UNIVERSITY OF CALGARY
FACULTY OF SCIENCE

Department of Physics & Astronomy
Science B 605
403 220-5385
phasoffice@ucalgary.ca

COURSE OUTLINE

1. **Course:** PHYS 449, Statistical Mechanics I - Fall 2020

   Lecture 01: TR 11:00 - 12:15 - Online

Instructor	Email	Phone	Office	Hours
Dr Joern Davidsen	davidsen@phas.ucalgary.ca	403 210-7964	SB 505	by appointment

   I will respond to your email inquiries about the course within 24 hrs except on weekends and holidays.

   In Person Delivery Details:

   Tutorials

   Wednesdays 3-3:50pm (group 1) and Thursdays 11-11:50am (group 2, ROOM TO BE CONFIRMED)

   Due to the design of the course, attendance is not mandatory. Worksheets with solutions will be uploaded to D2L after each tutorial.

   More information about safety protocols and other relevant info for in-person meetings will be provided to students prior to or during the first week of classes.

   Online Delivery Details:

   Some aspects of this course are being offered in real-time via scheduled meeting times. For those aspects you are required to be online at the same time.

   Lectures

   Synchronous component: Tuesdays 11-12:15

   Similar to a flipped classroom approach, students are expected to review the assigned reading and other learning materials each week followed by group discussions centered on specific questions related to this material during the synchronous component (via Zoom, not recorded, but the questions will be posted on D2L afterwards). The synchronous component will also contain a general Q&A part. While attendance of the synchronous component is not mandatory, it is an important learning opportunity and it provides direct feedback on the individual learning progression. Note also that the individual learning modules of this course build on one another.

   The technology requirements for the synchronous component are:

   - A device with a supported operating system for Zoom;
   - Webcam/Camera (built-in or external);
   - Microphone and speaker (built-in or external), or headset with microphone;
   - Stable internet connection

   Course Site:

   D2L: PHYS 449 L01-(Fall 2020)-Statistical Mechanics I

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

2. **Requisites:**

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

   Prerequisite(s):
   Physics 343; and 229 or 325; and Mathematics 375 or 376; and Mathematics 367 or 377.

3. **Grading:**

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

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

Assignments (8): 64%
Group presentations (pre-recorded): 10% (October 23 or November 20 depending on the topic of the group)
Final project: 26% (tentatively December 15)

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

4. **Missed Components Of Term Work:**

The university has suspended the requirement for students to provide evidence for absences. Please do not attend medical clinics for medical notes or Commissioners for Oaths for statutory declarations.

In the event that a student legitimately fails to submit any online assessment on time (e.g. due to illness 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. Absences not reported within 48 hours will not be accommodated. If an excused absence is approved, then the percentage weight of the legitimately missed assignment could also be pro-rated among the components of the 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.

Assignments and supporting learning 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 ELearning online website.

7. **Examination Policy:**

The final take-home exam should be completed without consulting with other students and any external help.

Students should also read the Calendar, Section G, on Examinations.

8. **Approved Mandatory And Optional Course Supplemental Fees:**

None.

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 E.2 of the University Calendar.

10. **Human Studies Statement:**

    See also [Section E.5](#) 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 I.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 form 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 [I.1](#) and [I.2](#) of the University Calendar

    b. **Final Exam:** The student shall submit the request to Enrolment Services. See [Section I.3](#) 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 Center:** For more information, see [www.ucalgary.ca/wellnesscentre](#) or call [403-210-9355](#).

    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 ([svsa@ucalgary.ca](#)) or phone at [403-220-2208](#). The complete University of Calgary policy on sexual violence can be viewed at [(https://www.ucalgary.ca/policies/files/policies/sexual-violence-policy.pdf)](#)

    d. **Misconduct:** Academic misconduct (cheating, plagiarism, or any other form) is a very serious offence that will be dealt with rigorously in all cases. A single offence may lead to disciplinary probation or suspension or expulsion. The Faculty of Science follows a zero tolerance policy regarding dishonesty. Please read the sections of the University Calendar under [Section K](#). Student Misconduct to inform yourself of definitions, processes and penalties. Examples of academic misconduct may include: submitting or presenting work as if it were the student's own work when it is not; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; collaborating in whole or in part without prior agreement of the instructor; borrowing experimental values from others without the instructor's approval; falsification/ fabrication of experimental values in a report. **These are only examples**.

    e. **Academic Accommodation Policy:** Students needing an accommodation because of a disability or medical condition should contact Student Accessibility Services in accordance with the procedure for accommodations for students with disabilities available at [procedure-for-accommodations-for-students-with-disabilities.pdf](#).

    Students needing an accommodation in relation to their coursework or to fulfill requirements for a graduate degree, based on a protected ground other than disability, should communicate this need, preferably in writing, to the Associate Head of the Department of Physics & Astronomy, Dr. David Feder by email phas.ahugrd@ucalgary.ca or phone 403-220-8127. Religious accommodation requests relating to class, test or exam scheduling or absences must be submitted no later than **14 days** prior to the date in question. See [Section E.4](#) of the University Calendar.

    f. **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 [Legal Services](#) website.

    g. **Student Union Information:** [VP Academic](#), Phone: [403-220-3911](#) Email: [suvpaca@ucalgary.ca](#). SU Faculty

Rep., Phone: [403-220-3913](tel:403-220-3913) Email: sciencerep@su.ucalgary.ca. [Student Ombudsman](), Email: ombuds@ucalgary.ca.

h. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction ([USRI]()) 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.

i. **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.

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 differentials, partial derivatives, integrating factor.

HW 1 (due Friday, noon, Sept 18)

- 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.

HW 2 (due Friday, noon, Sept 25)

- 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.

HW 3 (due Friday, noon, Oct 2)

- Module 1.6: **Thermodynamic entropy.** Learning outcomes: Derive 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.

HW 3 (due Friday, noon, Oct 9)

- 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

HW 4 (due Friday, noon, Oct 16)

Module 2: **Probability theory** (2 ½ 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.

NO HW (Oct 23) but group presentations (Thermodynamics) instead

- 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: high-dimensional integrals, Stirling's formula, series expansion (ln, exp), delta function

HW 5 (due Friday, noon, Oct 30)

- 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 ½ weeks)

Learning outcomes: Explain how we can obtain 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.

HW 6 (due Friday, noon, Nov 6)

- 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

NO HW (Nov 20) but group presentations (Probability theory) instead

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.

HW 7 (due Friday, noon, Nov 27)

- Module 4.2: **Applications of statistical mechanics**. Learning outcomes: Apply ensemble theory to calculate the thermodynamic properties for a given system. Mathematical background: l'Hopital's rule, high-dimensional integrals, spherical coordinates, Gamma function.

HW 8 (due Friday, noon, Dec 4)

- Module 4.3: **Indistinguishable particles.** Learning outcomes: Explain Gibbs paradox and how it can be resolved in the classical context, apply it in a given application.

General course information

i) *Textbook & class notes:*
As none of the currently available textbooks satisfactorily covers all aspects of the course, there are 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 posted class notes and 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 other 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.

ii) *Grading philosophy:*
Because I try to encourage participation as much as possible, I have put a heavier accent on assignments than is maybe customary.

iii) *Group presentations:*
Each group will consist of three or four students and prepare a 15 minute presentation on a given topic. Topics will fall into one of two categories: Thermodynamics and Probability theory. Each group will have at least a week to prepare and prerecord the presentation. Powerpoint slides with voice recordings are sufficient.

iv) *Final project:*
The final project will be a mix of a regular homework assignment and a topic paper. You will have at least 4 days to complete it.

v) *Class participation:*
The emphasis in this course will be on discussion and critical thinking. Given this, your active class participation throughout the semester will be essential. You will be challenged in class to defend your thinking by appropriate reasoning or by references to material covered in the lectures and reading. If you don't understand something during 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.

vi) *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.

vii) *Homework assignments:*
There will be continuous homework assignments over the term, which will typically be posted on D2L on Thursdays and are due the following Thursday before class. 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. (Paper is cheap compared to the time needed for you to complete the assignments and for me to grade your assignments.) 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 be written out by hand on paper. Please use ink, not pencil. Numerical and graphical answers involve output that are best printed out on a laser printer, then stapled 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.

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 24 2020 10:18

Department Approval

Electronically Approved - Aug 26 2020 15:40

Associate Dean's Approval