11:00 am (75 Minutes)	in-person	In Class				
Registrar Scheduled Final Exam	40%	Will be available when the final exam schedule is released by the Registrar	in person	Will be available when the final exam schedule is released by the Registrar				

 $[\]overline{{}^{1}}$ The date of the midterm is tentative.

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows.

	A+	A	A-	B+	В	B-	C+	С	C-	D+	D
Minimum % Required	90 %	85 %	80 %	75%	70%	65 %	60 %	55%	50%	45 %	40 %

This course will have a Registrar Scheduled Final exam that will be delivered in-person and on campus. <u>The Final Examination Schedule</u> will be published by the Registrar's Office approximately one month after the start of the term. The final exam for this course will be designed to be completed within 3 hours.

The University of Calgary offers a <u>flexible grade option</u>, Credit Granted (CG) to support student's breadth of learning and student wellness. Faculty units may have additional requirements or restrictions for the use of the CG grade at the faculty, degree or program level. To see the full list of Faculty of Science courses where CG is not eligible, please visit the following website: https://science.ucalgary.ca/current-students/undergraduate/program-advising/flexible-grading-option-cg-grade

4. Missed Components Of Term Work:

In the event that a student legitimately fails to submit any online or in-person assessment on time (e.g. due to illness, domestic affliction, etc...), please contact the course coordinator, or the course instructor if this course does not have a coordinator to arrange for a re-adjustment of a submission date, or possible exemption and reweighing of components. Absences not reported within 48 hours will not be accommodated. Students may be asked to provide supporting documentation (Section M.1) for an excused absence, SeeFAQ.

If an excused absence is approved, options for how the missed assessment is dealt with is at the discretion of the coordinator or course instructor. Some options such as an exemption and pro-rating among the components of the course may not be a viable option based on the design of this course.

5. Scheduled Out-of-Class Activities:

There are no scheduled out of class activities for this course.

6. Course Materials:

Recommended Textbook(s):

- W. Greiner, L. Neise, H. Stoecker, Thermodynamics and Statistical Mechanics: Springer,
- H. Gould , J. Tobochnik, Statistical and Thermal Physics: Princeton University Press.

Class notes, assignments, and supporting lecture materials will be posted on the course D2L website.

In order to successfully engage in their learning experiences at the University of Calgary, students taking online, remote and blended courses are required to have reliable access to the following technology:

- A computer with a supported operating system, as well as the latest security, and malware updates;
- A current and updated web browser;
- Webcam/Camera (built-in or external);
- Microphone and speaker (built-in or external), or headset with microphone;
- Current antivirus and/or firewall software enabled;
- Stable internet connection.

For more information please refer to the UofC <u>ELearning</u> online website.

2023-08-25 2 of 7

7. Examination Policy:

Final exam and midterm test are closed book. No aids, calculators, or laptops will be allowed.

Students should also read the Calendar, <u>Section G</u>, on Examinations.

8. Approved Mandatory And Optional Course Supplemental Fees:

There are no mandatory or optional course supplemental fees for this course.

9. Writing Across The Curriculum Statement:

For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) can be a factor in the evaluation of the work. See also Section <u>E.2</u> of the University Calendar.

10. Human Studies Statement:

Students will not participate as subjects or researchers in human studies.

See also <u>Section E.5</u> of the University Calendar.

11. Reappraisal Of Grades:

A student wishing a reappraisal, should first attempt to review the graded work with the Course coordinator/instructor or department offering the course. Students with sufficient academic grounds may request a reappraisal. Non-academic grounds are not relevant for grade reappraisals. Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See Section 1.3 of the University Calendar.

- a. **Term Work:** The student should present their rationale as effectively and as fully as possible to the Course coordinator/instructor within **ten business days** of either being notified about the mark, or of the item's return to the class. If the student is not satisfied with the outcome, the student shall submit the Reappraisal of Graded Term work <u>form</u> to the department in which the course is offered within 2 business days of receiving the decision from the instructor. The Department will arrange for a reappraisal of the work within the next ten business days. The reappraisal will only be considered if the student provides a detailed rationale that outlines where and for what reason an error is suspected. See sections <u>I.1</u> and <u>I.2</u> of the University Calendar
- b. **Final Exam:**The student shall submit the request to Enrolment Services. See <u>Section I.3</u> of the University Calendar.

12. Other Important Information For Students:

- a. **Mental Health** The University of Calgary recognizes the pivotal role that student mental health plays in physical health, social connectedness and academic success, and aspires to create a caring and supportive campus community where individuals can freely talk about mental health and receive supports when needed. We encourage you to explore the mental health resources available throughout the university community, such as counselling, self-help resources, peer support or skills-building available through the SU Wellness Centre (Room 370, MacEwan Student Centre, Mental Health Services Website) and the Campus Mental Health Strategy website (Mental Health).
- b. **SU Wellness Services:** For more information, see their <u>website</u> or call <u>403-210-9355</u>.
- c. Sexual Violence: The Sexual Violence Support Advocate, Carla Bertsch, can provide confidential support and information regarding sexual violence to all members of the university community. Carla can be reached by email (<u>svsa@ucalgary.ca</u>) or phone at <u>403-220-2208</u>. The complete University of Calgary policy on sexual violence can be viewed <u>here.</u>
- d. <u>Student Ombuds Office:</u> A safe place for all students of the University of Calgary to discuss student related issues, interpersonal conflict, academic and non-academic concerns, and many other problems.
- e. **Student Union Information:** <u>SU contact</u>, Email your SU Science Reps: <u>science1@su.ucalgary.ca</u>, <u>science2@su.ucalgary.ca</u>, <u>science3@su.ucalgary.ca</u>,

f. Academic Accommodation Policy:

It is the student's responsibility to request academic accommodations according to the University policies and procedures listed below. The student accommodation policy can be found at: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Student-Accommodation-Policy.pdf

2023-08-25 3 of 7

Students needing an accommodation because of a disability or medical condition should communicate this need to Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Accommodation-for-Students-with-Disabilities-Procedure.pdf.

Students needing an accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, by filling out the Request for Academic Accommodation Form and sending it to Dr. David Feder by email phas.ahugrd@ucalgary.ca preferably 10 business days before the due date of an assessment or scheduled absence.

g. **Misconduct:** Academic integrity is the foundation of the development and acquisition of knowledge and is based on values of honesty, trust, responsibility, and respect. We expect members of our community to act with integrity. Research integrity, ethics, and principles of conduct are key to academic integrity. Members of our campus community are required to abide by our institutional <u>Code of Conduct</u> and promote academic integrity in upholding the University of Calgary's reputation of excellence. Some examples of academic misconduct include but are not limited to: posting course material to online platforms or file sharing without the course instructor's consent; submitting or presenting work as if it were the student's own work; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; borrowing experimental values from others without the instructor's approval; falsification/fabrication of experimental values in a report. Please read the following to inform yourself more on academic integrity:

Student Handbook on Academic Integrity
Student Academic Misconduct Policy and Procedure
Faculty of Science Academic Misconduct Process
Research Integrity Policy

Additional information is available on the Student Success Centre Academic Integrity page

- h. **Copyright of Course Materials:** All course materials (including those posted on the course D2L site, a course website, or used in any teaching activity such as (but not limited to) examinations, quizzes, assignments, laboratory manuals, lecture slides or lecture materials and other course notes) are protected by law. These materials are for the sole use of students registered in this course and must not be redistributed. Sharing these materials with anyone else would be a breach of the terms and conditions governing student access to D2L, as well as a violation of the copyright in these materials, and may be pursued as a case of student academic or non-academic misconduct, in addition to any other remedies available at law.
- i. **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). Students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page. For more information, see <u>Legal Services</u> website.
- j. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction (<u>USRI</u>) survey and the Faculty of Science Teaching Feedback form provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses. Your responses make a difference please participate in these surveys.

Course Description

Overall learning goals:

- Explain how to describe macroscopic physical systems in thermal equilibrium.
- Identify suitable, reliable, and understandable reference material and critique original peer-reviewed literature on thermodynamics and statistical mechanics.
- Solve problems individually and in teams and communicate your own understanding of a given topic in the area of thermodynamics and statistical mechanics clearly in written and oral form

Course Schedule

Module 1: Thermodynamics (5 weeks)

Learning outcomes: Explain how to describe macroscopic physical systems in thermal equilibrium from a macroscopic perspective and what the laws of thermodynamics are.

- Module 1.1: **Thermodynamic systems and equilibrium.** Learning outcome: Explain the concept of equilibrium, thermodynamic coordinates, and quasi-static changes for macroscopic physical systems.
- Module 1.2: Energy and energy transfer. Learning outcome: Explain the concepts of work and heat to
 precisely formulate the 1st law of thermodynamics. Mathematical background: exact and inexact

2023-08-25 4 of 7

differentials, partial derivatives, path integrals, integrating factors.

- Module 1.3: **Temperature.** Learning outcomes: Explain the 0th law of thermodynamics to precisely formulate the concept of temperature. Mathematical concept: Implicit function theorem.
- Module 1.4: **Simple thermodynamic processes.** Learning outcomes: Explain the concept of heat capacities, adiabats & isotherms. Mathematical background: Ordinary differential equations.
- Module 1.5: Restrictions on energy conversion and efficiency. Learning outcomes: Explain the concepts
 of heat engine and refrigerator to precisely formulate the 2nd law of thermodynamics (Kelvin/Clausius).
 Explain the concept of a Carnot engine and prove Carnot's theorem.
- Module 1.6: **Thermodynamic entropy.** Learning outcomes: Derive the Clausius theorem, explain its relation to thermodynamic entropy, and apply it to reformulate the 2nd law (Planck).
- Module 1.7: Absolute zero temperature. Learning outcomes: Precisely formulate the 3rd law of thermodynamics as formulated by Nernst and derive its consequences.
- Module 1.8: **Thermodynamic potentials.** Learning outcomes: Explain the concept of thermodynamic potentials, derive the relationship between them including the Maxwell relations, and derive their extremal properties. Mathematical background: Legendre transformation

Module 2: **Probability theory** (2 1/2 weeks)

Learning outcomes: Explain how to describe random events and how to quantify information.

- Module 2.1: **Introduction.** Learning outcomes: Explain how to define probability and why there are different interpretations of probability. Formulate the law of large numbers in the context of the Bernoulli process. Mathematical background: Binomial coefficient, Binomial theorem.
- Module 2.2: Gaussian distribution and continuous random variables. Learning outcomes: Apply probability theory for discrete and continuous random variables to derive the central limit theorem. Mathematical background: Stirling's formula, series expansion (In, exp), delta function, high-dimensional integrals
- Module 2.3: **Information & Shannon entropy.** Learning outcomes: Explain the concepts of information and Shannon entropy, and apply the maximum entropy principle. Mathematical background: Calculus of variations, Lagrange multipliers.

Module 3: **Kinetic theory of gases** (1 1/2 weeks)

Learning outcomes: Explain how we can obtain the macroscopic properties of a gas from its microscopic description.

- Module 3.1: **Phase space density.** Learning outcomes: Explain the basic concepts of microstates, macrostates, and phase space density to define ensemble averages. Background: Hamiltonian dynamics.
- Module 3.2: The concept of equilibrium and the arrow of time. Learning outcomes: Explain the concept
 of ergodicity and Liouville's theorem and explain the implications for the concept of equilibrium and time
 reversibility. Background: Continuity equation

Module 4: Classical statistical mechanics (3 weeks)

Learning outcomes: Explain how to describe macroscopic physical systems in thermal equilibrium from a microscopic perspective.

- Module 4.1: **Ensemble theory.** Learning outcomes: Explain the basic concepts of classical statistical mechanics and their underlying assumptions and the relationship between the different ensembles.
- Module 4.2: **Applications of statistical mechanics.** Learning outcomes: Apply ensemble theory to calculate the thermodynamic properties of a given system. Mathematical background: l'Hopital's rule, spherical coordinates, Gamma function.
- Module 4.3: **Indistinguishable particles.** Learning outcomes: Explain Gibbs paradox and how it can be resolved in the classical context, and apply it in a given application.

General course information

- 1. **Textbook & class notes:** As none of the currently available textbooks satisfactorily covers all aspects of the course, I have posted my own class notes on D2L. There are also two textbooks listed under course material. For more information on the two textbooks and their supporting online material including free downloads, please see our course D2L website. On D2L, I have also listed a number of additional books and other reference material that might be helpful for you to follow up on specific aspects covered in class. I strongly encourage you to look at other books on the course topics as well since some of you might find the presentation in a given book (more) accessible while others might not. Being able to identify suitable, reliable, and understandable reference sources on a given topic (if necessary) is one of the keys to success in this class and beyond. While some students learn best in class by taking detailed notes, for others this is more a distraction from following and understanding the key concepts and identifying my mistakes in class. It is important to figure out which approach works best for you and act accordingly. It also might be helpful to team up with other students to share class notes and discuss specific topics.
- 2. **Grading philosophy:** Because I try to encourage participation as much as possible, I have put a heavier accent on assignments than is maybe customary.
- 3. Midterm: The in-class midterm (75 min long) will focus on the material covered up to and including the last

2023-08-25 5 of 7

homework assignment before the midterm.

- 4. **Final:** The final exam (3 h long) will focus predominantly on the material covered after the midterm. Note that you can't forget what you have learned in the first half, because the second-half material builds on it.
- 5. Class participation & reading assignments: The emphasis in this course will be on discussion and critical thinking. Given this, your active class participation throughout the semester will be essential and you need to be prepared by doing the reading assignments. You will be challenged in class to defend your thinking by appropriate reasoning or by references to material covered in the lectures or reading assignments. If you don't understand something during a lecture or from the assigned reading, please don't be shy, ask questions! If something catches your interest and you want to learn more, ask questions.
- 6. **Tutorials:** Weekly tutorials will be offered to review and expand on the material covered in class and to discuss the solutions to the homework problems as necessary.
- 7. **Homework assignments:** There will be continuous homework assignments over the term, which will typically be posted on D2L on Thursdays and are typically due the following Friday. These are the backbone of the course in that it is through these assignments that you will build up and apply your understanding of the various concepts and techniques. Please keep the following in mind as you work on and write up your assignments:
 - Your main two goals in writing up your homework are to be clear (so that it is understandable what you have written) and to demonstrate insight. Writing clearly means using readable handwriting. You should avoid tiny script and avoid trying to cram many sentences and equations onto a single page. Leave plenty of space between symbols and between successive lines of equations. Leave plenty of space between the ending of one homework problem and the beginning of the next. Spread your answers out over many pages if necessary. If we cannot read and understand your assignments easily, you will get little or no credit.
 - Demonstrating insight means using complete sentences that explain what you are doing and why. Cryptic brief answers like "yes", "no", "24", or "f(x)" will not be given credit. Instead, explain what you are doing and why, e.g., as if to a friend who is not familiar with this course. Your homework must show that you understand how you got your answer and that you appreciate the significance of your answer. A well-written complete answer is one that you will be able to understand yourself a month after you have written the answer, even if you don't remember the original question.
 - You are allowed to collaborate on the homework assignments (this is realistic, scientists collaborate all the time in research) but as much as possible you should attempt the assignments on your own since you will learn the most that way. Whether or not you collaborate, you must write up your homework on your own, in your own words, and with your own understanding. You must also acknowledge explicitly at the beginning of your homework anyone who gave you substantial help, e.g., classmates, myself, or other people. (Again, scientists usually acknowledge in their published articles colleagues that helped to carry out the research.) Failure to write your homework in your own words and failure to acknowledge help when given can lead to severe academic penalties so please play by the rules.
 - The assignments will require typically a mixture of analytical, numerical, and graphical approaches. The mathematical derivations or analyses for the analytical problems should preferably be written out by hand on paper. Please use ink, not pencil. Numerical and graphical answers involve output that is best printed out on a laser printer, then attached to your handwritten sheets. A hand-sketch of a graphical plot with essential features described is also acceptable.
 - Please pay attention to details as you write your assignments. All symbols should be given names the first time you introduce them, e.g., say "the momentum p" or "the flux F" instead of just using the symbols p and F. Physical units should be given for any answer that is a physical quantity, e.g., say "the angular momentum was A=0.02 J-sec" or "the angle was mu=0.32 radians." Numerical answers should have the minimum number of significant digits that is consistent with the given data. For example, if you have a product or ratio of numbers of which the least accurate number has two significant digits, the final answer should have only two significant digits. Graphs should have their axes clearly labeled by the corresponding variables and by the variables' physical units. Each graph should have a title that explains the graph's purpose. A good way to learn how to write effectively is to imitate the style of published articles, e.g., those published in Physical Review Letters.
 - If you use using Mathematica or any other software package in a homework assignment, please do not hand in the output of your entire session. Instead, just give us enough output to convince us that you have answered the question correctly. You should also include any code that you write so that we can try to understand how you obtained your answers.

Course Learning Incomes

Students taking PHYS 449 are expected to have prior knowledge in higher dimensional calculus, integrating factors, calculus of variations, Gamma functions, series expansions, and geometric series as covered in the required math courses. They also are expected to have prior knowledge of (i) discrete states typical for quantum mechanical systems as covered in PHYS 229 or PHYS 325, and (ii) phase space, Hamiltonian dynamics, Legendre transformation, calculus of variations, and Lagrange multipliers as covered in PHYS 343.

2023-08-25 6 of 7

Course Outcomes:

- The student can explain the concepts of work, heat, temperature, heat engine, thermodynamic entropy, equilibrium and quasi-static changes to precisely formulate the laws of thermodynamics, derive the relationship between different formulations and explain the consequences
- The student can explain the concept of a Carnot engine and prove Carnot's theorem
- The student can derive Clausius theorem and explain its relation to thermodynamic entropy
- The student can explain the concept of thermodynamic potentials and derive the relationship between them and derive their extremal properties
- The student can apply probability theory for discrete and continuous random variables to derive the central limit theorem
- The student can explain the concepts of information and Shannon entropy and apply the maximum entropy principle
- The student can explain the basic concepts of microstates, macrostates and phase space density. The student can apply them to formulate the concept of ergodicity and Liouville's theorem and explain the implications for the concept of equilibrium and time-reversibility
- The student can explain the basic concepts of classical statistical mechanics and their underlying assumptions, the relationship between the different ensembles and use them to calculate the thermodynamic properties in a given application
- The student is able to identify suitable, reliable and understandable reference material and critique original peer-reviewed literature on thermodynamics and statistical mechanics
- The student can solve problems individually or in teams and communicate his/her own understanding of a given topic clearly in written and oral form

Electronically Approved - Aug 25 2023 15:42

Department Approval

2023-08-25 7 of 7