

CHEM 703 / CHPH 703 / PHYS 703
Introduction to Nonequilibrium Statistical Physics

Spring 2020, three credits

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Description:

This course will provide an introduction to the analysis and microscopic modeling of systems away from thermal equilibrium. Topics will include linear response theory, ergodicity, Brownian motion, Monte Carlo modeling, thermal ratchets, and fluctuation relations. An organizing theme will be the second law of thermodynamics: how it can be understood from microscopic principles and how it applies to both large and small systems. Students will be introduced to the theoretical tools used to describe nonequilibrium phenomena, and will apply these tools to a variety of situations of interest in physics, chemistry and biology.

Prerequisites: PHYS 603 or CHEM 687 or permission of instructor.

Textbook: There is no required textbook for this course. I plan to teach from my own notes, occasionally drawing on other sources for particular topics. However, students might find the following books to be useful:

- J.R. Dorfman, *An introduction to chaos in nonequilibrium statistical mechanics*
Cambridge University Press, 1999
- R. Zwanzig, *Nonequilibrium statistical mechanics*
Oxford University Press, 2001
- N.G. van Kampen, *Stochastic processes in physics and chemistry*, 3rd edition
Elsevier, 2007

Office hours: Mondays, 3-4pm, 2106 IPST.

Course homepage:

http://terpconnect.umd.edu/~cjarzyns/CHEM-CHPH-PHYS_703_Spr_20/

Lectures: Attendance and participation are expected.

Academic Honor Principle: Students are expected to observe the University's Code of Student Conduct.

Grading: Grades will be based on problem sets (60%) and a final exam (40%). The format of the final exam (take-home or in class) will be determined during the semester.

Tentative Schedule of Lectures

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| Week 1 | Review of thermodynamics, equilibrium statistical mechanics and relevant mathematics |
| Week 2 | Hamiltonian dynamics: review and ergodicity |
| Week 3 | Hamiltonian dynamics: mixing |
| Week 4 | Hamiltonian dynamics: deterministic chaos, adiabatic invariants |
| Week 5 | Diffusive processes: introduction, examples, operator formalism |
| Week 6 | Diffusive processes: stochastic energetics, entropy, thermal ratchets |
| Week 7 | Linear response theory |
| Week 8 | Case study: goodness of ergodic adiabatic invariants |
| Week 9 | Discrete state processes: introduction, matrix analysis, Perron-Frobenius theorem |
| Week 10 | Discrete state processes: detailed balance, cycle decomposition |
| Week 11 | Discrete state processes: heat, work and entropy |
| Week 12 | Discrete state processes: chemical kinetics, analysis of models |
| Week 13 | Far-from-equilibrium systems: nonequilibrium work relations |
| Week 14 | Far-from-equilibrium systems: fluctuation theorems |