

Index

- adjoint equation, 86, 113
- Armijo condition, 223, 231
- Arzelà–Ascoli theorem, 140
- azimuthal quantum number, 24

- BFGS method, 228
- black-box methods, 222
- Bloch sphere, 65
- Bochner space, 359
- Bohr radius, 348
- Born–Oppenheimer approximation, 42
- Bose–Einstein condensate, 39
- bosons, 17, 39
- bra and ket vectors, 28

- canonical momentum, 16
- Carathéodory’s theorem, 76
- cascadic black-box schemes, 230
- charged particle, 16
- coercivity of the Hessian, 98
- commutation relation, 15
- commutator, 12, 15
- conical eigenvalue intersection, 169, 179
- connectivity graph of the control Hamiltonian, 168
- continuation for initializing optimization schemes, 274
- continuation technique, 292
- continuity equation, 51
- control constraints, 231
- control Hamiltonian, 164, 354
- control-to-state map, 77
- controlled Fokker–Planck equation, 66
- convolution theorem, 132
- correlation potential, 129
- Coulomb gauge condition, 16
- Coulomb potential, 44, 49, 347
- Crank–Nicolson scheme, 182

- de Broglie’s wave hypothesis, 8
- density functional theory, 43
- density functional theory (DFT), 43
- density matrix, 27, 29, 31
- density operator as a rank-one-projector, 29
- DFT’s function sets, 44
- differentiability
 - real-Fréchet, 133
 - real-Gâteaux, 133
- dipole approximation, 331, 343
- Dirac formalism, 28
- discretize-before-optimize, 236, 254
- Duhamel form, 140

- Ehrenfest’s theorem, 12, 15
- eigenvalue problem, 14
- electric scalar potential, 16
- electron density, 43
- ensemble of quantum states, 27
- exact and approximate controllability, 163
- exact-controllability problem, 291
- exchange potential, 129
- exponential midpoint scheme, 183

- fermions, 17
- fidelity, 318
- finite-dimensional Schrödinger–Pauli equation, 27
- Fokker–Planck equation, 65
- Fréchet differentiability, 79, 104, 133, 253

- Gâteaux differentiability, 79
- Galerkin projection, 282
- generalized Bloch vectors, 67
- generalized Jacobian, 245
- generalized Laguerre polynomials, 348
- global phase, 44
- group velocity, 9
- gyromagnetic ratio, 18

- Hamilton operator of a spherical symmetric problem, 345
- Hamiltonian dynamics, 62
- Hartree potential, 50, 128
- Hermitian operator, 11
- Hessian, 245, 256
- heteronuclear spins, 33
- hierarchy of objectives, 281
- Hohenberg–Kohn theorem, 47
- homodyne measurements, 64
- homotopy continuation scheme, 275

- implicit midpoint scheme, 182, 235
- implicit-function theorem, 77
- infinite-barrier well potential, 155
- infinite-well potential, 14
- intrinsic angular momentum, 17

- KKT system, 111
- Kohn–Sham (KS) approach, 49
- Krotov method, 232
- Krylov–Newton methods, 242
- KS potential, 50, 128

- Lagrange framework, 88
- Landau levels, 16

- Laplacian in spherical coordinates, 345
- Larmor frequency, 19, 33
- Legendre polynomials and Rodrigues formula, 347
- Lindblad operator, 63
- Lindblad–Kossakowski equation, 31, 63
- linearized constraint equation, 86
- Liouville–von Neumann equation, 31, 59
- Lorenz force, 16
- magnetic moment of a particle, 18
- magnetic quantum number, 25
- magnetic resonance imaging, 19
- mixed quantum state, 28
- momentum-stress tensor, 52
- monotonic scheme, 232
- multigrid optimization (MGOPT) method, 277
- multiparticle quantum system, 37
- multiple controls, 164
- necessary optimality conditions, 87, 119
- nonlinear complementarity problem (NCP) functions, 259
- nonlinear conjugate gradient (NCG) method, 224
- nonlinear multigrid methods, 276
- nuclear magnetic resonance (NMR), 19
- nuclear magneton, 18
- open quantum system, 65
- operator controllability, 164
- optimality condition, 86
- optimality system, 93, 109
- optimize-before-discretize, 236, 253
- orbital angular momentum, 17
- parity operator, 38
- Pauli matrices, 20
- Pauli principle, 38, 50
- Planck’s constant, 8
- posterior state vector, 64
- precession, 19
- principal quantum number, 24
- probability density function, 65
- projection method, 231
- pure quantum state, 28
- quadratic and superlinear convergence, 244
- quadratic model of the objective, 281
- quantum filtering equation, 161
- quantum Liouville equation, 57
- quantum nondemolition principle, 161
- quantum numbers, 24
- quasi-Newton methods, 228
- radial quantum number, 24
- radiofrequency pulse or control, 19, 37
- reachable set, 163, 293
- real-linear, 133
- reduced cost functional, 84
- reduced generalized Jacobian, 265
- reduced gradient, 84
- reduced Hessian, 248
- reduced Planck’s constant, 8
- rotating-frame transformation, 33
- Schrödinger equation (SE), 9, 12, 14
- Schur reduction, 257
- semiclassical limit, 61
- Sherman–Morrison–Woodbury formula, 228
- shooting-type method, 299
- Slater determinant, 38, 46
- Slater permanent, 38
- spherical Bessel functions, 349
- spherical harmonics, 23, 346, 350
- spin, 17
- spin-down, 17
- spin quantum number, 18, 25
- spin-spin interaction graph, 172
- spin-up, 17
- spinor, 19
- stability in the sense of Hadamard, 76
- steepest descent method, 223
- stimulated Raman adiabatic passage (STIRAP), 73
- stochastic Belavkin model, 65
- stochastic diffusion process, 64
- stochastic Schrödinger equation (SE), 64
- subdifferential, 119, 245
- subgradients, 262
- sufficient optimality conditions, 87
- symmetric or antisymmetric wavefunction, 38
- symplectic matrix, 183
- time reversibility, 182
- time-dependent density functional theory (TDDFT), 50
- time-dependent Kohn–Sham (TDKS) model, 56
- two-level system, 167
- uncertainty principle, 16
- unitary orbit, 171
- unitary propagator, 182
- van Leeuwen, theorem of, 55
- vector potential, 20
- wave packet, 9
- weak sequential continuity, 80
- Wigner function, 57, 58
- Wirtinger calculus, 253
- Wolfe condition, 224, 231
- Young’s inequality, 132
- Zeeman effect, 18, 25
- Zowe–Kurcyusz constraint qualification, 90