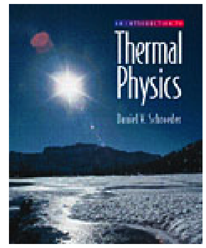
Physical Chemistry I / Thermal Physics and Statistical Mechanics

"Thermodynamics is the only physical theory of universal content which, within the framework of the applicability of its basic concepts, I am convinced will never be overthrown." — Albert Einstein

Instructor: Willetta Greene-Johnson, Ph. D.[1], Room 307 Cudahy Science 773-508-3537

Office Hours: Wednesday 4:00 PM and by appointment
wgreene@luc.edu



Textbook: Thermal Physics, 1st edition, Daniel V. Schroeder (Addison Wesley), 1999 ISBN **13: 9780201380279**

Supplementary Material: (not required)

- Physical Chemistry, 11th Ed., Atkins & de Paula ISBN 9780198769866 (required for C302)
- The 2nd Law, Atkins, ISBN: 978-0716750048
- MIT Open Course Ware, Thermodynamics and Kinetics. http://ocw.mit.edu/courses/chemistry/5- 60-thermodynamics-kinetics-spring-2008/

Meetings: Lectures are scheduled T Th in CSH-313, 10:00 A – 11:15 A.

CHEM 301 Discussion: T, CSH-313, 8:55 A – 9:45 A. See page 3 for more details.

Course Description: This course covers concepts of temperature and heat, equations of state, laws of thermodynamics and applications, fundamental principles and simple applications of statistical mechanics. Specifically, we consider what laws govern the behavior of a huge number of particles (10^{24} ~ mole) near/at equilibrium, and trace the relation between statistical mechanics (atomic systems) and thermodynamics (macroscopic/mesoscopic systems).

PHYSICS 328	PHYSICAL CHEMISTRY 301
Prerequisites: PHYS 235, PHYS 301, MATH 264 (The quantum mechanics encountered in PHYS 235 is quite sufficient prerequisite for this course).	**Prerequisites: CHEM 222** or **224/226** (Organic), **PHYS 112K** (College Physics w/ **Calculus**), and **Math 263** (Multivariate Calculus) No quantum mechanics required; what formulas are needed will be supplied.
If you have not completed the course prerequisites, you may be administratively dropped from the class.	

Exam Days: **Sept. 27, Nov. 1, Nov. 29, Dec. 11**
Final Exam Tuesday Dec. 11; 11:00 A –1:00 P in classroom to be announced.
Exam Style: In class, closed book
Calculators: Any scientific calculator is sufficient.

Grade Scale	B+ 87-89	C+ 77-79	D+ 67-69
A ≥ 93	B 83-86	C 73-76	D 63-66
A- 90-92	B- 80-82	C- 70-72	F < 63

[1] **Who am I: A chemical physicist trained in statistical mechanics. I'm interested in (1) thermodynamics (1) Swarming (2) Heat Engines and impact on resources (3) producer, pianist, composer, orchestrator, sequencer, and conductor. My vocal ensemble also has recorded three compact discs—hopefully can do an EP later this year. One of my songs was doubly tracked on a Grammy award winning vocal CD in 2004. The same song was recorded on DVD (released April 2008). Actually that song has been recorded by six artists. I'm also getting more orchestral arrangement contracts—I have had works performed by The Chicago Sinfonietta and The Memphis Symphony Orchestra. I just conducted a commissioned work this past May, 2018. Orchestras rock!**

Assignment Weights: Attendance: 10%, Homework 20%, Three Midterms **45% total**, Final 25%

Computational Aspects: *Some* assignments problems will require use of Mathematica and/or Excel.

Attendance: **Taken every lecture.**

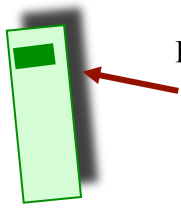
Attendance % = 10 × (28 - M) / 28 where 28 = number of meets, M = unexcused missed meets

SAKAI Connection:

Copies of syllabus, homework assignments, any supplementary handouts, and, worked out homework solutions will be posted in SAKAI course Resource Folder.

Homework: A pivotal part of this course and the student's learning experience.

1. Homework is graded out of 40 points.
2. **NO LATE HOMEWORK IS ACCEPTED.**
3. **Frequency:** Handed out Thursdays in class, returned in class ~1 week later.
4. Format
   Staple Fold the long way, **print clearly at top on outside**:



LAST NAME, FIRST NAME
Chem. 301 / Phys. 328
Date

5. You are encouraged to conquer homework with classmates, consult other books, etc., but ***ultimately turn in one's own work***.
   No carbon copies or scans from books. Use your own words. For example, I shouldn't see verbatim "copied-from-each-other" explanations from four students. This is an invitation for homework to become *more challenging* in order to weed out the "leeches". No science major should be leeching at this point in her / his career.
6. Homework will usually be returned within one week from assigned date.
7. Solutions to homework will be provided, usually within one week from assigned date.

Exams Format and Content:

Exams are in-class and closed book. They are based upon both homework and lecture content (includes short movies or discussions*, etc.,* if it applies.) A crib sheet will be provided.

Academic Integrity:

All students are responsible for exercising the highest level of academic honesty while taking exams. The University policy on plagiarism, and cheating is stated at:

http://www.luc.edu/academics/catalog/undergrad/reg_academicintegrity.shtml

During examinations, you must perform your own work. There must be severe, policy-imposed consequences if integrity is determined to be breached. It will *minimally* cost the offender a grade of "zero" for the item that was submitted and this grade cannot be dropped. Additionally, the incident must be reported to the Department Chair and the Office of the CAS Dean, and becomes a permanent item on all transcripts. Depending upon the seriousness of the incident, additional sanctions may be imposed.

Chem 301 Discussion details:

Attendance will be taken and the extent of the student's participation will be noted. Discussions will consist of working 2-3 exercises that pertain to that week's material. Remaining time may be used to clarify lecture topics or to casually survey physical chemistry targeted applications.

Course Content Detail and Learning Objectives:

Physics 328 / Physical Chemistry I addresses thermodynamics, statistical mechanics, and the properties of many-body systems. A main objective of thermodynamics is to determine how systems behave at or near equilibrium. Thermodynamics is widely used to quantify the energetics of physiochemical systems. The phenomenological description of such systems (classical thermodynamics, macroscopic phenomena) is reconciled with their microscopic properties (statistical mechanics). Another objective is for students to have some exposure to solving *some* problems via Mathematica, or similar platform. This is an essential job-competitive skill.

Finally, selected technological applications confirm the contemporary relevance of the subject. For example, amongst the foremost challenges that chemists and physicists are well trained to solve is the development of new and clean energy sources. Thermodynamics is key to surmounting the obstacles to realizing clean fuels. The central expectation of this course is that the student gainfully applies concepts covered in the course to "critically gauge the accuracy and potential competency of political / scientific (!) solutions to problems that, in your lifetime, will only grow in significance".[i]

Statement of Intent: By remaining in this course, students are agreeing to accept this syllabus and to abide by the guidelines outlined in the document. Students will be informed should there be a necessary change to the syllabus.

Intellectual Property: All lectures, notes, Power Points and other instructional materials in this course are the intellectual property of the professor. As a result, **they may not be distributed** or shared in any manner, either on paper or virtually without my written permission. Lectures may not be recorded without my written consent; when consent is given, those recordings may be used for review only and may not be distributed. Recognizing that your work, too, is your intellectual property, I will not share or distribute your work in any form without your written permission.

Special Circumstances—Receiving Assistance: Students are urged to contact me should they have questions concerning course materials and procedures. If you have any special circumstance that may have some impact on your course work, please let me know so we can establish a plan for assignment completion. If you require assignment accommodations, please contact me early in the semester so that arrangements can be made with Services for Students with Disabilities (SSWD) (http://www.luc.edu/sswd/).

Student Support Resources:

• ITS HelpDesk ○ helpdesk@luc.edu ○ 773-508-4487	• Services for Students with Disabilities ○ http://www.luc.edu/sswd/
	• Writing Center ○ http://www.luc.edu/writing/
• Library ○ Subject Specialists: http://libraries.luc.edu/specialists	• Ethics Hotline ○ 855.603.6988 http://luc.edu/sglc/aboutus/

Assessment Expectations:

By the conclusion of this course, the student should experience the following outcomes:

1. Understand the fundamental principles and constructs of classical thermodynamics
2. Understand the central role of entropy in determining thermal equilibrium and status of observables.
3. Understand appropriate deployment of the thermodynamic potentials U, S, F, G and H
4. Know how to construct and utilize partition functions
5. Recognize thermodynamic principles in pioneering research and novel technologies

Specifically, the motivated student should improve in his or her ability to

- Implement the following principles or constructs:

(1) Be able to calculate statistical entropy and to derive potentials, e.g.,Helmholtz energy…

(2) Given entropy function S(U,V,N) of a system, be able to determine the energy function: U(T,V,N). (Determine dependence of average energy upon temperature, or *vice versa*.)

(3) Know how to construct and employ the Boltzmann and Gibbs partition functions

(4) Be able to analyze a cyclic process and evaluate or closely estimate its efficiency.

(5) Utilize the appropriate thermodynamic potentials U, S, F, G, H for system analysis

(6) Be familiar with the following constructs: ideal gas, phase diagram, heat engine, binary (spin ½) system, partition function, connection between thermodynamic differentials and experiments, Einstein / Debye solids, mixtures, photon and Fermi gases.

(7) Be able to solve reasonable problems using Mathematica, Excel, etc.

- Assess outcome feasibility: **estimate energy costs of simpler processes compare to $k_B T$**
- Work and exchange ideas with others: **cordially solve weekly homework together**
- Appreciate the role of thermodynamics in **daily life, novel technology and cutting edge research.**

Later this semester, you will receive an emailed invitation to assess me via the **IDEA** (Individual Development and Educational Assessment). The form provides a thorough diagnostic of how successfully students think the instructor realized the objectives boxed above, as well as the value of the course and other contextual experiences. This opportunity will be available online at http//www.luc.edu/IDEA for a one-week time window only.

IDEA manual states: "As student raters, please be aware that the results of your ratings for this class will be included as part of the information used to make decisions about promotion/tenure/salary increases for this instructor. Fairness to both the individual and the institution require *accurate and honest* answers."

Approximate Lecture Schedule

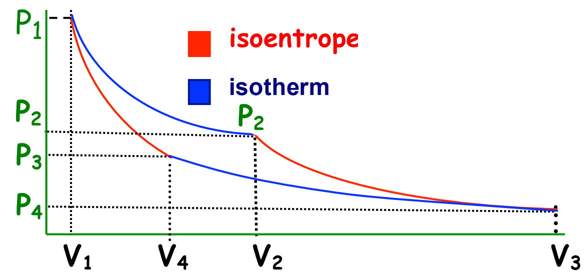
August	28, 30	Introduction, Ideal Gas Law, degrees of freedom, equi-partition theory, heat capacity, Dulong-Petit Law, 1st Law, adiabatic/ isothermal work, Cycles, particle-in-a-box	Ch. 1 pg1-4, 6,10-13, 14-17,17-22, 23-26,28-31, 32-35 [rates: 37-48]
September	4, 6	2nd Law, Entropy, Multiplicity, Stirling's Law, Large Numbers, irreversibility	Ch. 2 pp 49-mid 57
	11, 13	Multiplicity of Ideal Gas, Sackur Tetrode Eq'n; Statistical def'ns of Temperature / Pressure; various macroscopic entropy relations;	Ch. 2 pp 60-83 Ch. 3 85-95,95-99, Fig 3-8 & 3-10,103-106, 108-111, 112-113
	18, 20	Mechanical and Diffusive Equilibrium, Thermodynamic Identity. 2nd Law: Heat Engine, Efficiency, Carnot Cycle, Clausius, Kelvin, Heat Pump/Fridge, various cycles	Ch. 3 115-119,120-121 Ch. 4 122-24,125,127-129,131-32, 134-35, 137-138, 144-147
	25,	various cycles, Throttling, Joule-Thompson effect, some REVIEW 1-3	Ch. 4 139-140, 141-143, 144-147
	27	**Exam 1**	**1-3**
October	10-2,4	Heat Reservoir, Boltzmann Statistics; Boltzmann factor, Partition F'n "Z", Helmholtz Energy, Equipartition Theory,	Ch. 6 220-224, 225-27, 229-230, equipartition 238-240
	10-8,9	**BREAK**	
	11,	Maxwell Boltzmann Distribution; Applications. (1) binary system, (2) paramagnetic; (3) ideal gas, (4) Harmonic oscillator (5) ideal rotator, [(6) elastomer]	Ch. 6 232-33, 234-236, MB: 242-46, 247-251; IG: 251-55
	16,18	Thermodynamic Potentials, Maxwell Relations, Chemical Potential; phase diagrams. phase stability & Transitions, Clausius/Clapeyron Equation, [Application of CC eq'n to magnetocaloric system. magnetic cooling]	Ch. 5 149-155 156-158, 161-162, 163-65, 166-171, 172-174, 180-184 **Handouts: Phases, Mixtures**
	23, 25	simple sol'ns: μ & other partial molar quantities, gas, pure liquid, ideal sol'n, Raoult & Henry Laws, osmotic pressure, colligative properties, phase diagrams, [distillation/azeotrope]	Ch. 5 186-191, 192-94, 200-204, 206-208, 208-213, 214-15, Henry: 216-217, Saha: 218-19
	30	Remaining Ch. 5 topics. some **REVIEW 4-6**	
November	11-1	**Exam 2**	**4-6**
	6, 8	Blackbody Radiation, Harmonic Osc; Partition F'n, occupancy, Planck Distribution; Stefan-Boltzmann Law, Kirchhoff, Wien, Spectral radiation, CMB	Ch. 7 288-293, 294, 295-296, 300-303
	13, 15	Johnson-Nyquist noise. Phonons, Debye Solid, heat capacity	Ch. 7 NJ: lect. Appendix 1,2 Debye Theory 307-312
	20	Grand Partition F'n, Gibbs factor. Osmosis, Adsorption; Application: Ideal Gas; Chemical pot'L & Diffusive Systems;	Ch. 7 257-250
	27	Intro to Fermi & Boson distributions some REVIEW	Ch. 7 262-265,267-69,
	29	**Exam 3**	**6–7**
December	4 6	Fermi-Dirac distribution, density of state, Fermi metals, Fermi gas, neutron stars, white dwarfs, Bose-Einstein distribution, ~0 K, BEC, Atom-laser; some REVIEW	Ch. 7 271-275, 315-323,
12/11		**FINAL EXAM 1P – 3P DEC 11**	**1-7**

Approx. Schedule of Topics [2]

August / September

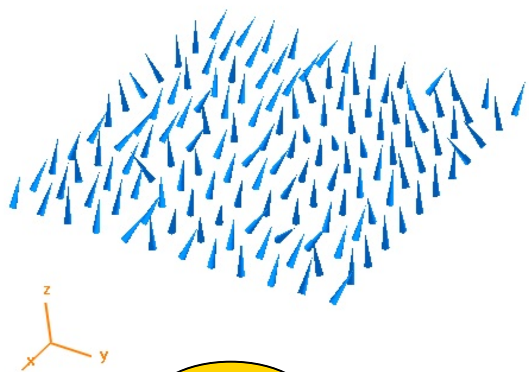
Ch. 1: Thermodynamics

Thermal equilibrium; Ideal Gas
Equipartition Theory; Heat and Work;
Heat Capacity; Latent Heats
Enthalpy; Standard Enthalpies of Formation;



Ch. 2: Entropy (statistical definition)

Two State System
Probability vs. Possibility
Einstein Solid,1-D Paramagnetic
Ideal Gas (from Boltzmann's Multiplicity)
Entropy of Ideal Gas
2^{nd} Law (statistical statement)



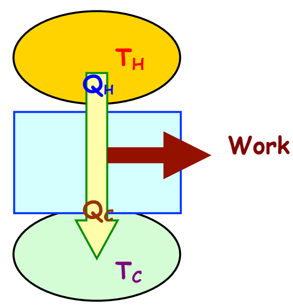
Ch. 3: Statistical Temperature

Heat flow; Negative Heat Capacity
Mechanical Equilibrium; Pressure

October

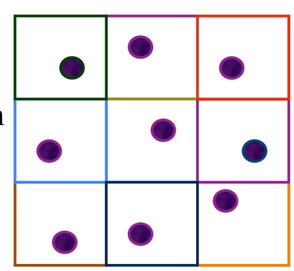
Ch. 4 : Carnot Cycle

- Efficiency and the 2^{nd} Law of Thermodynamics
- Refrigerators, Air Conditioners and Heat Pumps
- Applications:
  - i. Geothermal Heat Pump
  - ii. Ocean Thermal Energy Cycle (OTEC)
  - iii. Magnetic Refrigeration

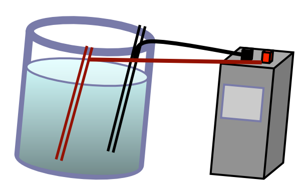


Ch. 6: Boltzmann Statistics

- Definition; Proof of Equi-partition Theorem
- Maxwell Boltzmann Distribution Function
- Helmholtz Energy
- Partition Function of selected systems: atom in box, harmonic oscillator, *etc.*
- Thermodynamic Identity



an ensemble of identically prepared systems



Ch 5: Free Energy and Chemical Thermal Dynamics

- Thermodynamic Potentials
- Free energy ↔ available work
- Chemical potential: relation to Gibbs energy
- Maxwell Relations: significance to experiment
- Single Component Phase Diagram; Ideal Mixture
- Entropy of Ideal Mixtures
- Mixtures, Ideal, Partial Miscible, Azeotropes

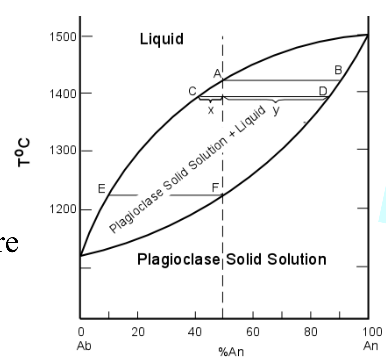
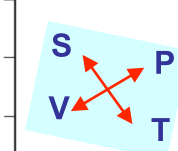


Figure 3



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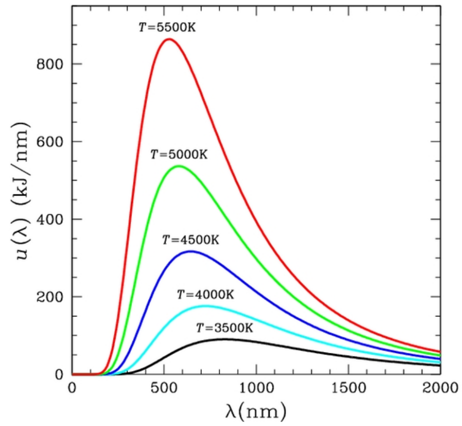
[2] approximate

November / December

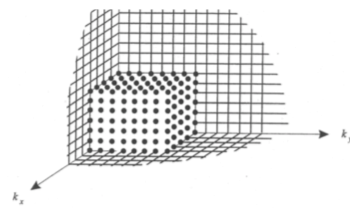
Ch. 7: Bose and Fermi Statistics
Blackbody Radiation

- Planck Distribution
- Stefan-Boltzmann Law
- Phonons: Debye Theory
- Heat Capacity of Solid



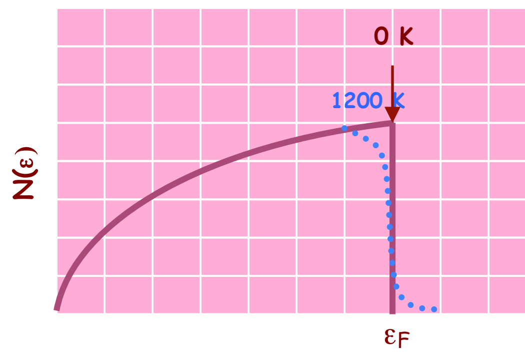
Open and Diffusive Systems

- Grand Partition Function
- Chemical Potential
- Examples including osmosis



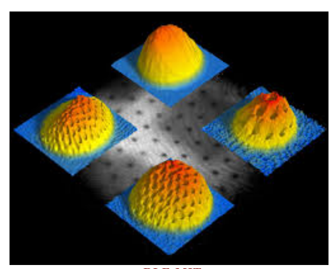
Fermions

- Fermi-Dirac Distribution Function
- Fermi Gas
  - Ground State; Density of State
  - Electronic Heat Capacity
  - Fermi metals
  - Electron Degeneracy Pressure
  - White Dwarfs, Nuclear matter



Bosons

- Bose-Einstein Distribution Function
- Temperature dependence of Orbital Occupancy
- Chemical Potential (T ~ 0 K)
- Bose Gas
  - He-4: Bose-Einstein Condensation
  - atom laser [3]



RLE-MIT

Final Exam 11:00 A – 1:00 P, Tuesday, Dec. 11, 2018 (room tba)

[i] Dan Killelea, Assoc. Prof. of Chemistry, Loyola

[3] http://visions.iop.org/v16.html