Index

Acceptance-rejection method, 62	Configuration interaction, 20
Anti-symmetric geminal power	Constrained-path quantum Monte Carlo, 219
Constrained optimization, 246	Continuous time, 179, 196
Definition, 237	Correlated sampling, 59
Area law, 31	Correlation energy, 243
Atomic orbitals, 238	Correlation time, 73
Contracted, 241	Covariance, 45
Gaussian type, 240	Cumulative probability, 43
Periodic systems, 241	Cusp conditions, 239
Slater type, 240	
Twisted boundary conditions, 241	Delayed updates, 121, 227
Auxiliary-field quantum Monte Carlo	Direct sampling, 60
Attractive Hubbard model, 228	Distribution function
Backward propagation, 221	Bernulli, 46
Forward propagation, 221	Binomial, 46
Pseudo-partition function, 220	Gaussian, 46
Repulsive Hubbard model, 229	Poisson, 46
Sequential updates, 223	Uniform, 46
Sign problem, 221	
	Energy derivatives, 134
Backflow correlations, 21, 122	Errorbars
Bayes formula, 43	Block analysis, 83
BCS Hamiltonian, 27, 115, 125	Bootstrap method, 78
BCS wave function, 26, 125	Error propagation, 77
Block analysis, 83	Jackknife method, 81
Boltzmann distribution, 86, 90	
Bootstrap method, 78	Fermionic wave function
Bosonic wave function	Determinant, 112
Condensed state, 110	Fast update of determinants, 116
Fast update of the Jastrow factor, 111	Fast update of Pfaffians, 126
Permanent, 111	Green's functions, 119, 128
Box-Muller trick, 65	Pfaffian, 123
Brownian motion, 86	Fixed-node approximation, 204, 209, 255
	Fixed-node energy
Central limit theorem, 53	Expectation value, 212
Changing random variables, 47	Ground-state value, 211
Characteristic function, 45	Upper-bound property, 211
Chebyshev's inequality, 48	Fixed-node error, 212
Cholesky decomposition, 222	Fixed-node Hamiltonian, 210, 255
Classical mapping, 33	Fixed-phase approximation, 204

Index 273

Fokker-Planck equation, 90 Laughlin wave function, 25, 237 Approach to equilibrium, 92 Light cone, 163 Schrödinger equation, 91 Linear method, 132, 147, 248 "Strong" zero-variance property, 149 Generalized eigenvalue equation, 149 Gram-Schmidt orthogonalization, 222 Green's function Monte Carlo Local energy, 105, 172, 175, 191 Local estimator, 104 Accumulated weight, 173, 176, 184 Branching, 181 Markov chains Continuous time, 179 Forward walking, 176, 186 Auxiliary-field quantum Monte Carlo, 223 Definition, 66 Guiding function, 173 Importance sampling, 173 Detailed balance, 70 Ergodicity, 70 Master equation, 169 Mixed average, 177 Green's function Monte Carlo, 169, 200 Sign problem, 168 Master equation, 67 Periodicity, 70 Single walker technique, 170 Gutzwiller factor, 17 Reducibility, 70 Gutzwiller projector, 18, 107 Reptation Monte Carlo, 191 Gutzwiller wave function, 17 Stationary solution, 70 Mean value, 44 Metropolis-Hastings algorithm, 74 Haldane-Shastry wave function, 23 Acceptance probability, 74 Hartree-Fock wave function, 4, 15 Trial probability, 74 Heisenberg model, 10 Molecular orbitals, 243 Heitler-London wave function, 3 Hellmann-Feynman theorem, 212 Mott insulator, 9 Mott transition, 10 Hessian matrix, 148 Multideterminant wave function, 20 Hubbard model (bosonic), 12 Hubbard model (fermionic), 7 Hubbard-Stratonovich transformation, 218 Newton-Raphson optimization, 132 Nodal surface, 202 Imaginary-time propagation, 35, 202, 205, 214 Importance sampling, 61 Optimization Linear method, 147 Jackknife method, 81 Reweighting technique, 132 Jastrow factor Steepest descent, 137 Stochastic reconfiguration, 139 One-body (electron-ion on the continuum), Two-body (electron-electron on the continuum), Pairing (geminal) function, 243 Particle-hole transformation, 115, 229 Path integral Monte Carlo, 190, 220 Two-body (electron-electron on the lattice), 19, 107 Pauli surface, 202 Jastrow wave function, 18, 107 Perron-Frobenius theorem, 72, 199, 210 Pfaffian, 123 Jastrow-Slater wave function, 20, 107, 237 Power method, 34 Probability Langevin dynamics Accelerated dynamics, 96 Conditional, 42 Detailed balance, 92 Definition (frequentist), 41 Discretization, 87 Joint, 42 Marginal, 42 Discretization error, 95 First-order equations, 85, 140 Reproducibility of the experiments, 40, 52 Probability density, 43 Master equation, 90 Second-order equations, 86 Projection technique, 34, 167, 189, 214, 253 Pseudo-random numbers Large deviations, 55 Definition, 261 Lattice regularization, 235 Fibonacci (lagged) generators, 261 Electron-ion potential, 253 Periodicity, 261 Laplacian, 253 Size consistency, 258 Zero-variance property, 256 Quantum quench, 161

274 Index

Random process, 66
Random variable, 42
Real-time propagation, 156
Reptation Monte Carlo
Bounce algorithm, 195
Continuous time, 196
Importance sampling, 190
Master equation, 195
Pseudo-partition function, 189
Sign problem, 190
Simple update, 191
Resonating-valence bond wave function, 5, 29, 237, 244
Reweighting technique, 59

Sampling, 56
Continuous distribution, 64
Discrete distribution, 62
Sign problem, 199
Size consistency, 244
Size extensivity, 31
Slater determinant, 4
Sparse Hamiltonian matrix, 35
Standard deviation, 45
Steepest descent, 88, 132, 137, 248
Stochastic reconfiguration, 132, 139, 248
Covariance property, 142
Preconditioning, 143
Projection, 146
Regularization, 143, 147

Scale invariant regularization, 144

Signal to noise ratio, 144

Thermalization time, 73, 172, 176, 193
Time-dependent Hartree-Fock, 156
Time-dependent variational Monte Carlo
Continuous-time limit, 159
Energy conservation, 160
Equations, 158
Norm conservation, 160
Stationary action, 160
Trotter approximation, 216
Trotter error, 180, 196, 216

Vandermonde determinant, 22
Variance, 45
Variational Hamiltonian, 209
Variational Monte Carlo
Expectation value, 104
Local basis set, 108
Local energy, 105
Local estimator, 104
Zero-variance property, 105
Variational principle
Accuracy on the correlations, 14
Accuracy on the energy, 13
Generalities, 13

Wave function metric, 139 Weak law of large numbers, 52 White noise, 85 Wick theorem, 119, 128, 224

Zero-variance property, 105