Course Concepts

Ch En 593R: Statistical Thermodynamics
Fall 2024

Course Topics

1. Probability theory and stochastic processes
2. Classical and Quantum Mechanics
3. Phase space and ensemble theory
4. Pure components: gases, liquids, solids, phase behavior
5. Soft matter: polymers, colloids, electrolytes
6. Nonequilibrium statistical mechanics and stochastic kinetics

Lecture 1: Probability Theory and Stochastic Processes

Reading:

- Kaznessis §2.1-§2.10
- Kaznessis §13.1-§13.3

I. Probability Basics

Things you should know

(1.I.a) Set notation (subset, union, intersection, compliment)

(1.I.b) Definition and meaning of mutually exclusive (disjoint sets) and independence

(1.I.c) Four types of probability (classical, statistical, subjective, axiomatic)

(1.I.d) Four probability axioms and resulting properties of probability

(1.I.e) Definition of conditional probability

(1.I.f) Bayes theorem and law of total probability

(1.I.g) Identify different cases of combinatorics problems (ordering/not, distinguishability/not, replacement/not)

Calculations you should be able to do

(1.I.α) Bayes theorem problems

(1.I.β) Compute quantities and probabilities using combinatorics

(1.I.γ) Compute large factorials using Stirling's approximation

II. Probability Distributions

Things you should know

(1.II.a) Understand the meaning of, properties for, and relationships between probability mass functions, probability density functions, and cumulative distribution functions

(1.II.b) Identify examples of pmfs, pdfs, and cdfs and physical situations where those distributions arise

(1.II.c) Identify the names and meanings of (centered) moments.

(1.II.d) Understand the meaning and the properties of characteristic functions (and related transforms)

(1.II.e) Understand the Law of Large Numbers and the Central Limit Theorem

Calculations you should be able to do

(1.II.α) Normalize pdfs and compute probabilities using pmfs, pdfs, and cdfs

(1.II.β) Make plots of pmfs, pdfs, and cdfs and be able to convert between them (e.g., get a cdf from a pdf).

(1.II.γ) Use the expectation operator to compute moments and centered moments and use properties of the expectation operator in derivations as needed

(1.II.δ) Determine the characteristic function, moment generating function, cumulant generating function, and probability generating function from a pmf or pdf

(1.II.ε) Use transformations of the pmf/pdf to compute moments and cumulants

(1.II.ζ) Derive the $N \to \infty$ limit of a pmf/pdf and/or $N \to \infty$ limit of the moments of a pmf/pdf

III. Multivariate Random Variables

Things you should know

(1.III.a) The difference between a joint and marginal distribution (for pmf, pdf, and cdf) for bivariate and multivariate distributions.

(1.III.b) Moments of bivariate and multivariate distributions: mean, variance, correlation, covariance, cross-covariance (and corresponding vectors/matrices)

(1.III.c) Definition of conditional pmfs and pdfs for bivariate and multivariate distributions.

(1.III.d) Difference between independence and uncorrelated. Mathematical properties for independent distributions.

(1.III.e) The bivariate normal distribution and its characteristic function, what the moments are, and how the distribution changes with different moments.

(1.III.f) The multivariate normal distribution and its characteristic function

(1.III.g) Vector-function analogy for vectors, operators, inner products

(1.III.h) The concept of a functional, functional derivative, and functional integral

(1.III.i) Definition of a probability density functional, moments, and characteristic functional for random fields

(1.III.j) The probabilty density functional and characteristic functional for Gaussian random fields

Calculations you should be able to do

(1.III.α) Obtain a marginal distribution (marginalization) from a joint distribution for bivariate and multivariate distributions

(1.III.β) Convert between pmf, pdf, and cdf for bivaraiate and multivariate distributions

(1.III.γ) Compute moments of a bivariate or multivariate distribution (e.g., correlation and covariance matrix) using the pmf/pdf or the characteristic function

(1.III.δ) Compute conditional pmfs and pdfs and conditional moments.

(1.III.ε) Use properties of independence and the chain rule of probability theory to relate marginal and joint distributions.

(1.III.ζ) Compute bivariate/multivariate characteristic functions

IV. Stochastic Processes

Things you should know

(1.IV.a) Not this year ...

Calculations you should be able to do

(1.IV.α) Not this year ...

Lecture 2: Mechanics and Phase Space

Reading:

- Kaznessis §3.1-§3.4

I. Classical Mechanics

Things you should know

(2.I.a) Newton's equation of motion for N particles

(2.I.b) Relation between force and potential and pairwise potentials

(2.I.c) Lennard-Jones potential, meaning of parameters

(2.I.d) Meaning of the action, Lagrangian, generalized coordinates, Euler-Lagrange equation

(2.I.e) Classical harmonic oscillator example

(2.I.f) Pendulum (linear and nonlinear) example

(2.I.g) Meaning of generalized momentum, Hamiltonian, and Hamilton's equations, Poisson Bracket, phase space

(2.I.h) Why Hamiltonian? Symplectic geometry and Noether's theorem

(2.I.i) What is Liouville's equation

Calculations you should be able to do

(2.I.α) Compute dynamics using Newton's equation of motion

(2.I.β) Construct a Lagrangian from the kinetic and potential energy using generalized coordinates and compute an equation of motion using the Euler-Lagrange equation

(2.I.γ) Construct a Hamiltonian from the total energy and compute an equation of motion using Hamilton's equations

(2.I.δ) Solve classical mechanics problems using Newtonian, Lagrangian, or Hamiltonian formalisms

II. Quantum Mechanics

Things you should know

(2.II.a) Wave equation, solutions for traveling and standing waves, meaning of parameters (e.g., speed, wavenumber, angular frequency, etc.), complex exponentials

(2.II.b) Uncertainty principle of Fourier conjugates and waves, physical intuition

(2.II.c) Concepts of wave-particle duality, Planck-Einstein formulas (for E and $\boldsymbol{p}$)

(2.II.d) The Schrödinger equation as a PDE, both versions (time dependent/independent)

(2.II.e) Postulates of quantum mechanics: state vector, observables, eigenvalues, probabilities, collapse, Schrödinger's equation.

(2.II.f) Interpret solutions of Schrödinger's equation in terms of the postulates

Calculations you should be able to do

(2.II.α) Verify that an expression is a solution to the wave equation

(2.II.β) De Broglie wavelength for a physical situation

(2.II.γ) Use separation of variables to solve Schrödinger's equation

Lecture 3: Ensemble Theory

Coming soon . . .

Lecture 4: Pure Components

Coming soon . . .

Lecture 5: Soft Matter

Coming soon ...

Lecture 6: Nonequilibrium Stat Mech and Stochastic Kinetics

Coming soon ...