

Index

- $3j$ symbol, 17, 365–368
- $6j$ symbol, 154, 156–158, 369–370, 394–397
- Absorption
 - Circularly polarized radiation, 242–244
 - Coefficient, 239–241
 - Cross section, 243
 - Induced absorption rate, 238–239
 - Linearly polarized radiation, 241–242
 - Lineshape models, 247–253
 - Rate coefficient, 239
- Angular momentum operator, generalized, 30–32
- Atomic hydrogen
 - Spin–orbit splitting, 29
- Atomic hydrogen
 - Electric dipole moment, coupled representation, 143–146
 - Electric dipole moment, uncoupled representation, 139–143
 - Radial integrals, 140
 - Solution, Schrödinger wave equation, 22–26
 - Spontaneous emission coefficients, 147–148
- Atomic nitrogen, 38–39
- Band strength, diatomic molecules, 165
- Born–Oppenheimer approximation, 56, 58–60
- CARS
 - Broadband, 330–332
 - Collisional narrowing, 334–339
 - Electric field modeling, 326–327
 - Example problem, dual-pump CARS, 353–359
 - Example problem, parallel polarization, 348–353
 - Femtosecond, time-dependent equations, 342–343
 - Nonresonant susceptibility, 322
 - Polarizability, orientation averaging, 317–318
 - Polarizability, pure rotational, 319–320
 - Polarizability, vibrational, 320–321
 - Scanning, monochromatic laser fields, 327–328
 - Scanning, narrowband lasers, 329–330
 - Scanning, narrowband Stokes, 328–329
 - Signal amplitude formula, 325
 - Signal irradiance formula, 325
 - Susceptibility, general expression, 321–322
 - Transition linewidths, 332–334
- Center of mass coordinates, 57
- Centrifugal stretching, 62
- Central-field approximation, 33
- Central potential, 22
- Classical electron oscillator model, 3–11
- Clebsch–Gordan coefficients, 17, 28, 45, 138
 - Relation to $3j$ symbols, 28, 47
- Closure relations, 264
- Collisional broadening, 239
- Density matrix, 134–136
 - Coherence decay terms, 136
 - Energy interaction terms, 134–136
 - Multistate system, 236–237
 - Two-state system, 237–238
- Diatomic molecules
 - Electronic transitions, 164–166
- Dielectric permittivity, 6
- Dirac
 - Bra and ket notation, 17
 - Inner product, 18
- Dirac wave equation, 16, 22, 27
- Doppler broadening, 248–249
- Doppler linewidth, 257
- Doublet electronic levels
 - $^2\Lambda$, $\Lambda > 0$ levels, 82–96
 - $^2\Pi$ levels, 82–96
 - $^2\Sigma$, 90–100
 - $\Lambda > 0$, matrix elements, including higher order, 91–92
- Effective Hamiltonian, 68
- Electric dipole interaction
 - Long wavelength approximation, 125–127
- Electric dipole moment, 1–4
 - Atomic hydrogen, 136–146
 - Reduced density matrix element, 148
- Electric dipole oscillator
 - Radiative decay, 12–15
- Electric quadrupole moment, 1, 3

- Electromagnetic field
 Plane wave approximation, 11
 Propagation in dielectric medium, 11
- Electronic transition moment
 MOLPRO code, 203
 NH $X^3\Sigma^-A^3\Pi$, 230
 NO $X^2\Pi-A^2\Sigma^+$, 203
 OH $X^2\Pi-A^2\Sigma^+$, 203
- Electronic transitions
 Diatomic molecules, 164–166
 Doublet transitions, diatomic molecules, $^2\Pi-^2\Sigma$, 198–199
 Doublet transitions, diatomic molecules, $^2\Sigma-^2\Pi$, 191–194
 Doublet transitions, diatomic molecules, $^2\Sigma-^2\Sigma$, 184–186
 Doublet transitions, diatomic molecules, F_1-F_1 , 178–182
 Doublet transitions, diatomic molecules, $\Delta\Lambda = -1$, 196–198
 Doublet transitions, diatomic molecules, $\Delta\Lambda = +1$, $\Lambda > 0$, 188–191, 193–195
 Doublet transitions, diatomic molecules, $\Delta\Lambda = 0$, $\Lambda, \Lambda' > 0$, 186–189
 Forbidden transitions, diatomic molecules, 232–233
 Singlet transitions, diatomic molecules, $^1\Pi-^{1\Sigma}$, 170–174
 Singlet transitions, diatomic molecules, $^1\Sigma-^{1\Sigma}$, 166–170
 Singlet transitions, diatomic molecules, $\Lambda > 0$, $\Lambda' > 0$, 174–177
 Triplet transitions, diatomic molecules, $^3\Sigma-^3\Pi$, 216–222
 Triplet transitions, diatomic molecules, $^3\Sigma-^3\Sigma$, 211–216
 Triplet transitions, diatomic molecules, $\Lambda > 0$, $\Lambda' > 0$, 222–229
- Euler angles, 42–43
- Franck–Condon factors, 166
- Galatry profile, 252–253
- Gauge invariance, 121–125
- Hard collision model, 253
- Harmonic oscillator potential, 57
- Harmonic oscillator wavefunction, 56–61
- Homogeneous broadening, 239
- Hönl–London factors, 165–166
 Singlet transitions, diatomic molecule, $^1\Sigma-^{1\Sigma}$, 169–170
 Singlet transitions, diatomic molecules, $^1\Pi-^{1\Sigma}$, 173–174
 Singlet transitions, diatomic molecules, $\Lambda > 0$, $\Lambda' > 0$, 175–177
- Hund's case (a), 56–118
 Basis wavefunctions, 65–66
- Eigenvalues, 66–67
- Hamiltonian, 79
- Matrix elements, 66–67
- Matrix elements, centrifugal distortion, rotation, 72–75
- Matrix elements, centrifugal distortion, spin–orbit interaction, 76
- Matrix elements, lambda-doubling, 76–77
- Matrix elements, rotation, 68–71
- Matrix elements, spin–orbit interaction, 71
- Matrix elements, spin–rotation interaction, 71–72
- Matrix elements, spin–spin interaction, 72
- Parity of wavefunctions, 65–66
- Hund's case (b), 56–118
- Hyperfine interaction
 Effect on absorption coefficient, 393–397
 Effect on spontaneous emission rate coefficient, 393–397
- Hyperfine splitting
 Atomic hydrogen, 29
- Inhomogeneous broadening, 248–249
- Irreducible spherical tensor operators, 49–50
 Scalar product, 52
- Irreducible spherical tensors, 49–50, 148–150
- Jacobi polynomial, 44
- jj coupling, 16, 39
- Lamb shift, 29
- Lorentz classical electron oscillator model, 3
- Lorentzian lineshape, 239
- Lowering operator, 30
- LS coupling, 16, 38
 Radiative transitions, atomic oxygen, 156–159
 Single-photon transition selection rules, 155
- Macroscopic polarization, 5
- Magnetic permeability, 11
- Morse potential, 61–62
- Multielectron atoms, 16
 Electron configuration, 33–34
 Orbital angular momentum, 35–36
 Quantum numbers, 33
 Spin angular momentum, 35–36
 Wavefunction, 34–35
- NH
 $A^3\Pi$ ($v=0$) Hund's case (a) coefficients, 56–113
 $A^3\Pi$ ($v=0$) level energies, 112
 $A^3\Pi$ ($v=0$) spectroscopic parameters, 111
 $X^3\Sigma^-A^3\Pi$ vibrational band strengths, 229–232
 $X^3\Sigma^-A^3\Pi$ (0,0) Einstein coefficients, 384–392
 $X^3\Sigma^-A^3\Pi$ Einstein coefficients, 232
- NIST Atomic Spectra Database, 38
- NO
 $X^2\Pi$ ($v=0$) Hund's case(a) coefficients, 93–94

- X²Π (v=0) level energies, 93–94
- X²Π (v=0) spectroscopic parameters, 92
- X²Π-A²Σ⁺ (0,0) Einstein coefficients, 206–210
- X²Π-A²Σ⁺ electronic transition moment, 203
- X²Π-A²Σ⁺ vibrational band strengths, 201–206
- Nuclear rotation angular momentum, 64–119
- OH
 - X²Π (v=0) Hund's case (a) coefficients, 93–96
 - X²Π (v=0) level energies, 93–96
 - X²Π (v=0) spectroscopic parameters, 95
 - X²Π-A²Σ⁺ (0,0) Einstein coefficients, 206–210
 - X²Π-A²Σ⁺ electronic transition moment, 203
 - X²Π-A²Σ⁺ vibrational band strengths, 201–206
- Operators, quantum mechanical, 17–18
 - Hermitian, 18
 - Orbital angular momentum, 23
- Oscillator strength, 244
- Pair coupling, 16, 39–40
- Parity, 39
- Pauli exclusion principle, 32–33
- Pauli spinor, 27
- Perturbation analysis
 - Multiphoton resonances, 131–134
 - Raman resonances, 133–134
 - Single-photon resonances, 128–131
 - Two-photon absorption, 133
- Poynting vector, 14
- Principal moments of inertia, 62
- Pure dephasing collisions, 5–6
- Quantum Liouville equation, 134–136
- Rabi frequency, 238
- Radial wavefunctions
 - Atomic hydrogen, 26
- Radiative transitions
 - Doublet transitions, diatomic molecules, ²Π-²Σ, 198–199
 - Doublet transitions, diatomic molecules, ²Σ-²Π, 191–194
 - Doublet transitions, diatomic molecules, ²Σ-²Σ, 184–186
 - Doublet transitions, diatomic molecules, F₁-F₁, 178–182
 - Doublet transitions, diatomic molecules, ΔΛ = -1, 196–198
 - Doublet transitions, diatomic molecules, ΔΛ = +1, Λ > 0, 188–191, 193–195
 - Doublet transitions, diatomic molecules, ΔΛ = 0, Λ, Λ' > 0, 186–189
 - Doublet transitions, diatomic molecules, ΔΛ = -1, Λ > 1, 193–200
 - Effect of hyperfine splitting, 153–154
 - Forbidden transitions, diatomic molecules, 232–233
 - Hund's case (a) basis states, 163–164
 - LS coupling multiplet terms, 156–159
 - LS coupling selection rules, 155
 - Oscillator strength, 244
 - Pure rotational, 161–162
 - Singlet transitions, diatomic molecules, ¹Π-¹Σ, 170–174
 - Singlet transitions, diatomic molecules, ¹Σ-¹Σ, 166–170
 - Singlet transitions, diatomic molecules, Λ > 0, Λ' > 0, 174–177
 - Spontaneous emission rate coefficient, 152–153
 - Triplet transitions, diatomic molecules, ³Σ-³Π, 216–222
 - Triplet transitions, diatomic molecules, ³Σ-³Σ, 211–216
 - Triplet transitions, diatomic molecules, Λ > 0, Λ' > 0, 222–229
 - Vibrational, 162–163
- Raising operator, 30
- Raman polarizability
 - Irreducible spherical tensor representation, 264–266
 - Operator, 264
 - Placzek theory, 262–276
 - Relation between space-fixed and molecule-fixed tensor components, 266–268
 - Rotation operator, 266–267
 - Taylor series expansion, 270
- Raman scattering
 - Cross section, 290–291
 - Cross section, Stokes Q-branch, 291–305
 - Depolarization ratio, 275–276
 - Example problem, 298–305
 - H₂Q(1) line, 300–302
 - Intensity formulae, 273–275
 - N₂O(6) line, 302–305
 - N₂Q-branch, 298–300
 - Polarizability, definition, 259–262
 - Scattering geometry, 259–262
- Raman transitions
 - O₂³Σ⁻ transitions, 276–290
 - Placzek–Teller coefficients, 272–273
 - Pure rotational Raman transitions, 273
 - Pure rotational tensor components, 271–273
 - Vibrational tensor components, 273
 - Vibrational transitions, 273
- Reduced matrix element, 50–51
 - Coupled angular momenta, 51
- RKR calculations
 - LEVEL code, 201
 - OH and NO X²Π-A²Σ⁺, 201–203
- Rotating wave approximation, 238
- Rotation operator, 41–45
 - Integral relations, 46–48
 - Relation with spherical harmonics, 45–48
- Russell–Saunders coupling, 16

- Schrödinger wave equation, 16
 - Cartesian coordinates, 19
 - External electromagnetic fields, 120–125
 - Separation of variables, 19–20
 - Solution atomic hydrogen, 22–26
 - Two-particle, 60
- Secular matrix
 - Doublet levels, $\Lambda > 0$, 85
 - Triplet levels, $\Lambda > 0$, 101
- Singlet electronic levels
 - $^1\Pi$ levels, 80–82
 - $^1\Sigma$ levels, 79–80
- Soft collision model, 252–253
- Speed of light, 11
- Spherical harmonics, 25–26
 - Relation with rotation operators, 45
- Spin orbital function, 137
- Spin wavefunction, 27, 137
- Spin–orbit interaction
 - Atomic hydrogen, 29
 - Calcium atom, 52–55
 - Multielectron atoms, 33
 - Spherical tensor analysis, 52–55
- Spontaneous emission
 - Angular distribution, 253–255
 - Polarization, 253–255
 - Zeeman-state dependence, 253–255
- Spontaneous emission rate coefficient, 147, 152–153, 165, 182
- Stimulated emission rate, 238–239
- Susceptibility, 6
 - Linear, 244–247, 306–309
 - Second-order, 309–311
 - Third-order, 311–317
- Symmetric top molecule wavefunction, 62–64
- Symmetry operation σ_v , 191
- Term symbol, 36
- Triplet electronic levels
 - $\Lambda > 0$, 99–109
 - $\Lambda > 0$, diagonal matrix elements, 109
 - $\Lambda > 0$, off-diagonal matrix elements, 110
- Velocity-changing collisions, 250–253
- Voigt function
 - Table of values, 399–404
- Voigt lineshape, 249–250, 257
- Wigner–Eckart theorem, 17, 52, 120, 150
 - Electric dipole transitions, 148–153
 - Reduced density matrix elements, 148–153