

SUBJECT INDEX

- Ab initio calculations, P,T-odd interactions, 253–259
 - barium fluoride molecule, 256–259
 - ytterbium molecule, 254–256
- Adiabatic probability:
 - Monte Carlo heat flow simulation, 69–70
 - nonequilibrium statistical mechanics, microstate transitions, 44–46
 - nonequilibrium thermodynamics, 7
 - time-dependent mechanical work, 52–53
 - transition probability, 53–57
- Angular momentum, one- vs. three-photon excitation, coherence spectroscopy, 163–166
- Anharmonicity, transition state trajectory, stochastically moving manifolds, 218–222
- Archimedean point, transition state trajectory, 201–213
- Asymmetry:
 - transport matrix, linear thermodynamics, 19–20
 - two-pathway excitation, coherence spectroscopy, atomic systems, 170–171
- Atomic systems, two-pathway excitation, coherence spectroscopy, 170–171
- Autonomous system, transition state trajectory, 202–203
- Barium fluoride (BaF) molecule, P,T-odd interactions, 242, 249–250, 254–256
- Barrier potential, transition state trajectory, stochastically moving manifolds, 221–222
- Basis functions, Cartesian Gaussian spinors, 259–261
 - spherical harmonics, 261
- Best current datum, electric dipole moment search, 242
- Binary collision dynamics, reactive hybrid MPC-molecular dynamics, 132–133
- Birth-death probabilistic rules, multiparticle collisions, reactive dynamics, 109–111
- Block-asymmetric matrix, linear thermodynamics, quadratic expansion, 12–13
- Block-diagonal coefficients, linear thermodynamics:
 - regression theorem, 17–20
 - time scaling, 15–16
- Boltzmann distribution, time-dependent mechanical work, transition probability, 55–57
- Boltzmann's constant:
 - Monte Carlo heat flow simulation, 68–70
 - steady-state probability distribution, nonequilibrium statistical mechanics, 40–43
- Born-Oppenheimer approximation, permanent electric dipole moment, 246–249
- Bottleneck, transition state theory, 193–195
- Bottom-up approaches, geometric transition state theory, 195–201
- Bounded states, coherence spectroscopy, one- vs. three-photon excitation, 163–166
- B-particle momentum, multiparticle collision dynamics, single-particle friction and diffusion, 115–118
- Breit-Wigner phase, two-pathway excitation, coherence spectroscopy:
 - energy domain, 180–182
 - low-lying resonance, continuum excitation, 169–170
 - molecular systems, 175–177

- Brownian motion, multiparticle collision
 - dynamics, hydrodynamic
 - interactions, 118–121
- Canonical ensemble, multiparticle collision
 - dynamics, single-particle friction and diffusion, 116–118
- Cartesian Gaussian spinors:
 - basis functions using spherical harmonics, 261
 - P,T-odd interaction operator, 252–253
 - basis functions, 259–261
- Casimir's generalization, nonlinear
 - thermodynamics, time scaling, 34–36
- Channel phases:
 - transition state trajectory, deterministically moving manifolds, 228–231
 - two-pathway excitation, coherence spectroscopy, 148–149
 - energy domain, 179–182
 - one- vs. three-photon excitation, 165–166
- Chapman-Enskog method, multiparticle
 - collision dynamics, hydrodynamic equations, 105–107
- Charge conjugation (C), space inversion
 - symmetry and, 240–241
- Clebsh-Gordon coefficient, relativistic molecular orbitals, 250–251
- Coarse-grained approaches, multiparticle
 - collision dynamics, 90–92
- Coarse velocity, linear thermodynamics,
 - regression theorem, 18–20
- Coherence spectroscopy, two-pathway excitation:
 - atomic systems, 170–171
 - channel phases, 148–149
 - energy domain, 178–182
 - extended systems and dissipative environments, 177–185
 - future research issues, 185–186
 - isolated resonance, coupled continuum, 168–169
 - isolated resonance, uncoupled continuum, 167–168
 - long-range effects, resonance separation, 160–163
 - low-lying resonance, 169–170
 - measurement techniques, 154–159
 - molecular systems, 171–177
 - one- vs. three-photon case, 163–166
 - qualitative physics, 150–154
 - structureless, coupled continuum, 167
 - structureless, uncoupled continuum, 166
 - time domain, 182–185
- Collapse dynamics, multiparticle collision
 - dynamics, polymers, 124–127
- Collision operators, multiparticle collision
 - dynamics, 97–99
- Colloidal suspensions, multiparticle collision
 - dynamics, 121–122
- Colored noise, transition state trajectory, 208–209
- Configuration interaction (CI), ab initio
 - calculations, P,T-odd interactions, 254–259
- Continuum excitation, coherence spectroscopy:
 - isolated resonance:
 - coupled continuum, 168–169
 - uncoupled continuum, 167–168
 - low-lying resonance, 169–170
 - structureless:
 - coupled continuum, 167
 - uncoupled continuum, 166
- Cope's rule, nonequilibrium thermodynamics, 84
- Core polarization, ab initio calculations, P,T-odd
 - interactions, 255–259
- Correlation matrix, linear thermodynamics,
 - regression theorem, 17–20
- Coupled cluster (CC), ab initio calculations,
 - P,T-odd interactions, 254–259
- Coupled continuum, two-pathway excitation,
 - coherence spectroscopy:
 - isolated resonances, 168–169
 - structureless excitation, 167
- CPT theorem:
 - basic principles, 240–241
 - electron electric dipole moment, particle physics implications, 242–243
 - permanent electric dipole moment, 245–246
- Critical velocity, transition state trajectory,
 - stochastically moving manifolds, 219–222
- Crowded environments, reactive hybrid MPC-
 - molecular dynamics, 131–133
- Damping effects, transition state trajectory:
 - deterministic driving, 209–213
 - stochastically moving manifolds, 215–222
- De Broglie wavelength, two-pathway
 - excitation, coherence spectroscopy, 165–166
- Decoherence, two-pathway excitation,
 - coherence spectroscopy:

- energy domain, 181–182
- time domain, 183–185
- Degrees of freedom, transition state trajectory, stochastically moving manifolds, 215–222
- Delta function limit, two-pathway excitation, coherence spectroscopy, 183–185
- Deterministic force, transition state trajectory, 209–213
 - future research issues, 232
 - stochastically moving manifolds, 214–222
 - time-dependent invariant manifolds, 222–231
 - harmonic approximation, 222–223
 - Hénon-Heiles system, 228–231
 - nonlinear corrections, 223–228
 - white noise, 203–207
- Diatomic molecules:
 - electric dipole moment search, 242
 - internal electric field computations, 249–250
 - P,T-odd interactions, ab initio calculations, 253–259
 - barium fluoride molecule, 256–259
 - ytterbium molecule, 254–256
- Diffusion equation, multiparticle collision dynamics, macroscopic laws and transport coefficients, 99–104
- Dimer velocity, multiparticle collision dynamics, self-propelled objects, 134–136
- Dipole matrix elements, one- vs. three-photon excitation, coherence spectroscopy, 163–166
- Dirac delta function, transition state trajectory, white noise, 203–207
- Dirac-Fock (DF) level, ab initio calculations, P,T-odd interactions, 253
- Dirac matrices, P,T-odd interaction operator, 251–253
- Discrete-time velocity correlation function, multiparticle collision dynamics, macroscopic laws and transport coefficients, 103–104
- Dissipative structures:
 - nonequilibrium thermodynamics, 84
 - two-pathway excitation, coherence spectroscopy, 177–185
- Dividing surface, transition state trajectory, stochastically moving manifolds, 218–222
- Doob formula, linear thermodynamics, quadratic expansion, 13
- Dynamic structure factor, multiparticle collision dynamics, polymers, 124
- Eigenvalues, transition state trajectory:
 - colored noise, 209
 - stochastically moving manifolds, 214–222
 - white noise, 203–207
- Einstein relation, multiparticle collision dynamics, single-particle friction and diffusion, 115–118
- Elastic scattering, two-pathway excitation, coherence spectroscopy, 166–170
 - isolated resonance, uncoupled/coupled continuum, 167–169
 - low-lying resonance, continuum excitation, 169–170
 - molecular systems, 172–177
 - structureless, coupled continuum, 167
 - structureless, uncoupled continuum, 166
- Electric dipole moment (EDM):
 - ab initio calculations, 253–259
 - electron EDM, particle physics implications, 242–243
 - measurement principles, 244–245
 - permanent EDMS mechanisms, 245–249
 - P,T-odd interactions, 241–242
 - space inversion and time reversal symmetries, 240–241
- Electron density, permanent electric dipole moment, 249
- Electron electric dipole moment (EDM), particle physics implications, 242–243
- Electronic structure reference calculations:
 - computational procedure:
 - diatomic molecule internal electric field, 249–250
 - P,T-odd interaction operator, matrix elements, 251–253
 - relativistic molecular orbitals, 250–251
 - electric dipole moment:
 - electron EDM, particle physics implications, 242–243
 - measurement principles, 244–245
 - permanent EDMS mechanisms, 245–249
 - P,T-odd interactions, 241–242
 - space inversion and time reversal symmetries, 240–241
- Electrons, permanent electric dipole moment, 246

- Energy-domain approach, two-pathway
 - excitation, coherence spectroscopy, 153–154
- extended systems and dissipative environments, 178–182
- Entropy:
 - heat flow:
 - production rate, 64–65
 - second entropy, 60–65
 - thermodynamic variables, 58–60
 - linear thermodynamics:
 - macrostates, 9–11
 - production rate, 20–23
 - quadratic expansion, 11–13
 - regression theorem, 18–20
 - reservoirs, 23–25
 - time scaling, 13–16
 - nonequilibrium statistical mechanics,
 - microstate forward and reverse transitions, 49–51
 - nonequilibrium thermodynamics, 4–6
 - first vs. second entropy, 82–84
 - nonlinear thermodynamics:
 - production rate, 39
 - quadratic expansion, 27–28
 - reservoir exchange, 36–38
 - time scaling, 29–36
 - time-dependent mechanical work, transition probability, 56–57
- Equilibrium density, multiparticle collision dynamics, macroscopic laws and transport coefficients, 100–104
- Escape actions, transition state trajectory, deterministically moving manifolds, 230–231
- Evolution operators, multiparticle collision dynamics, 97–99
 - macroscopic laws and transport coefficients, 100–104
- Extended systems, two-pathway excitation, coherence spectroscopy, 177–185
- Fano's formalism, coherence spectroscopy, one- vs. three-photon excitation, 164–166
- Fermi nucleus, P,T-odd interaction operator, 252–253
- Feshbach's partitioning network, two-pathway excitation, coherence spectroscopy, 160–163
- Finitely extensible nonlinear elastic (FENE)
 - interactions, multiparticle collision dynamics, polymers, 122–128
- Flow simulation, multiparticle collision dynamics, hydrodynamic equations, 107
- Fluctuation-dissipation theorem, transition state trajectory, white noise, 203–207
- Fluctuation theorem, nonequilibrium thermodynamics, 6–7
- Fluid flows, multiparticle collision dynamics, polymers in, 127–128
- Forward transitions:
 - nonequilibrium statistical mechanics,
 - microstates, 47–51
 - time-dependent mechanical work, transition probability, 55–57
- Fourier's law of heat conduction, reservoirs, second entropy, 63–64
- Fourier transform:
 - multiparticle collision dynamics:
 - hydrodynamic equations, 105–107
 - macroscopic laws and transport coefficients, 99–104
 - transition state trajectory:
 - deterministically moving manifolds, 226–228
 - white noise, 205–207
- Friction interactions, multiparticle collision dynamics, single-particle friction and diffusion, 114–118
- Friction kernel, transition state trajectory, colored noise, 209
- Galilean invariance, multiparticle collision dynamics, 95–96
- Gaussian approximation, heat flow, 60
- Gaussian distribution, transition state trajectory, white noise, 206–207
- Gaussian-Markov process, linear thermodynamics, quadratic expansion, 13
- Gaussian nucleus, P,T-odd interaction operator, 252–253
- Gaussian probability, linear thermodynamics:
 - quadratic expansion, 12–13
 - regression theorem, 17–20
- Gaussian-type orbitals (GTOs), 257–258
- Gauss's law, diatomic molecules, internal electric field computations, 249–250

- Generalized relativistic effective core potentials (GRECP), *ab initio* calculations, P,T-odd interactions, 253–259
- Gene transcription, multiparticle collisions, reactive dynamics, 108–111
- Geometric transition state theory, 195–201
- Gillespie's algorithm, multiparticle collisions, reactive dynamics, 109–111
- Golden Rule approximation, two-pathway excitation, coherence spectroscopy, 160–163
- Gouy phase shift, two-pathway excitation, coherence spectroscopy, 155–159
- molecular systems, 174–177
- Green-Kubo theory:
- Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 73–74, 77–81
 - multiparticle collision dynamics:
 - hydrodynamic equations, 105–107
 - macroscopic laws and transport coefficients, 102–104
 - single-particle friction and diffusion, 114–118
 - nonequilibrium statistical mechanics, 43–44
 - Monte Carlo procedures, 83
 - nonequilibrium thermodynamics, second law, 5
- Green's function, reactive hybrid MPC-molecular dynamics, 131–133
- Grid shifting algorithm, multiparticle collision dynamics, 95–96
- collision and evolution operators, 98–99
- Grote-Hynes reaction frequency, transition state trajectory, colored noise, 209
- Gyration radius, multiparticle collision dynamics, polymer collapse, 125–127
- Hamiltonian equations:
- electric dipole moment measurement, 244–245
 - linear thermodynamics, macrostates, 10–11
 - transition state trajectory:
 - deterministically moving manifolds, 225–228
 - deterministic driving, 209–213
 - future research issues, 232
 - two-pathway excitation, coherence spectroscopy, 161–163
- Harmonic approximation, transition state trajectory:
- deterministically moving manifolds, 222–223
 - stochastically moving manifolds, 220–222
- Heat flow:
- Gaussian approximation, 61
 - Monte Carlo simulations, 67–81
 - dynamics, 75–81
 - Metropolis algorithms, 70–71
 - nonequilibrium molecular dynamics, 71–74
 - structure profiles, 74–75
 - system details, 67–70
 - phase space probability distribution, 65–67
 - second entropy, 61–65
 - isolated system, 61–62
 - production rate, 64–65
 - reservoirs, 62–64
 - thermodynamics variables, 58–60
 - time-dependent mechanical work, transition probability, 56–57
- Heaviside function, multiparticle collision dynamics, hydrodynamic equations, 105–107
- Helmholtz free energy, time-dependent mechanical work, transition probability, 57
- Hénon-Heiles system, transition state trajectory, deterministically moving manifolds, 228–231
- Hybrid multiparticle collision-molecular dynamics, 111–112
- collapse dynamics of polymers, 124–127
 - reactive hybrid MPC-molecular dynamics, 128–133
 - crowded environments, 131–133
- Hydrodynamic equations, multiparticle collision dynamics, 104–107
- collapse dynamics of polymers, 126–127
 - interactions, 118–121
 - self-propelled objects, 135–136
- Immiscible fluids, multiparticle collision dynamics, 138–139
- Inhomogeneous polynomials, transition state trajectory, deterministically moving manifolds, 224–228
- Instantaneous locations, transition state trajectory, stochastically moving manifolds, 216–222
- Interaction operator, P,T-odd interaction, matrix elements, 251–253, 260–263
- Interference term, two-pathway excitation, coherence spectroscopy, energy domain, 180–182

- Interferometric method, two-pathway excitation, coherence spectroscopy, time domain, 184–185
- Intermediate regimes:
 - heat flow, second entropy, isolated systems, 60–62
 - linear thermodynamics, 25–27
 - nonlinear thermodynamics, time scaling, 31–36
- Internal electric field, diatomic molecules, 250–251
- Ionization, two-pathway excitation, coherence spectroscopy, molecular systems, 172–177
- Island complexes, transition state trajectory, deterministically moving manifolds, 230–231
- Isolated systems:
 - heat flow, second entropy, 60–62
 - two-pathway excitation, coherence spectroscopy, coupled/uncoupled continuum, 167–169
- Isotope effect, two-pathway excitation, coherence spectroscopy, molecular systems, 173–177
- Jacobian matrices, multiparticle collision dynamics, 94–95
- Kinetically balanced molecular orbitals, 257–258
- Lagrangians, nonequilibrium thermodynamics, 5–6
- Langevin equation:
 - linear thermodynamics, quadratic expansion, 13
 - Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 79–81
 - multiparticle collision dynamics:
 - hydrodynamic interactions, 118–121
 - single-particle friction and diffusion, 114–118
 - transition state trajectory:
 - colored noise, 208–209
 - deterministic driving, 209–213
 - future research issues, 232–233
 - stochastically moving manifolds, 214–222
 - white noise, 203–207
- Laplace transform, transition state trajectory, colored noise, 208–209
- Laser technology, two-pathway excitation, coherence spectroscopy, 154–159
- Lees-Edwards boundary, multiparticle collision dynamics, polymer fluid flow, 127–128
- Legendre polynomials, two-pathway excitation, coherence spectroscopy, 152–154
- Lennard-Jones interactions:
 - Monte Carlo heat flow simulation, 67–70
 - nonequilibrium molecular dynamics, 75–81
 - multiparticle collision dynamics:
 - collapse dynamics of polymers, 124–127
 - hydrodynamic interactions, 120–121
 - polymers, 122–128
- Lepton flavor-change, electron electric dipole moment, 242–243
- Linear combination of molecular orbitals (LCAO), computational procedures, 250–251
- Linear limit, nonlinear thermodynamic coefficients, 36
- Linear momentum (L) operator, time reversal symmetry and, 243–244
- Linear scaling, multiparticle collision dynamics, nonideal fluids, 137
- Linear thermodynamics:
 - entropy production, 20–23
 - formalities, 8–11
 - intermediate regime and maximum flux, 25–27
 - quadratic expansion, 11–13
 - regression theorem, 16–20
 - reservoirs, 23–25
 - time scaling, 13–16
- Liouville equation:
 - multiparticle collision dynamics:
 - collision and evolution operators, 98–99
 - hydrodynamic interactions, 119–121
 - time-dependent mechanical work, 52–53
 - two-pathway excitation, coherence spectroscopy:
 - energy domain, 178–182
 - extended systems and dissipative environments, 178–185
- Long-range effects, two-pathway excitation, coherence spectroscopy, 160–163
- Low-lying resonances, two-pathway excitation, coherence spectroscopy, continuum excitation, 169–170

- Macroscopic laws:
 - multiparticle collision dynamics, 99–104
 - reactive hybrid MPC-molecular dynamics, 128–133
- Macrostates:
 - linear thermodynamics, 9–11
 - nonequilibrium thermodynamics, 5–6
 - steady-state probability distribution, nonequilibrium statistical mechanics, 41–43
- Manifolds:
 - time-dependent invariant manifolds, transition state theory, 213–231
 - deterministically moving manifolds, 222–231
 - harmonic approximation, 222–223
 - nonlinear corrections, 223–228
 - driven Hénon-Heiles system, 228–231
 - stochastically moving manifolds, 214–222
 - two-pathway excitation, coherence spectroscopy:
 - extended systems and dissipative environments, 177–185
 - resonance manifolds, 160–163
- Markov chain formulation, multiparticle collision dynamics:
 - collision and evolution operators, 98–99
 - hydrodynamic equations, 104–107
 - macroscopic laws and transport coefficients, 99–104
- Markov decay time, Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 80–81
- Markov procedure:
 - linear thermodynamics, intermediate regimes and maximum flux, 26–27
 - nonlinear thermodynamics, time scaling, 29–36
- Matrix elements, P,T-odd interactions, 251–253, 260–263
- Maximum Dissipation Principle, linear thermodynamics, entropy production, 21–23
- Maximum flux, linear thermodynamics, 25–27
- Maxwell-Boltzmann distribution, multiparticle collision dynamics, 95
- Mesoscale simulation of complex systems, multiparticle collision dynamics, basic principles, 90–92
- Metropolis algorithm, Monte Carlo heat flow simulation, 70–71
 - molecular dynamics, 76–81
- Microcanonical ensemble, multiparticle collision dynamics, single-particle friction and diffusion, 116–118
- Microstate transitions, nonequilibrium statistical mechanics, 44–51
 - adiabatic evolution, 44–46
 - forward and reverse transitions, 47–51
 - stationary steady-state probability, 47
 - stochastic transition, 46–47
- Minimum Dissipation Principle, linear thermodynamics, entropy production, 21–23
- Minimum entropy production, nonequilibrium thermodynamics, 6
- Mirror paths, time-dependent mechanical work, transition probability, 54–57
- Modulation depth, two-pathway excitation, coherence spectroscopy, 155–159
- Molecular beam detector, two-pathway excitation, coherence spectroscopy, 157–159
- Molecular dynamics (MD):
 - hybrid multiparticle collision-molecular dynamics, 111–112
 - Monte Carlo heat flow simulation, 75–81
 - multiparticle collision dynamics:
 - basic principles, 91–92
 - polymers, 123–124
- Molecular systems, two-pathway excitation, coherence spectroscopy, 171–177
- Monomials, transition state trajectory, deterministically moving manifolds, 225–228
- Monte Carlo simulations, heat flow, 67–81
 - dynamics, 75–81
 - Metropolis algorithms, 70–71
 - nonequilibrium molecular dynamics, 71–74
 - structure profiles, 74–75
 - system details, 67–70
- Multicomponent systems, multiparticle collision dynamics, 96–97
- Multi-Higgs, left-right symmetry, electron electric dipole moment, 242–243
- Multiparticle collision dynamics:
 - basic principles, 92–93
 - collision operators and evolution equations, 97–99
 - colloidal suspensions, 121–122
 - Galilean invariance and grid shifting, 95–96
 - hybrid MPC-molecular dynamics, 111–112

- Multiparticle collision dynamics (*continued*)
 - hydrodynamic equations, 104–107
 - flow simulation, 107
 - friction interactions, 118–121
 - immiscible fluids, 138–139
 - macroscopic laws and transport coefficients, 99–104
 - Gree-Kubo expression, 102–104
 - mesoscale simulation of complex systems:
 - basic principles, 90–92
 - real system simulations, 113–114
 - multicomponent systems, 96–97
 - nonideal fluids, 136–137
 - polymers, 122–128
 - collapse dynamics, 124–127
 - dynamical properties, 123–124
 - fluid flows, 127–128
 - properties of, 94–95
 - reactive dynamics, 107–111
 - reactive hybrid MPC-molecular dynamics, 128–133
 - crowded environments, 131–133
 - self-propelled objects, 133–136
 - single-particle friction and diffusion, 114–118
- Nanoscale analysis, multiparticle collision
 - dynamics, self-propelled objects, 134–136
- Nonequilibrium molecular dynamics (NEMD):
 - Monte Carlo heat flow simulation, 71–74
 - theoretical background, 6
- Nonequilibrium probability, time-dependent
 - mechanical work, 51–53
- Nonequilibrium quantum statistical mechanics, 57–58
- Nonequilibrium statistical mechanics:
 - Green-Kubo theory, 43–44
 - microstate transitions, 44–51
 - adiabatic evolution, 44–46
 - forward and reverse transitions, 47–51
 - stationary steady-state probability, 47
 - stochastic transition, 46–47
 - steady-state probability distribution, 39–43
- Nonequilibrium thermodynamics:
 - second law of:
 - basic principles, 2–3
 - future research issues, 81–84
 - heat flow:
 - Gaussian approximation, 61
 - phase space probability distribution, 65–67
 - second entropy, 61–65
 - isolated system, 61–62
 - production rate, 64–65
 - reservoirs, 62–64
 - thermodynamics variables, 58–60
- linear thermodynamics:
 - entropy production, 20–23
 - formalities, 8–11
 - intermediate regime and maximum flux, 25–27
 - quadratic expansion, 11–13
 - regression theorem, 16–20
 - reservoirs, 23–25
 - time scaling, 13–16
- Monte Carlo simulations, heat flow, 67–81
- dynamics, 75–81
- Metropolis algorithms, 70–71
- nonequilibrium molecular dynamics, 71–74
- structure profiles, 74–75
- system details, 67–70
- nonequilibrium quantum statistical
 - mechanics, 57–58
- nonequilibrium statistical mechanics:
 - Green-Kubo theory, 43–44
 - microstate transitions, 44–51
 - adiabatic evolution, 44–46
 - forward and reverse transitions, 47–51
 - stationary steady-state probability, 47
 - stochastic transition, 46–47
 - steady-state probability distribution, 39–43
- nonlinear thermodynamics:
 - coefficients linear limit, 36
 - entropy production rate, 39
 - parity, 28–29
 - quadratic expansion, 27–28
 - reservoir exchange, 36–38
 - time scaling, 29–36
- theoretical background, 4–8
- time-dependent mechanical work:
 - phase space probability, 51–53
 - transition probability, 53–57
- statistical mechanics and, 4
- Nonideal fluids, multiparticle collision
 - dynamics, 136–137
- Nonlinear coefficients, linear limit, 36
- Nonlinear corrections, transition state trajectory,
 - deterministically moving manifolds, 223–228

- Nonlinear Hamiltonian system, geometric transition state theory, 200–201
- Nonlinear thermodynamics:
 - coefficients linear limit, 36
 - entropy production rate, 39
 - parity, 28–29
 - quadratic expansion, 27–28
 - reservoir exchange, 36–38
 - time scaling, 29–36
- Nonuniqueness properties, transition state trajectory, deterministic driving, 210–213
- Nonzero electron electric dipole moment, 247–249
- Normal form coordinates, transition state trajectory, deterministically moving manifolds, 227–228
- Normally hyperbolic invariant manifold (NHIM):
 - geometric transition state theory, 195–201
 - transition state trajectory, 201–213
 - deterministically moving manifolds, 223–228
 - time-dependent manifolds, 213–231
- Nucleons, permanent electric dipole moment, 246
- One-photon excitation, coherence spectroscopy, 163–166
 - extended systems and dissipative environments, 178–182
- Onsager-Machlup functional:
 - Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 79–81
 - nonequilibrium thermodynamics, 5–6
- Onsager's regression hypothesis:
 - heat flow, reservoirs, second entropy, 63–64
 - linear thermodynamics:
 - quadratic expansion, 13
 - regression theorem, 16–20
 - nonequilibrium thermodynamics, 4
 - nonlinear thermodynamics:
 - reservoir exchange, 38
 - time scaling, 34–36
- Optimum point:
 - linear thermodynamics, time scaling, 14–16
 - nonlinear thermodynamics, time scaling, 29–36
- Orthogonality, nonlinear thermodynamics, time scaling, 32–36
- Parity nonconservation (PNC) effects, electric dipole moment search, 242
- Parity operator:
 - nonlinear thermodynamics, 28–29
 - time reversal symmetry and, 243–244
- Pauli spin matrices, permanent electric dipole moment, 246–249
- Peclet number, multiparticle collision dynamics, real-time systems, 114
- Periodic boundary conditions, Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 79–81
- Periodic-orbit dividing surface (PODS):
 - geometric transition state theory, 196–201
 - transition state trajectory, 202–213
- Perturbation theory, transition state trajectory, deterministically moving manifolds, 224–228
- Phase lag spectrum, two-pathway excitation, coherence spectroscopy, molecular systems, 175–177
- Phase space probability:
 - geometric transition state theory, 197–201
 - heat flow, 65–67
 - Monte Carlo heat flow simulation, nonequilibrium molecular dynamics, 71–74
 - nonequilibrium statistical mechanics, 83–84
 - time-dependent mechanical work, 51–53
- Phase space trajectory, nonequilibrium thermodynamics, 8
- Phase space volumes, multiparticle collision dynamics, 94–95
- Photoionization, two-pathway excitation, coherence spectroscopy, atomic systems, 170–171
- Poisson brackets, transition state trajectory, deterministically moving manifolds, 226–228
- Poisson distribution, multiparticle collision dynamics, macroscopic laws and transport coefficients, 102–104
- Polyatomic molecules, coherence spectroscopy, two-pathway excitation, 174–177
- Polymers, multiparticle collision dynamics, 122–128
 - collapse dynamics, 124–127
 - dynamical properties, 123–124
 - fluid flows, 127–128

- Position operator (Q), time reversal symmetry and, 243–244
- Power law decay, reactive hybrid MPC-molecular dynamics, 130–133
- Precession frequency, electric dipole moment measurement, 244–245
- Probability distribution, nonequilibrium thermodynamics, 7–8
- Projection theorem, electric dipole moment measurement, 244–245
- P,T-odd interactions:
 ab initio calculations, 253–259
 barium fluoride molecule, 256–259
 ytterbium molecule, 254–256
 electric dipole moment, 241–242
 interaction operator, matrix elements, 251–253, 260–263
 spherical polar coordinates, 261–262
- Pulse duration, two-pathway excitation, coherence spectroscopy, time domain, 183–185
- Quadratic expansion:
 linear thermodynamics, 11–13
 entropy production, 22–23
 Monte Carlo heat flow simulation, 75–81
 nonlinear thermodynamics, 27–28
- Qualitative physics, two-pathway excitation, coherence spectroscopy, 150–154
- Quasiclassical approximation, two-pathway excitation, coherence spectroscopy, 151–154
- Rate constants, reactive hybrid MPC-molecular dynamics, 129–133
- Rayleigh parameters, two-pathway excitation, coherence spectroscopy, 155–159
- Reaction-diffusion equations, multiparticle collisions, reactive dynamics, 108–111
- Reaction rates:
 transition state theory, 192–194
 transition state trajectory, stochastically moving manifolds, 218–222
- Reactive dynamics:
 geometric transition state theory, 196–201
 multiparticle collisions, 107–111
 transition state trajectory, stochastically moving manifolds, 218–222
- Real-time systems, multiparticle collision dynamics, 113–114
- Reduction condition:
 linear thermodynamics, quadratic expansion, 13
 nonlinear thermodynamics, time scaling, 31–36
- Regression theorem, linear thermodynamics, 16–20
- Relativistic effective core potentials (RECP), ab initio calculations, 253
- Relativistic molecular orbitals, computational procedure, 250–251
- Relaxation times, Monte Carlo heat flow simulation, molecular dynamics, 76–81
- Reservoirs:
 heat flow, second entropy, 62–64
 linear thermodynamics, 23–25
 nonequilibrium statistical mechanics, microstate forward and reverse transitions, 50–51
 nonlinear thermodynamics, 36–38
- Resonance manifolds, two-pathway excitation, coherence spectroscopy, 160–163
- Restricted active space self-consistent field (RASSCF) scheme, ab initio calculations, P,T-odd interactions, 253–259
- Reverse transitions:
 nonequilibrium statistical mechanics, microstates, 47–51
 time-dependent mechanical work, 55–57
- Reynolds number, multiparticle collision dynamics:
 hydrodynamic equations, 107
 real-time systems, 113–114
- Rotation matrix orthogonality, two-pathway excitation, coherence spectroscopy, 162–163
- Rothman-Keller immiscible fluid model, multiparticle collision dynamics, 138–139
- Rouse modes, multiparticle collision dynamics, polymers, 123–124
- Rydberg states, two-pathway excitation, coherence spectroscopy, molecular systems, 172–177

- Scalar equations, transition state trajectory:
 - deterministically moving manifolds, 224–228
 - stochastically moving manifolds, 214–222
- Scattering theory, two-pathway excitation,
 - coherence spectroscopy, 151–154
- Schiff's theorem, permanent electric dipole moment, 247–248
- Schmidt number, multiparticle collision dynamics,
 - real-time systems, 113–114
- Schrödinger equation:
 - nonequilibrium quantum statistical mechanics, 57–58
 - two-pathway excitation, coherence spectroscopy, 153–154
- Second entropy. *See* Entropy
- Self-consistent field (SCF), *ab initio* calculations, P,T-odd interactions, 254–259
- Self-propelled objects, multiparticle collision dynamics, 133–136
- Semiclassical approximation, two-pathway excitation, coherence spectroscopy, 152–154
- S-functionals, transition state trajectory:
 - deterministic driving, 212–213
 - white noise, 206–207
- Single-particle friction and diffusion,
 - multiparticle collision dynamics, 114–118
- Slater determinant, P,T-odd interaction operator, 252–253
- Solvent properties, transition state trajectory,
 - future research issues, 232–233
- Space inversion symmetry (P):
 - ab initio* calculations, 253–259
 - barium fluoroide molecules, 256–259
 - ytterbium molecule, 254–256
 - electric dipole moment search, 241–242
 - nonconservation, 239–241
- Spatial neighbor tables, Monte Carlo heat flow simulation, 68–70
- Spherical harmonics, Cartesian Gaussian basis functions, 261
- Spherical polar coordinates, P,T-odd interactions, 261–262
- Standard model (SM), particle physics, electron electric dipole moment, 242–243
- Stark effect, permanent electric dipole moment, 245–249
- Static probability distribution:
 - Monte Carlo heat flow simulation, 74–75
 - nonequilibrium statistical mechanics, 40–43
- Stationary steady-state probability,
 - nonequilibrium statistical mechanics, microstate transitions, 47
- Statistical mechanics, nonequilibrium thermodynamics, 82–84
- Steady-state probability distribution:
 - heat flow, phase space, 65–67
 - nonequilibrium statistical mechanics, 39–43
- Stochastically moving manifolds, transition state trajectory, 214–222
- Stochastic rotation, multiparticle collision dynamics and, 93
- Stochastic transition:
 - nonequilibrium statistical mechanics, microstate transitions, 46–47
 - time-dependent mechanical work, transition probability, 53–57
- Stokes law, multiparticle collision dynamics,
 - single-particle friction and diffusion, 117–118
- Supersymmetry (SUSY), electron electric dipole moment, particle physics implications, 242–243
- Symmetric-matrix valued function, transition state trajectory, colored noise, 208–209
- Symmetry rules, linear thermodynamics, macrostates, 11
- Taylor expansion, transition state trajectory,
 - deterministically moving manifolds, 224–228
- Terminal velocity, linear thermodynamics:
 - intermediate regimes and maximum flux, 25–27
 - regression theorem, 18–20
- Test particle density, multiparticle collision dynamics, macroscopic laws and transport coefficients, 100–104
- Thermodynamic variables:
 - heat flow, 58–60
 - nonequilibrium thermodynamics, 83–84
- Three-manifold model, two-pathway excitation,
 - coherence spectroscopy, extended systems and dissipative environments, 177–185
- Three-photon excitation, coherence spectroscopy, 163–166

- Time-correlation matrix, linear
 - thermodynamics, quadratic expansion, 12–13
- Time-dependent invariant manifolds, transition state theory, 213–231
 - deterministically moving manifolds, 222–231
 - harmonic approximation, 222–223
 - nonlinear corrections, 223–228
 - driven Hénon-Heiles system, 228–231
 - future research issues, 231–232
 - stochastically moving manifolds, 214–222
- Time-dependent mechanical work:
 - phase space probability, 51–53
 - transition probability, 53–57
- Time-domain analysis, two-pathway excitation, coherence spectroscopy, 153–154, 182–185
- Time reversal symmetry (T):
 - basic principles, 240–241
 - electric dipole moment search, 241–242
 - parity operator, 243–244
- Time scaling:
 - linear thermodynamics, 13–16
 - intermediate regimes and maximum flux, 25–27
 - nonequilibrium statistical mechanics, microstate transitions, 47–51
 - nonlinear thermodynamics, 29–36
 - two-pathway excitation, coherence spectroscopy, energy domain, 180–182
- Top-down approaches, geometric transition state theory, 195–201
- Trajectory calculations:
 - geometric transition state theory, 198–201
 - linear thermodynamics, intermediate regimes and maximum flux, 26–27
 - Monte Carlo heat flow simulation, 69–70
 - time-dependent mechanical work, transition probability, 53–57
 - transition state theory, 201–213
 - colored noise, 208–209
 - white noise, 203–207
- Transition matrix, two-pathway excitation, coherence spectroscopy, 161–163
- Transition probability, time-dependent mechanical work, 53–57
- Transition state theory (TST):
 - basic principles, 192–195
 - future research, 231–233
 - geometric test, 195–201
- time-dependent invariant manifolds, 213–231
 - deterministically moving manifolds, 222–231
 - harmonic approximation, 222–223
 - nonlinear corrections, 223–228
 - driven Hénon-Heiles system, 228–231
 - stochastically moving manifolds, 214–222
- trajectory, 201–213
 - colored noise, 208–209
 - deterministic driving, 209–213
 - white noise, 203–207
- Transport coefficient:
 - linear thermodynamics, intermediate regimes and maximum flux, 25–27
 - multiparticle collision dynamics, macroscopic laws and, 99–104
 - nonequilibrium statistical mechanics, Green-Kubo theory, 43–44
 - nonequilibrium thermodynamics, 5
- Transport matrix:
 - linear thermodynamics:
 - asymmetry of, 19–20
 - entropy production, 20–23
 - regression theorem, 18–20
 - nonlinear thermodynamics, time scaling, 34–36
- Transverse damped oscillations, transition state trajectory, stochastically moving manifolds, 216–222
- Two-dimensional constant matrix, transition state trajectory, white noise, 203–207
- Two-pathway excitation, coherence spectroscopy:
 - atomic systems, 170–171
 - channel phases, 148–149
 - energy domain, 178–182
 - extended systems and dissipative environments, 177–185
 - future research issues, 185–186
 - isolated resonance, coupled continuum, 168–169
 - isolated resonance, uncoupled continuum, 167–168
 - long-range effects, resonance separation, 160–163
 - low-lying resonance, 169–170
 - measurement techniques, 154–159
 - molecular systems, 171–177
 - one- vs. three-photon case, 163–166
 - qualitative physics, 150–154

- structureless, coupled continuum, 167
- structureless, uncoupled continuum, 166
- time domain, 182–185
- Two-photon photoemission (2PPE)
 - spectroscopies, two-pathway
 - excitation, coherence spectroscopy:
- extended systems and dissipative environments, 178–183
- time domain, 182–185
- Umbrella weight, Monte Carlo heat flow simulation, 70–71
- Unconditional transition probability:
 - linear thermodynamics, macrostates, 10–11
 - nonequilibrium statistical mechanics, microstate forward and reverse transitions, 47–51
- Uncoupled continuum, two-pathway excitation, coherence spectroscopy:
 - isolated resonances, 167–168
 - structureless continuum, 166
- Unrestricted Dirac-Fock (UDF), *ab initio* calculations, P,T-odd interactions, 253–259
- Volume fraction dependence, reactive hybrid MPC-molecular dynamics, 132–133
- Weissenberg number, multiparticle collision dynamics, polymer fluid flow, 127–128
- White noise, transition state trajectory, 203–207
- stochastically moving manifolds, 222
- Work theorem:
 - nonequilibrium thermodynamics, 6–7
 - time-dependent mechanical work, transition probability, 56–57
- Yamada-Kawasaki distribution:
 - nonequilibrium thermodynamics, 7
 - time-dependent mechanical work, 52–53
- Ytterbium-fluoride (YbF) molecule, P,T-odd interactions, 242, 249–250, 254–256
- Zeroth temperature, heat flow, thermodynamic variables, 59–60
- Zimm theory, multiparticle collision dynamics, polymers, 123–124

