

Contents

Preface	xi
1. The physics of many-particle systems	1
1.1. Classical mechanics of many-particle systems	1
1.1.1. Hamiltonian dynamics	1
1.1.2. A model for N interacting atoms	2
1.2. Quantum mechanics of many particle systems	4
1.2.1. Wavefunctions	5
1.2.2. A model for a magnet	5
1.3. Macroscopic variables	7
1.3.1. Extensive and intensive variables	8
1.3.2. Densities	8
1.3.3. Macroscopic description of fluids	9
1.3.4. Macroscopic description of magnets	11
1.4. Correlation functions and structure functions	14
1.5. Computer simulation	18
1.6. An example: molecular dynamics in two dimensions	19
1.6.1. Chaotic behavior	20
1.6.2. Molecular dynamics in Python	21
Suggested reading	22
Problems	22
2. Physics and probability	27
2.1. Pressure and temperature in a gas	28
2.1.1. Kinetic definition of pressure	28
2.1.2. Temperature and temperature scales	30
2.1.3. Virial theorem	31
2.1.4. Dense gases; the van der Waals' equation	34
2.2. Classical systems	35
2.2.1. Phase space and phase trajectories	36
2.2.2. Time averages and phase-space averages	37
2.2.3. Ergodicity and mixing	38
2.2.4. Objections to the theory	44
2.2.5. Relaxation times	46

2.3. Quantum systems	46
2.3.1. Random phases	47
2.3.2. Density matrix	48
2.4. Method of the most probable distribution	48
2.4.1. Maxwell-Boltzmann distribution	48
2.4.2. Fermi distribution	50
2.4.3. Bose distribution	51
2.4.4. Classical limit	51
Suggested reading	52
Problems	52
3. Entropy and thermodynamics	57
3.1. Classical thermodynamics	57
3.2. Boltzmann's definition of entropy	61
3.2.1. Examples	62
3.2.2. Properties of the statistical entropy	64
3.3. Thermodynamic processes	65
3.4. Temperature, pressure and chemical potential	66
3.4.1. Temperature	66
3.4.2. Force	68
3.4.3. Chemical potential	68
3.5. Measuring entropy	70
3.5.1. Entropy and heat	70
3.5.2. Entropy and equations of state	71
3.5.3. Third law of thermodynamics	72
3.6. Entropy of mixing	76
3.7. Legendre transforms and free energies	77
3.7.1. Helmholtz free energy	77
3.7.2. Enthalpy	80
3.7.3. Gibbs free energy	81
3.8. Grand potential	82
3.9. Statistical physics of polymers	83
3.9.1. Ideal polymers	83
3.9.2. Flory theory of excluded volume	86
Suggested reading	87
Problems	87
4. Canonical ensemble	93
4.1. Averages and the partition function	93
4.2. Canonical averages and equipartition	94
4.2.1. Distributions of additive degrees of freedom	94
4.2.2. Boltzmann equipartition theorem	95

4.3.	The partition function and the free energy	98
4.3.1.	First proof: average of F	98
4.3.2.	Second proof: energy fluctuations	98
4.4.	The canonical recipe	100
4.4.1.	Recipe	100
4.4.2.	Phase space density and density matrix	101
4.5.	Examples	101
4.5.1.	Ideal paramagnet	101
4.5.2.	Ideal gas	102
4.5.3.	Ideal gas with internal degrees of freedom: di- atomic molecules	103
4.5.4.	Low temperature solids in the Einstein model	105
4.5.5.	Interacting fluid	105
4.6.	Simulations in the canonical ensemble	108
4.6.1.	Statistical sampling at fixed T	108
4.6.2.	Markov processes	109
4.6.3.	Metropolis algorithm	113
4.6.4.	Monte Carlo simulations	113
	Suggested reading	115
	Problems	116
5.	Grand Canonical Ensemble	119
5.1.	Averages and the grand partition function	119
5.2.	Grand partition function and grand potential	120
5.2.1.	First proof: average of Ω	120
5.2.2.	Second proof: number fluctuations	120
5.2.3.	Density fluctuations	121
5.2.4.	Density fluctuations, $g(R)$, and $S(\mathbf{q})$	122
5.3.	The grand canonical recipe	122
5.4.	Examples using the grand canonical ensemble	123
5.4.1.	Ideal gas	123
5.4.2.	Langmuir adsorption isotherm	124
5.4.3.	Quantum ideal gases	125
5.5.	Using the chemical potential	127
5.5.1.	Theory of dilute solutions	127
5.5.2.	Chemical reactions	130
5.5.3.	Screening	131
	Suggested reading	135
	Problems	135
6.	Quantum statistical physics of Bosons	139
6.1.	Quantum statistical mechanics	139
6.1.1.	Gas degeneracy	139

6.1.2.	Many particle wavefunctions	140
6.1.3.	Free particle orbitals	142
6.1.4.	Classical limit	143
6.1.5.	Interacting systems	144
6.2.	Black-body radiation and photons	145
6.2.1.	Thermodynamics of light	145
6.2.2.	Statistical mechanics of light	147
6.2.3.	Quantum statistical mechanics of photons	149
6.2.4.	Applications of the Planck radiation law	149
6.3.	Phonons	152
6.3.1.	Sound in classical physics	153
6.3.2.	Lattice vibrations and normal modes	155
6.3.3.	Phonons and heat capacity	158
6.4.	Bose-Einstein condensation and superfluidity	160
6.4.1.	Non-interacting bosons	161
6.4.2.	Wavefunctions	163
6.4.3.	Two-fluid model	165
6.4.4.	Superfluidity and excitations	167
6.4.5.	Wavefunction for phonons and rotons	170
	Suggested reading	172
	Problems	173
7.	Quantum statistical physics of fermions	175
7.1.	Wavefunctions	176
7.2.	Non-interacting electrons	176
7.2.1.	Ground state of the free electron gas	177
7.2.2.	Excited states	179
7.2.3.	Thermionic emission	183
7.2.4.	Plasma oscillations	184
7.2.5.	Metals, insulators, and semiconductors	186
7.3.	Interacting electrons	191
7.3.1.	Screening in degenerate Fermi gases	191
7.3.2.	Quasiparticles and Fermi liquid theory	192
7.4.	Superconductivity	193
7.4.1.	The superconducting ground state	194
7.4.2.	Supercurrents and the London equation	198
7.4.3.	Magnetism and superconductivity	201
7.4.4.	Flux quantization and Type-II superconductors	202
	Suggested reading	204
	Problems	205

8. Phase transitions and phase equilibrium	207
8.1. Phases and phase diagrams	207
8.1.1. Fluids	207
8.1.2. Magnets	207
8.1.3. Salt & water	209
8.2. Thermodynamic limit	211
8.3. Phase equilibrium	211
8.3.1. Pure fluid	211
8.3.2. Clausius-Clapeyron equation	212
8.3.3. First order and continuous transitions	213
8.3.4. Gibbs phase rule	214
8.3.5. van der Waals' theory revisited	215
8.3.6. Spinoidal curves and nucleation	219
8.3.7. Eutectics and the common tangent construction	220
8.4. Simulations of phase coexistence	222
8.4.1. Constant volume Monte Carlo	222
8.4.2. Gibbs ensemble	223
Suggested reading	227
Problems	227
9. Continuous phase transitions	231
9.1. Bragg-Williams and Weiss theories	231
9.2. Lattice gas mapping	234
9.3. Landau theory of phase transitions	235
9.3.1. Continuous phase transitions and order parameters	236
9.3.2. The Landau free energy	237
9.3.3. Uniform order parameter	239
9.3.4. Ornstein-Zernike theory and correlation lengths	240
9.3.5. Ginzburg criterion	242
9.4. Order and dimensionality	243
9.4.1. Lower critical dimension	243
9.4.2. One dimensional Ising model	245
9.4.3. Two dimensional Ising model	246
9.4.4. Higher dimensions	248
9.5. Scaling, universality and renormalization	249
9.5.1. Scaling	250
9.5.2. Kadanoff construction	253
9.5.3. Renormalization flows	254
9.5.4. Renormalization transformations	256
9.6. High temperature expansions	260
9.6.1. Expanding around $T = \infty$	260
9.6.2. Graphical expansion of the partition function	261

9.6.3.	Graphs in one and two dimensions	262
9.6.4.	Disconnected diagrams and the linked cluster theorem	263
9.7.	Monte Carlo methods near T_c	265
9.7.1.	Potts model	265
9.7.2.	Wolff algorithm	266
9.7.3.	Swendsen-Wang algorithm	269
9.8.	Percolation	270
9.8.1.	Bond and site percolation	270
9.8.2.	Percolation as a phase transition	272
9.8.3.	Percolation on a Cayley tree	272
9.8.4.	Percolation and Potts models	274
	Suggested reading	275
	Problems	276
A.	Mathematical background	279
A.1.	An identity about partial derivatives	279
A.2.	Legendre transform	279
A.3.	Gaussian integrals	281
A.4.	Laplace (saddle-point) method for integration	282
A.5.	Stirling's approximation	283
A.6.	Fourier series	283
A.7.	Fourier transforms	284
A.7.1.	Examples	284
A.7.2.	Fourier representation of the delta function	285
A.7.3.	Convolutions and the Weiner-Khinchin theorem	285
A.7.4.	Parseval's theorem	287
A.7.5.	Fourier series and Fourier transforms	287
B.	Python	289
B.1.	Obtaining and learning Python	289
B.2.	simplemd.py	289
B.2.1.	Periodic boundary conditions	291
B.3.	sinaibilliard.py	292
B.4.	isingdemon1d.py	293
B.5.	randomcoil.py	294
B.6.	LJ2dMC.py	295
B.7.	LJ2dgibbs.py	298
B.8.	wolff.py	305
	Index	316