CSE 389D / Course identifier: 61055 / Spring 2020

Introduction to Mathematical Modeling in Science and Engineering II

Room: PAR 101
Classes: M 12:30-2:30 / W 12:30-2
Recitations: F 2-4

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Office hours M 3-4 / W 2:30-3:30

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Office hours T/Th 1:30-2:30

Syllabus

1. Quantum Mechanics

Lagrangian mechanics and Hamiltonian mechanics. Hamilton-Jacobi theory. Schrödinger equation and interpretation of the wavefunction. General solution of the Schrödinger equation for the one-dimensional square well. Brief review of the hydrogen atom. Operators and matrix elements. Dirac Notation. Poisson brackets, commutators, and canonical quantization. Ladder operators and quantum harmonic oscillator. Dirac equation and spin. Identical particles. Hartree-Fock method. The chemical bond.

2. Statistical Mechanics

Microstates, macrostates, phase space, and ensembles. Liouville's theorem. Microcanonical and canonical ensembles. Gibbs distribution. Maxwell-Boltzmann distribution and temperature. Grand canonical ensemble. Fermi statistics. Fermi gas. Bose-Einstein statistics. Phonon gas. Quantization of the electromagnetic field and photons. Black body radiation. Entropy. Curie-Weiss model and phase transitions. Free energy analysis of phase transitions. Critical exponents.

Online material: Lecture notes and homework assignments will be posted through Canvas.

Homework: There will be homework assignments every two weeks. Problem sets will be assigned on the Monday and due the Friday of the following week at the recitation.

Examination and grading: Homework: 30%, Midterm: 30%, Final: 40%. The midterm exam will take place Wednesday, 11 March (instead of the class). The comprehensive final will take place Saturday, 16 May.

Textbooks:

H. Goldstein, *Classical Mechanics*, 3rd Ed., Pearson, 2014.
E. Merzbacher, *Quantum Mechanics*, 3rd Ed., Wiley, 1997.
D. J. Griffiths, *Introduction to Quantum Mechanics*, 2nd Ed., Pearson, 2005.
P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th Ed., Oxford, 1958.
F. Giustino, *Materials modelling using density functional theory*, Oxford, 2014.
R. C. Tolman, *The Principles of Statistical Mechanics*, Dover, 1938.
L. D. Landau and E. M. Lifschitz, *Statistical Physics*, 2nd Ed., Pergamon, 1970.
R. P. Feynman, *Statistical Mechanics: A set of lectures*, CRC Press, 2018.
E. Fermi, *Molecules, Crystals, and Quantum Statistics*, Benjamin, 1966.
D. Chandler, *Introduction to modern statistical mechanics*, Oxford, 1987.