

Contents

<i>Preface</i>	<i>page</i> xi
Part I Monte Carlo basics	1
1 Introduction	3
1.1 The Monte Carlo method	3
1.2 Quantum Monte Carlo	5
1.3 Classical Monte Carlo	6
2 Monte Carlo basics	11
2.1 Some probability concepts	11
2.2 Random sampling	15
2.3 Direct sampling methods	17
2.3.1 Discrete distributions	17
2.3.2 Continuous distributions	20
2.4 Markov chain Monte Carlo	23
2.4.1 Markov chains	24
2.4.2 Stochastic matrices	25
2.5 Detailed balance algorithms	28
2.5.1 Metropolis algorithm	28
2.5.2 Generalized Metropolis algorithms	31
2.5.3 Heat-bath algorithm	33
2.6 Rosenbluth's theorem	35
2.7 Entropy content	38
Exercises	40
3 Data analysis	43
3.1 Equilibrating the sampling	43
3.2 Calculating averages and estimating errors	46
3.3 Correlated measurements and autocorrelation times	49

3.4	Blocking analysis	50
3.5	Data sufficiency	52
3.6	Error propagation	55
3.7	Jackknife analysis	57
3.8	Bootstrap analysis	59
3.9	Monte Carlo computer program	61
	Exercises	63
4	Monte Carlo for classical many-body problems	66
4.1	Many-body phase space	66
4.2	Local updates	68
4.3	Two-step selection	69
4.4	Cluster updates	70
4.4.1	Swendsen-Wang algorithm	71
4.4.2	Graphical representation	73
4.4.3	Correlation functions and cluster size	75
4.5	Worm updates	76
4.6	Closing remarks	80
	Exercises	82
5	Quantum Monte Carlo primer	84
5.1	Classical representation	84
5.2	Quantum spins	86
5.2.1	Longitudinal-field Ising model	86
5.2.2	Transverse-field Ising model	87
5.2.3	Continuous-time limit	92
5.2.4	Zero-field XY model	98
5.2.5	Simulation with loops	103
5.2.6	Simulation with worms	106
5.2.7	Ergodicity and winding numbers	110
5.3	Bosons and Fermions	111
5.3.1	Bosons	111
5.3.2	Fermions	112
5.4	Negative-sign problem	114
5.5	Dynamics	115
	Exercises	117
	Part II Finite temperature	119
6	Finite-temperature quantum spin algorithms	121
6.1	Feynman's path integral	121

6.2	Loop/cluster update	124
6.2.1	General framework	124
6.2.2	Continuous-time loop/cluster update	127
6.2.3	XXZ models	129
6.2.4	Correlation functions	132
6.2.5	Magnetic fields	136
6.2.6	Large spins ($S > \frac{1}{2}$)	137
6.3	High-temperature series expansion	140
6.3.1	Stochastic series expansion	140
6.3.2	“Continuous-time” limit	144
6.4	Worm update	145
6.4.1	Freezing problem	146
6.4.2	Directed-loop algorithm	147
6.4.3	Violation of the detailed balance condition	153
6.4.4	Correlation functions	154
6.4.5	XXZ model	156
6.4.6	On-the-fly vertex generation	161
6.5	Toward zero temperature	164
6.5.1	Extrapolation to zero temperature	166
6.5.2	Quantum phase transitions	168
6.5.3	Finite-size scaling	170
6.6	Applications to Bosonic systems	174
	Exercises	179
7	Determinant method	180
7.1	Theoretical framework	180
7.1.1	Hubbard-Stratonovich transformations	181
7.1.2	Determinantal weights	185
7.1.3	Single-particle Green’s function	188
7.2	Finite temperature algorithm	189
7.2.1	Matrix representation	190
7.2.2	Metropolis sampling	192
7.2.3	The algorithm	194
7.2.4	Measurements	197
7.3	Hirsch-Fye algorithm	198
7.4	Matrix product stabilization	202
7.5	Comments	209
	Exercises	211
8	Continuous-time impurity solvers	214
8.1	Quantum impurity models	214

8.1.1	Chain representation	216
8.1.2	Action formulation	217
8.2	Dynamical mean-field theory	219
8.2.1	Single-site effective model	219
8.2.2	DMFT approximation	221
8.2.3	DMFT self-consistency loop	222
8.2.4	Simulation of strongly correlated materials	223
8.2.5	Cluster extensions	226
8.3	General strategy	228
8.4	Weak-coupling approach	230
8.4.1	Sampling	232
8.4.2	Determinant ratios and fast matrix updates	233
8.4.3	Measurement of the Green's function	234
8.4.4	Multi-orbital and cluster impurity problems	236
8.5	Strong-coupling approach	237
8.5.1	Sampling	240
8.5.2	Measurement of the Green's function	240
8.5.3	Generalization – Matrix formalism	244
8.5.4	Generalization – Krylov formalism	247
8.6	Infinite- U limit: Kondo model	249
8.6.1	Weak-coupling approach	249
8.6.2	Strong-coupling approach	252
8.7	Determinant structure and sign problem	254
8.7.1	Combination of diagrams into a determinant	254
8.7.2	Absence of a sign problem	256
8.8	Scaling of the algorithms	258
	Exercises	262
	Part III Zero temperature	265
9	Variational Monte Carlo	267
9.1	Variational Monte Carlo	267
9.1.1	The variational principle	267
9.1.2	Monte Carlo sampling	270
9.2	Trial states	272
9.2.1	Slater-Jastrow states	273
9.2.2	Gutzwiller projected states	274
9.2.3	Valence bond states	282
9.2.4	Tensor network states	287
9.3	Trial-state optimization	291
9.3.1	Linear method	293

9.3.2	Newton's method	296
9.3.3	Connection between linear and Newton methods	298
9.3.4	Energy variance optimization	298
9.3.5	Stabilization	299
9.3.6	Summary of the linear and Newton's optimization methods	299
	Exercises	301
10	Power methods	302
10.1	Deterministic direct and inverse power methods	302
10.2	Monte Carlo power methods	305
10.2.1	Monte Carlo direct power method	306
10.2.2	Monte Carlo inverse power method	310
10.3	Stochastic reconfiguration	314
10.4	Green's function Monte Carlo methods	320
10.4.1	Linear method	322
10.4.2	Diffusion Monte Carlo	324
10.4.3	Importance sampling	326
10.5	Measurements	327
10.6	Excited states	329
10.6.1	Correlation function Monte Carlo	329
10.6.2	Modified power method	331
10.7	Comments	334
	Exercises	337
11	Fermion ground state methods	338
11.1	Sign problem	338
11.2	Fixed-node method	341
11.3	Constrained-path method	345
11.4	Estimators	349
11.4.1	Mixed estimator	349
11.4.2	Forward walking and back propagation	352
11.5	The algorithms	355
11.6	Constrained-phase method	360
	Exercises	363
	Part IV Other topics	365
12	Analytic continuation	367
12.1	Preliminary comments	367
12.2	Dynamical correlation functions	370
12.3	Bayesian statistical inference	373

12.3.1 Principle of maximum entropy	375
12.3.2 The likelihood function and prior probability	378
12.3.3 The “best” solutions	380
12.4 Analysis details and the Ockham factor	383
12.5 Practical considerations	388
12.6 Comments	395
Exercises	396
13 Parallelization	398
13.1 Parallel architectures	398
13.2 Single-spin update on a shared-memory computer	399
13.3 Single-spin update on a distributed-memory computer	402
13.4 Loop/cluster update and union-find algorithm	403
13.5 Union-find algorithm for shared-memory computers	408
13.6 Union-find algorithm for distributed-memory computers	411
13.7 Back to the future	413
<i>Appendix A</i> Alias method	416
<i>Appendix B</i> Rejection method	418
<i>Appendix C</i> Extended-ensemble methods	420
<i>Appendix D</i> Loop/cluster algorithms: SU(N) model	425
<i>Appendix E</i> Long-range interactions	428
<i>Appendix F</i> Thouless’s theorem	432
<i>Appendix G</i> Hubbard-Stratonovich transformations	435
<i>Appendix H</i> Multi-electron propagator	441
<i>Appendix I</i> Zero temperature determinant method	445
<i>Appendix J</i> Anderson impurity model: chain representation	449
<i>Appendix K</i> Anderson impurity model: action formulation	451
<i>Appendix L</i> Continuous-time auxiliary-field algorithm	455
<i>Appendix M</i> Continuous-time determinant algorithm	459
<i>Appendix N</i> Correlated sampling	462
<i>Appendix O</i> The Bryan algorithm	464
<i>References</i>	469
<i>Index</i>	484