

Index

Symbols

$1 \times 1 \times 1$ cluster, 164
 $2 \times 2 \times 2$ cluster, 167
 $3 \times 3 \times 3$ cluster, 172
 $4 \times 4 \times 4$ cluster, 174
 12-term expansion, 48f, 52
N-electron wave function, 67

A

acceptance, 7, 25f, 85
 acceptance ratio, 30, 37, 80, 104, 125
 accuracy, 32, 46, 50, 53, 82, 85f, 91–97, 102, 104, 141, 178
 adiabatic decoupling, 40
 ALPHA, 50, 52, 55, 124–128, 135
 antibonding, 165
 antiferromagnetic, 165ff, 169, 171, 174f, 177f, 210, 217
 antisymmetric function, 64
 antisymmetrized wave function, 69
 antisymmetrizing operator, 65
 antisymmetry, 61ff, 258
 artificial periodicity, 168
 asymptotic behavior, 174
 atom
 – center, 151
 – corner, 151
 atomic aggregate, 147ff
 atomic orbital, 40
 – best superposition, 169
 atomic structure, 147
 atomic wave function, 218
 AUTOCORR, 243
 autocorrelation function, 221, 247
 AVVAR, 88

B

back-folding, 212, 216
 band theory, 211

basis set, 212

bcc

– arrangement, 148, 150
 – cube, 151
 – lattice, 154, 156

BETA1, 141

BETA2, 141

binding energy, 43, 50f

Bloch vector, 184

Bloch's theorem, 181

block, 92–95, 97

BLOCKING, 88, 110

blocking scheme, 63

Boltzmann, 40

– factor, 18

– probability density, 4, 7

bond distance, 51, 163

bonding, 165

Born–Oppenheimer approximation, 39, 185

Born–von Kármán boundary conditions, 183ff, 208, 216

boundary condition, 125

Brillouin zone, 168, 183ff, 211

bulk lattice constant, 172

C

central limit theorem, 7, 32, 91–95, 102, 166, 174

CHARGE, 248

check of determinant routines, 130

CJAS, 52, 55, 103, 117f, 126ff, 135, 141, 167, 171, 173, 175ff

Clementi and Roetti, 71

closed shell, 212

cluster, 136f, 143ff, 148ff, 156

– geometry, 153ff, 163

– shape, 153, 156

– size, 178

cluster expansion, 5

- cofactor, 76, 80
- compilation, 54
- compilation sequence, 115
- complete set of eigenfunctions, 61
- conditional probability, 133
- configuration-interaction, 103
- confined single-particle wave function, 122
- confined system, 121ff
- contour plot of energy, 144, 166f, 173, 175
- contour plot of the variance, 144f
- convergence, 18, 93, 102, 174
- correlated sampling, 117
- correlated system, 101
- correlation, 143
- correlation energy, 144
- cost of optimization, 116
- Coulomb interaction, 262
- Coulomb singularity, 193, 213
- COULTERM, 268
- cubic
 - box, 126, 129
 - group, 175
 - lattice, 263
 - point symmetry, 168
 - symmetry, 261
- cuspid condition, 149, 191f, 213, 215

- D**
- degenerate, 173, 177
- degenerate state, 170
- DENSITY, 248
- density, 22, 37, 132, 139, 142f
- density functional, 71, 131
- density functional theory, 121, 131
 - fundamentals, 137ff
- density–density correlation function, 131, 205
- DERFC, 195, 267
- determinant, 61ff, 80, 123, 141f, 149, 165,
 - 173f, 177, 209f
 - $N * N$, 67
 - change, 77
 - expansion, 76
 - spin-down, 73, 152
 - spin-up, 73, 152
 - structure, 150
 - trial, 169
 - update, 81
 - zero, 64
- DETUPD, 248
- DFT, *see* density functional theory
- diatomic molecule, 53
- diffusion, 230
 - constant, 224
 - equation, 224, 226
 - Monte Carlo, 103
- dimer, 151
- dipole force, 46
- dipole–dipole interaction, 53
- direct lattice, 260
- direct space, 262f
- double occupation, 44

- E**
- edge length, 156
- effective potential, 63, 138
- eigenfunction, 119
- eigenstate, 215, 224
- electron
 - spin-down, 165
 - spin-up, 165
- electron correlation, 185
- electron exchange, 249
- electron orbital, 71
- electronic density, 137
- electronic shell structure, 148
- electron–electron energy, 206
- electron–electron interaction, 187, 190, 204f, 220
- electron–nucleus interaction, 188, 190, 215
- electron–nucleus potential energy, 220
- electrostatic potential, 186
- energy, 93f, 98, 125, 142, 144, 164, 172, 176, 179
 - contour, 126f
 - expectation, 30, 32
 - minimization, 47
 - minimum, 85, 98, 102, 126ff
 - per electron, 206
 - surface, 40, 99f
 - variance, 47, 95
- equation of state, 3
- equilibrium distance, 48, 53
- equilibrium lattice constant, 221
- ERGLOC, 248
- ergodicity, 7, 226
- estimator, 174
- EWALD, 193, 195, 197, 200f
- Ewald
 - expression, 186
 - method, 189
 - potential, 184ff, 192, 195ff, 202f, 262f
 - sum, 192f, 202f, 207
 - summation, 190f, 204, 213, 217, 220, 259
 - summing procedure, 189
 - tabulation, 191
 - technique, 184
 - term, 216

EWALD_DEN_ARR, 207

EWALD_MOD, 265

exchange-correlation

– functional, 121

– hole, 133, 186, 204f

– potential, 138

excited state, 44

expansion, 44

expectation value, 92f

F

Fermi field operator, 131

FILLG95, 243

FILLRAN, 230

FILLTAO, 243

finite cluster, 262

finite size, 138

finite system, 179

finite-size correction, 197, 206

finite-size effects, 183ff, 204, 213, 217

five-term expansion, 46, 49

fluctuation, 95, 97, 100, 215

folding back, 153, 156

FOLDTOWSC, 154ff

force, 48, 50f

Fortran language command, 103

four-electron wave function, 68

Fourier series, 207

FOURIER_COS, 217

FOURIER_QUADRATURE, 207, 217

free energy, 3f

free particle, 225, 227

fundamental frequency, 51

G

Gaussian

– density, 228

– distributed variable, 7

– distribution, 92

– function, 228

– random number, 228

– two-particle interaction, 53

GCUTI, 177

GCUTR, 177

GENRAN, 109, 241, 243, 247

global electron, 80

global variable, 73, 87, 103

gnuplot, 20

G_{PLASM}, 165, 171

gradient, 77f, 90, 140, 193, 249

Green function *G*, 224ff

Green's theorem, 49, 127

ground state, 93, 126ff

ground-state energy, 101f, 165

guess, 116

H

Hamiltonian, 62, 127

– spin-independent, 61

hard-wall cube, 121

harmonic oscillator

– energy, 234

– energy spectrum, 230

– frequency, 234

– Schrödinger equation, 229ff

– wave function, 234

Hartree integration, 197

Hartree interaction, 206

Hartree term, 205, 207

Hartree–Fock, 63, 71, 82, 96, 142, 217ff

– calculation, 83, 143

– eigenvalue, 97

– orbital, 85f

high temperature asymptotics, 239

Hohenberg–Kohn theorem, 137

HOMO, 164

homogeneous function, 48

Hund's rule, 64, 71

hybrid orbital, 166f

hybrid state, 161, 164

hybridization, 44, 217

hydrogen atom, 23ff, 214

hydrogen molecule, 39ff, 45, 50, 52

I

ideal gas, 3

imaginary time, 224

importance sampling, 18, 25

indistinguishable, 68

infinite lattice, 183, 259

infinite solid, 262

INITEWALD, 195, 197

initialization, 104

INITLATTICE, 150, 156f

INITRAN, 242

INITVEWALD, 194

interacting classical gas, 1, 239

interaction energy, 96, 103

interaction potential, 15f

inverse matrix, 76–79, 130

J

JASEXP, 14, 16, 248

JASEXPATOM, 248

JASEXP2, 248, 252

JASEXPSOLID, 150, 161f

JASPEX, 14

- Jastrow, 149, 172
 Jastrow exponent, 53, 113, 125, 161, 215, 247
 – exponential form, 167
 Jastrow factor, 40, 42ff, 46, 49, 62, 68, 70, 73, 93, 98, 113, 192, 212–216, 220, 247, 262
 – one-particle function, 165
 Jastrow parameter, 42, 46, 49f, 96, 99ff, 218f
 jellium cluster, 122, 138–141
 JEXP, 90, 104
- K**
 kinetic energy, 28, 77, 79, 96, 103
 – Laplacian, 96
 – velocity form, 96
 Kohn–Sham eigenvalue, 138
 Kohn–Sham equations, 137f
 Kohn–Sham level, 139
 Kohn–Sham potential, 139
 Kohn–Sham wave function, 138f, 141f
- L**
 Lagrangian, 127
 Laplacian, 77f, 90, 130, 140, 214, 249
 Laplacian representation, 49
 LATCON, 168
 lattice constant, 153
 lattice sum, 259, 263
 lattice vector, 156
 LATTICE_SUM, 264
 LCAO, 43f, 53, 169f, 173, 175, 177, 208f, 217
 LCAO wave function, 156
 LCLUSTER, 123f, 128–131
 LDA, 141
 Lennard-Jones potential, 5, 21
 Li₂ molecule, 163f
 LIDIMER, 168, 170, 173, 177, 218
 LIDIMER geometry, 153ff
 limit cycle, 118
 linear combination of atomic orbitals, *see*
 LCAO
 lithium
 – atom, 61ff
 – biatomic molecule, 178
 – cluster, 147ff
 – HF system, 96
 – lithium atom orbital, 72
 – solid, 181
 local density approximation, 131, 138
 local energy, 24–28, 31, 41, 100
 local kinetic energy, 86, 213
 LOCAL_DENSITY, 217
 LUMO, 164
- M**
 Madelung constant, 192, 206, 262
 main Monte Carlo, 28f
 main program, 103, 124
 – Lcluster_hybrid.f, 150
 main run, 8, 29, 55
 MAKE_LATTICE, 156, 159, 197, 266
 MAKE_SUPERLATTICE, 156, 159
 many-body system, 18
 many-body wave function, 62, 182, 205, 208
 master equation, 26, 227
 maximum step width, 18
 MCMAX, 30, 32, 37, 50
 mean square deviation, 94
 metal cluster, 148
 metallic bonding, 210
 Metropolis algorithm, 7, 26
 minimal energy surface, 101
 minimization, 44
 minimum energy, 100
 minimum image convention (mic), 185
 minor, 76
 missing symmetry, 170
 MKVEW2DAT, 195, 200
 MKVEWDAT, 195, 200
 MKWEDGE, 195, 199
 model periodic Coulomb (mpC) interaction,
 186, 218, 220
 model system, 121
 module, 13, 115, 141
 – determinant, 79, 87, 125
 – ewald_cal_tab, 192, 195
 – highlevel, 54, 103, 108, 124
 – INITORB, 150
 – jastrow, 54, 103, 113, 150, 162, 248f
 – lattice_Lisolid, 150, 156, 195
 – M_determinant_Lcluster.f, 160
 – M_determinant_Lisolid_hybrid.f, 217
 – M_ewald_cal_tab.f, 217
 – midlevel, 54, 103, 108
 – M_jastrow, 141
 – M_jastrow_Lisolid_sinewald.f, 217
 – M_lattice_Lcluster.f, 173, 178, 217
 – M_observables_Lisolid.f, 217
 – M_orbital_cluster, 141
 – M_orbital_HF, 168
 – M_orbital_Lcluster_HF.f, 150
 – M_orbital_Lisolid_HF_hybrid.f, 218
 – M_orbital_Lisolid_HF_lcao.f, 217
 – M_output_Lisolid.f, 217
 – M_random_Lisolid.f, 217
 – M_variables_Lcluster.f, 159
 – M_variables_Lisolid.f, 217

- observable, 87
- orbital, 43, 54, 73, 123
- output, 13, 103, 114
- position, 13f, 19, 32
- random, 17, 54, 88, 103, 109, 124, 241

molecular orbital

- antibonding, 164
- bonding, 164

molecule, 44

Monte Carlo run, 27

Morse potential, 44f, 51f

multidimensional configuration point, 92

multiple minima, 102, 116

multiplet, 65

multiplicity, 64, 71

multipole expansion, 192

N

nanometer-sized system, 122

nanophysics, 147

NELOB, 105, 151

nodal surface, 64, 215

nondegenerate, 64

noninteracting system, 138

normalization, 25, 41, 68, 72, 132ff

normalization sum rule, 132

nuclear configuration, 178

nucleus

- center, 154, 164
- corner, 154, 164
- position, 168

nucleus position, 151, 155, 172

nucleus–nucleus interaction, 188, 190

nucleus–nucleus potential energy, 220

O

OBSERV, 88, 105, 125

observable, 28, 55, 85, 97, 101f, 125, 149

- electronic density, 86
- energy, 82
- kinetic energy, 82, 86
- single-energy part, 83, 86
- symmetric, 62, 67ff
- total energy, 86
- variance, 82

OBSERVSTATALL, 89, 105, 125, 135

OBSERVSTATEL, 88, 105

OCTANT, 194f, 201

one-electron radius r_s , 137

one-electron system, 23

one-particle spherical wave, 166

optimization, 115ff

optimization method, 102

ORBDER, 90, 124

orbital, 90

orbital decay parameter, 46

ORBWAV, 104, 124, 151f

orthogonal transformation, 176

orthorhombic quantum dot, 122

OSCDIF, 231

P

PAIRCORR, 125, 135

pair-correlation function, 125, 131ff

- average, 132
- on-top, 135
- spin-resolved, 134, 136

parameter space, 119

particle density, 18

partition function, 3f

Pauli principle, 213

periodic boundary condition, 191, 209

periodic continuation, 168

periodic image position, 191

periodicity, 168, 181ff, 260, 262

- relaxed, 169

permutation, 64, 66, 68

phase coefficient, 171, 173, 177f

phase factor, 182

phase factor matrix, 170

plane wave, 210f

point group symmetry, 163

point symmetry, 173, 175

Poisson's equation, 263

polarization field, 192

positive background charge, 136

potential energy, 28, 52, 96, 103

potential energy curve, 44f, 51f

power expansion, 49

prerun, 8, 28f, 55

pressure, 4

primitive lattice, 153

probability density, 24f, 32, 92

probability distribution, 85

probability interpretation, 18

product ansatz, 42f

proton distance, 46, 52

proton–proton repulsion, 45, 48

pseudorandom number, 228, 241

pseudorandom number generator, 241

PSIMAT, 104, 151f

Q

QMC, *see* quantum Monte Carlo

QUADRATURE_SCWSC, 217

quantum mechanical uncertainty, 174

- quantum mechanical variance, 45, 93f
- quantum Monte Carlo
 - auxiliary-field, 223
 - diffusion, 223
 - path-integral, 223
 - variational, 3, 23, 103, 223
- R**
- radial density, 85f, 125–131
- radial density distribution, 32
- radial electron distribution, 84
 - single electron
 - kinetic energy, 84
 - potential energy, 84
 - total interaction energy, 84
- random
 - number, 7, 109, 228, 241
 - number generator, 28, 109
 - random_number, 241
 - walk, 25ff, 224, 226f
 - walker, 230
- RANF, 234, 244
- rannumb, 109
- real gas, 3
- reciprocal lattice, 168, 173, 260
- reciprocal lattice vector, 211
- reciprocal space, 262
- Ritz variational principle, 24
- RLCAO, 178
- run time, 174
- S**
- scalability, 149
- scalable regime, 148
- scale transformation, 47
- screening length, 16
- self-adjoint, 47, 49
- self-image interaction, 189
- series expansion, 49, 51, 249
- Sherman–Morrison algorithm, 63, 77f, 80f
- SIMPLE_SUM, 267
- simulated annealing, 21
- simulation cell, 154, 156
- single-electron, 68
- single-electron state, 70
- single-electron wave function, 142, 150
- single-particle state, 67, 217
- single-particle wave function, 141
- singlet ground state, 39
- sink, 225f, 231
- SLAP, 103, 117f, 141, 166f, 171, 173, 175ff
- Slater determinant, 71, 76ff, 83, 150
- Slater function, 72
- Slater parameter, 42, 49, 93, 96, 99ff, 172, 217
- source, 225f, 231
- spherical harmonic, 23, 139
- spherical jellium cluster, 136
- spherical quantum dot, 136ff
- spin, 61ff, 257
 - contamination, 70
 - degenerate, 67
 - doublet, 72
 - eigenstate, 259
 - eigenvector, 63
 - flip operator, 258
 - pairing, 258
 - singlet, 64
 - state, 257
 - variable, 63
 - vector, 65
- square deviation, 93
- stability of matter, 71
- standard deviation, 32, 43, 46, 50f, 85, 172
- statistic, 1
- statistic, classical many-particle, 2
- statistical
 - accuracy, 174
 - average, 7
 - ensemble, 7
 - fluctuation, 85
 - mechanic, 3
 - scatter, 29
 - standard deviation, 174
 - uncertainty, 92
- step probability, 40
- step width, 28
- STEPMAX, 28f, 31, 37, 43, 50, 85f, 93, 98f, 103f
- stochastic process, 227
- SULATCON, 154
- sum rule, 133
- supercell, 154, 168
- superimposed 2s state, 173
- superlattice, 156, 168, 183, 185, 187, 191, 197, 212, 216, 260
- surface integral, 49
- symmetric combination, 177
- symmetry, 62–65
 - particle, 63
 - spin, 63
- symmetry element, 175
- symmetry transformation, 176
- T**
- temperature, 3, 15, 17
- test wave function, 116

thermalization, 55
 thermalizing step, 28
 thermodynamic, 2
 thermodynamical energy, 18
 total energy, 41, 96, 103
 transformed position, 176
 transition region, 52
 translational symmetry, 163, 181
 transposition, 61, 64
 trial wave function, 223
 Trotter-formula, 227
 two-body quantity, 131
 two-electron correlation, 247

U

uncorrelated, 82
 uncorrelated system, 63
 update, 174
 update iteratively, 93
 upper bound, 45, 100
 uppermost momentum state, 173
 Ursell–Mayer, 5

V

van der Waals, 3, 5
 – equation, 4f
 – law, 6
 – pressure, 15, 17
 variance, 26, 29, 31f, 37, 43, 47, 51, 86, 91–94,
 98, 100, 102, 118, 142, 174, 176, 215
 – block, 63
 – criterion, 26
 variance minimization, 117
 – unweighted, 116

variance minimum, 31, 127
 variational freedom, 44f
 velocity form, 50, 52, 127
 velocity representation, 49
 VEW, 195
 VEWGR, 193, 195, 201f
 VEWTAB, 193
 vibrational quantum, 45
 VIRIAL, 248
 virial, 47f, 51
 – energy, 48
 – equation, 46, 52
 – theorem, 47, 50f, 82, 96, 103, 220

W

wave, 257
 wave function, 41, 123, 149, 177, 249
 wave function node, 226
 wave function symmetry, 257
 wave vector, 169f, 173
 WEDGE, 194f, 197, 199
 Wigner–Seitz cell, 149ff, 153–156, 184, 193,
 203f, 208, 262f
 Wigner–Seitz radius, 128f
 WPHI, 151f

Y

Yukawa potential, 5

Z

ZBQLINI, 244
 ZBQLU01, 246