UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF PHYSICS AND ASTRONOMY
COURSE OUTLINE

1. **Course:** PHYS 449 Statistical Mechanics I Fall 2017

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   Lecture Sections: LEC 1 | TR 12:30-1:45 | SB 105

   Course Website: d2l.ucalgary.ca
   Departmental Office: SB 605, 403-220-5385, phasugrd@ucalgary.ca

2. **Prerequisites:** PHYS 325; and one of AMAT 219 or MATH 253 or 267 or 277. (Please see Calendar Description for more information).
   Note: The Faculty of Science policy on pre- and co-requisite checking is outlined in the 2015-2016 Calendar. A student may not register in a course unless a grade at least" C-" has been obtained in each pre-requisite course; it is the responsibility of students to ensure that their registrations are in order.
   See http://www.ucalgary.ca/pubs/calendar/current/sc-3-5.html for details.

3. **Grading:** The University policy on grading and related matters is described sections 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): 40%
   Midterm Exam: 20% (Oct. 26, during regular class hours)
   Final Examination: 40% (To be scheduled by the Registrar)

   Percentage to letter grade conversion scale:

> = 90 %	A +	> = 75 %	B +	> = 60 %	C +	> = 45 %	D +
> = 85 %	A	> = 70 %	B	> = 55 %	C	> = 40 %	D
> = 80 %	A -	> = 65 %	B -	> = 50 %	C -	< 40 %	F

4. **Missed Components of Term Work:** The regulations of the Faculty of Science pertaining to this matter are found in the Faculty of Science area of the Calendar in Section 3.6. It is the student's responsibility to familiarize himself/herself with these regulations. See also Section E.6 of the University Calendar.

5. **Scheduled out-of-class activities:** N/A.

   REGULARLY SCHEDULED CLASSES HAVE PRECEDENCE OVER ANY OUT-OF-CLASS-TIME-ACTIVITY. If you have a clash with this out-of-class-time-activity, please inform your instructor as soon as possible so that alternative arrangements may be made for you.

6. **Course Materials:** *Thermodynamics and Statistical Mechanics* (W. Greiner, L. Neise, H. Stoecker; Springer)

Statistical and Thermal Physics (H. Gould , J. Tobochnik; Princeton University Press)

Online Course Components: Assignments, and supporting lecture material will be posted on the course D2L website.

7. **Examination Policy**: Final exam and midterm test are closed book. No calculators or laptops will be allowed. 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:** In this course, the quality of the student's writing in homework assignments will be a factor in the evaluation of those assignments. See also Section E.2 of the University Calendar.

10. **Human studies statement:** Students in the course will not be expected to participate as subjects or researchers. See also Section E.5 of the University Calendar.

11. **OTHER IMPORTANT INFORMATION FOR STUDENTS:**

(a) **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.

(b) **Assembly Points:** In case of emergency during class time, be sure to FAMILIARIZE YOURSELF with the information on assembly points.

(c) **Student Accommodations:** 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 http://www.ucalgary.ca/policies/files/policies/procedure-for-accommodations-for-students-with-disabilities_0.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 and Astronomy, Dr. David Feder, by email (dfeder@ucalgary.ca) or by phone (403.220.3638).

(d) **Safewalk:** Campus Security will escort individuals day or night (http://www.ucalgary.ca/security/safewalk/). Call 220-5333 for assistance. Use any campus phone, emergency phone or the yellow phones located at most parking lot pay booths.

(e) **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). As one consequence, 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 also http://www.ucalgary.ca/secretariat/privacy.

(f) **Student Union Information:** VP Academic Phone: 220-3911 Email: suvpaca@ucagary.ca.
SU Faculty Rep: Phone: 220-3913
Email: science1@su.ucalgary.ca, science2@su.ucalgary.ca and science3@su.ucalgary.ca
Student Ombuds Office: 403 220-6420
Email: ombuds@ucalgary.ca; http://ucalgary.ca/provost/students/ombuds

(g) **Internet and Electronic Device Information:** You can assume that in all classes that you attend, your cell phone should be turned off unless instructed otherwise. Also, communication with other individuals, via laptop computers, Blackberries or other devices connectable to the Internet is not allowed in class time unless specifically permitted by the instructor. If you violate this policy you may be asked to leave the classroom. Repeated abuse may result in a charge of misconduct.

(h) U.S.R.I.: At the University of Calgary, feedback provided by students through the Universal Student Ratings of Instruction (USRI) survey provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses (www.ucalgary.ca/usri). Your responses make a difference - please participate in USRI Surveys.

12. OTHER COURSE RELATED INFORMATION:

(a) Course Description

State-counting; classical distributions; origins and role of entropy; equilibrium; microcanonical, canonical, and grand canonical ensembles; concepts of work, heat, and temperature; equations of state; heat capacity; equipartition theorem; engines; laws of thermodynamics; non-equilibrium systems; Maxwell-Boltzmann distribution; enthalpy and free energies.

(b) Course Learning Outcomes

The purpose of the course is to teach the student concepts and methods to describe many-particle systems from a classical mechanical point of view.

The aims of the course are that, upon completion of the course, the student is expected to have acquired the following knowledge and skills:

- 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 the arrow of time.
- 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.

(c) 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 discrete states typical for quantum mechanical systems as covered in PHYS 325.

(d) Syllabus

1. Thermodynamics
   - 1.1. Basic notation: thermodynamics systems, equilibrium
   - 1.2. Work: quasistatic changes, exact and inexact differentials, integrating factor
   - 1.3. Heat & 1st law of thermodynamics
   - 1.4. 0th law of thermodynamics & temperature
   - 1.5. Heat capacities: gas, magnet
   - 1.6. Adiabats & isotherms: ideal gas, black-body radiation or the photon gas
   - 1.7. 2nd law of thermodynamics: heat engines, efficiency, refrigerators, formulations by Kelvin and Clausius
   - 1.8. Carnot engines: reversible and cyclic processes, Carnot's theorem
   - 1.9. Thermodynamic temperature scale
   - 1.10. Clausius theorem, thermodynamic entropy and the 2nd law: formulation by Planck, reversible and irreversible processes
   - 1.11. Thermodynamic potentials: Maxwell relations, Legendre transformation, Helmholtz free energy, enthalpy, Gibbs free energy, grand potential
   - 1.12. Approach to equilibrium and equilibrium conditions: isolated system, closed systems
   - 1.13. 3rd law of thermodynamics: formulation by Nernst and consequences
2. Probability theory & statistics
   - 2.1. Basic notation: probability space, probability axioms, interpretations of probability, microstates, macrostates, binomial distribution
   - 2.2. Characteristics of probability distributions: mean, variance, standard deviation, relative uncertainty, law of large numbers
   - 2.3. Gaussian distribution and continuous random variables: Stirling's formula, cumulative distribution function, probability density function, change of random variable
   - 2.4. Many continuous random variables & central limit theorem: independent random variables, joint, unconditional and conditional probability density functions, Bayes' theorem
   - 2.5. Information & Shannon entropy: multinomial coefficient, maximum entropy principle and motivation of the central postulate of statistical mechanics
3. Kinetic theory of gases
   - 3.1. Hamiltonian dynamics & phase space: equivalence of Hamilton's equations of motion and Lagrange's equations of motion, equivalence of Hamiltonian and total mechanical energy
   - 3.2. Microstates, macrostates and phase space density: ensemble averages
   - 3.3. Liouville's theorem: conservation of probability, equilibrium at the macroscopic level from a microscopic description, possible solutions and the central postulate of statistical mechanics
   - 3.4. Ergodicity
   - 3.5. 2nd law of thermodynamics revisited: time-reversal symmetry of Hamilton's equations of motion (time permitting), implications of ergodicity and the arrow of time
4. Classical statistical mechanics
   - 4.1. Rules for large numbers: saddle point integration
   - 4.2. Microcanonical ensemble: central postulate of statistical mechanics, entropy equivalence (Shannon/Boltzmann vs. thermodynamic), recipe for deriving the thermodynamic properties of a system
   - 4.3. Canonical ensemble: partition function, Helmholtz free energy
   - 4.4. Examples: Two-level system (heat capacity), ideal gas (internal energy, equation of state, Maxwell-Boltzmann distribution, interpretation of temperature)

4.5. Mixing entropy and Gibbs paradox: indistinguishable particles, coarse-grained phase space, ideal gas revised
4.6. Gibbs canonical ensemble: ideal gas in isobaric ensemble (enthalpy, heat capacities), non-interacting Ising model with external magnetic field (magnetic susceptibility, heat capacity)
4.7. Grand canonical ensemble (time permitting): ideal gas (chemical potential), surfactant adsorption
4.8. Virial theorem (time permitting): average temperature of the sun, mass of distant galaxies
4.9. Equipartition theorem (time permitting)

(e) General course information

❖ Textbook & lecture 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 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.

❖ Grading philosophy:

Because I try to encourage participation as much as possible, I have put a heavier accent on assignments than is maybe customary.

❖ Midterm:

The in-class midterm (75 min long) will focus on the material covered up to and including the last homework assignment before the midterm.

❖ Final:

The final exam (3hrs 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.

❖ 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.

❖ Tutorials:

Weekly tutorials will be offered to discuss the solutions to the homework problems and to review the material covered in class as necessary.

❖ 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 μ=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.

Department Approval____Date____________________________