Course Concepts

Ch En 593R: Statistical Thermodynamics
Fall 2024

Learning Outcomes

The Learning Outcomes for this course are designed to align with the Aims of a BYU education. Accordingly, by the end of this course, students will be able to:

1. Foundations – Explain and apply the mathematical and physical foundations of statistical thermodynamics, including multivariate probability distributions, stochastic processes, classical dynamics, and quantum mechanics.

2. Core Statistical Thermodynamics – Apply ensemble theory and partition functions to connect microscopic models of single-component gases, liquids, and solids to macroscopic thermodynamic properties.

3. Scholarly Engagement – Engage with the academic literature on statistical thermodynamics to learn about more complex systems, and synthesize and clearly communicate these concepts through written reports and oral presentations.

4. Faith and Stewardship – Seek inspiration to understand and articulate how the principles of statistical thermodynamics teach about and testify of a loving Heav-enly Father, and apply those principles in ways that advance knowledge and serve God's children.

Unit I: Probability Theory and Stochastic Processes

Reading:

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

Lec 1 – Probability Basics

<u>Things you should know</u>

(I.1.K1) Set notation (subset, union, intersection, compliment)

(I.1.K2) Definition and meaning of mutually exclusive (disjoint sets) and independence

(I.1.K3) Four types of probability (classical, statistical, subjective, axiomatic)

(I.1.K4) Four probability axioms and resulting properties of probability

(I.1.K5) Definition of conditional probability

(I.1.K6) Bayes theorem and law of total probability

(I.1.K7) Identify different cases of combinatorics problems (ordering/not, distinguishability/not, replacement/not)

Calculations you should be able to do

(I.1.D1) Bayes theorem problems

(I.1.D2) Compute quantities and probabilities using combinatorics

(I.1.D3) Compute large factorials using Stirling's approximation

Lec 2 – Probability Distributions

Things you should know

(1.2.K1) Understand the meaning of, properties for, and relationships between probability mass functions, probability density functions, and cumulative distribution functions

(1.2.K2) Identify examples of pmfs, pdfs, and cdfs and physical situations where those distributions arise.

Calculations you should be able to do

(1.2.D1) Normalize pdfs and compute probabilities using pmfs, pdfs, and cdfs

(1.2.D2) Make plots of pmfs, pdfs, and cdfs and be able to convert between them (e.g., get a cdf from a pdf).

Lec 3 – Moments

Things you should know

(1.3.K1) Identify the names and meanings of centered moments.

Calculations you should be able to do

(1.3.D1) Use the expectation operator to compute moments and centered moments and use properties of the expectation operator in derivations as needed

(1.3.D2) Determine the characteristic function, moment generating function, cumulant generating function, and probability generating function from a pmf or pdf

(1.3.D3) Use the characteristic function, mgf, or cgf to compute moments and cumulants

Lec 4 – Central Limit Theorem

Things you should know

(1.4.K1) Understand the Law of Large Numbers and the Central Limit Theorem

Calculations you should be able to do

(1.4.D1) Derive the $N \to \infty$ limit of a pmf/pdf and/or $N \to \infty$ limit of the moments of a pmf/pdf

Lec 5 – Bivariate Random Variables

Things you should know

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

(1.III.b) Moments of bivariate distributions: mean, variance, correlation, covariance, cross-covariance

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

(1.III.d) Difference between independence and uncorrelated and 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.

Calculations you should be able to do

(1.III.α) Obtain a marginal distribution (marginalization) from a bivariate joint distribution

(1.III.β) Convert between a bivariate pdf and cdf

(1.III.γ) Compute moments of a bivariate distribution (e.g., correlation and covariance matrix) using the pdf

(1.III.δ) Compute conditional pdfs, conditional moments, and use the law of total probability

(1.III.ε) Compute bivariate characteristic functions and use it to compute moments

Lec 6 – Random Vectors

Things you should know

(1.III.a) The difference between a joint and marginal distribution for multivariate distributions.

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

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

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

Calculations you should be able to do

(1.III.α) Obtain a marginal distribution (marginalization) from a multivariate pdf

(1.III.β) Convert between a multivariate pdf and cdf

(1.III.γ) Compute moments of a multivariate distribution (e.g., correlation and covariance matrix) using the pdf

(1.III.δ) Compute conditional pdfs, conditional moments, and use independence and the chain rule to relate conditional, marginal, and joint distributions.

(1.III.ε) Compute multivariate characteristic functions and use it to compute moments

Lec 7 – Random Fields

Things you should know

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

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

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

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

Calculations you should be able to do

(1.III.α) Evaluate inner products between functions and/or operators, evaluate linear operators acting on functions, evaluate functionals

(1.III.β) Evaluate a functional derivative or a functional integrals using the definition (e.g., do a simple proof)

(1.III.γ) Use given differentiation or integration rules for functionals to compute a characteristic functional or calculate moments

Lec 8 – Stochastic Processes

Things you should know

(1.IV.a) The concept of a joint pdf for a stochastic process, its relation to random vectors, time-indexing, discrete versus continuous processes, marginal pdfs

(1.IV.b) The definition of moments and of the characteristic equation for a stochastic process

(1.IV.c) Assumptions leading to a Gaussian random process

(1.IV.d) Examples of a Gaussian random process: white noise, Wiener, Ornstein-Uhlenbeck

Calculations you should be able to do

(1.IV.α) Determine the joint pdf of a Gaussian process given the moments

(1.IV.β) Perform standard manipulations of joint/marginal pdfs of stochastic processes: e.g., determine the moments, compute the characteristic equation, marginalize the distribution, compute conditional pdfs, etc.

Lec 9 – Markov Processes

Things you should know

(1.IV.a) The property of conditional independence (Markov assumption) and of a transition probability density

(1.IV.b) What the Chapman-Kolmogorov (CK) equation is and what it means

(1.IV.c) What the Fokker-Planck (FP) equation is and what it means; what are the drift and diffusion coefficients

(1.IV.d) Examples of continuous Markov processes and their FP coefficients: Wiener process, Ornstein-Uhlenbeck

(1.IV.e) The concept of a stationary stochastic process

Calculations you should be able to do

(1.IV.α) Use the CK equation to propagate transition probability densities

(1.IV.β) Use the FP equation to compute transient and stationary probability densities for Markov processes

Lec 10 – Stochastic Differential Equations

Things you should know

(1.IV.a) What a Langevin equation and a stochastic differential equation (SDE) is, the physical meaning of the terms, and the connection with the FP equation

(1.IV.b) The relationship between white noise and the Wiener process; what dW is.

Calculations you should be able to do

(1.IV.α) Solve a simple SDE and/or compute moments from stochastic trajectories

Unit 2: Classical and Quantum Mechanics

Reading:

- Kaznessis §3.1-§3.4

Lec 10 – Lagrangian 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

Calculations you should be able to do

(2.I.α) 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.β) Solve classical mechanics problems using Newtonian or Lagrangian formalisms

Lec 11 – Hamiltonian Mechanics and Phase Space

Things you should know

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

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

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

Calculations you should be able to do

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

(2.I.β) Solve classical mechanics problems using Hamiltonian formalism

Lec 12 – Waves and Particles

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 $\boldsymbol{p}$)

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

Lec 13 – Quantum Mechanics

Things you should know

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

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

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

Calculations you should be able to do

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

Lecture 3: Phase Space and Ensemble Theory

Coming soon . . .

Lecture 4: Pure Components: gases, liquids, solids, phase behavior

Coming soon ...

Lecture 5: Soft Matter: polymers, colloids, electrolytes

Coming soon ...

Lecture 6: Nonequilibrium Stat Mech and Stochastic Kinetics

Coming soon ...