

# Index

---

---

- 2D exchange spectroscopy 529ff
- 2D exchange spectroscopy, experimental example 538
  - pulse sequence for 529
  - theory of 532
- 2D FT, definition of 105
- 2D INADEQUATE 431ff
- 2D INADEQUATE, experimental example 435
  - phase cycle 433
  - pulse sequence for 432
  - spectral appearance 434
  - States procedure 432
- 2D spectroscopy 92, 105ff
- 2D spectroscopy, phase-sensitive 114
  - pure absorption 109
  - pure phase 114
  - ultrafast 115
- 3D FT, definition of 114
- 3D spectroscopy 92, 114
- AA'BB' spin system, example of 464
- AA'XX' spin system, example of 464
- AB spin system, example of 464
  - form of spectrum 619
- absorption 40, 116
- absorption, stimulated 275
- abundance, natural 12
- acquisition time 76
- activation energy 523
- active spin 470, 493
- activity, kinetic 541
- adamantane 192, 217
- ADC 74ff
- adjoint of function 123
- adjoint of operator 130
- <sup>107</sup>Ag, nuclear properties of 12
- <sup>109</sup>Ag, nuclear properties of 12
  - shape of nucleus 174
- <sup>27</sup>Al 345
- <sup>27</sup>Al, nuclear properties of 12
  - quadrupole moment 207
- alphabet notation for spin systems 356, 463ff
- aluminium *see* <sup>27</sup>Al
- ammonium ion 207, 350, 455
- amplifier, for NMR signal 73
  - power 69
- amplitude, complex 94
- amplitude modulation 109
- AMX spin system, example of 467
- analogue-to-digital converter *see* ADC
- angular frequency 29, 40
- angular momentum 148ff
- angular momentum, classical 6
  - combination rule 8
  - intrinsic 7, 157
  - measurement of 232
  - orbital 7, 16, 224
  - quantization of 6
  - total 6, 500
- angular momentum operator 149ff
- angular momentum operator, cyclic commutation 143, 395, 484, 604ff
  - definition of 149
  - eigenstates and eigenvalues 152
  - matrix representation 156
  - rotation of 151
  - spin *see* spin angular momentum operator

- angular momentum operator, (*Continued*)  
 total 500  
 total square 153, 360
- anisotropic liquid 18, 443
- anisotropic liquid, AX systems in 443ff  
 chemical shift in 203  
 DD coupling in 216  
 J-coupling in 221  
 magnetically-equivalent spin pairs in 362  
 molecular motion in 187  
 motional averaging in 191  
 orientational average in 187  
 quadrupolar coupling in 209  
 spin-1 spectrum 329  
 spin-3/2 spectrum 341  
 spin-5/2 spectrum 348
- anomer 587
- anticorrelation of spin polarizations 389
- antiferromagnetism 37
- antimony *see* <sup>121</sup>Sb
- antiphase peaks 386, 428
- antiphase peaks, in 2D INADEQUATE 434  
 in COSY 416ff, 491ff  
 in INADEQUATE 423  
 in INEPT 439
- antisymmetric component of a tensor 224
- arrayed experiments 91
- Arrhenius equation 523
- arrow, double-headed, in pulse sequence diagrams 89  
 single-headed, in pulse sequence diagrams 92
- arrow, notation for coherence 262  
 notation for transition probability 550
- arsenic *see* <sup>75</sup>As
- <sup>75</sup>As 334
- assignment 409
- assignment, by 2D INADEQUATE 434  
 by COSY 409ff  
 by INADEQUATE 423  
 by TOCSY 497ff
- asymmetric unit, of crystal 225
- asymmetry parameter *see* biaxiality
- atom, structure of 15ff
- atomic number 11
- atomic orbitals 16, 154, 165
- <sup>197</sup>Au 334
- Aufbau principle 9
- aurora borealis 585
- autocorrelation function 545ff
- auto-relaxation rate constant, longitudinal 563  
 transverse 579
- average, planar 447  
 spherical 215, 447
- Avogadro constant 523
- AX spectrum 378ff
- AX spectrum, form of 366, 619  
 peak assignment 380
- AX spin system, energy levels of 364  
 example of 364  
 experiments on 409ff  
 heteronuclear 438ff, 443ff  
 homonuclear 369ff  
 meaning of 356  
 spectrum of 365, 378ff
- A<sub>3</sub>X<sub>2</sub> spin system, example of 464
- azimuthal quantum number *see* quantum number, azimuthal
- <sup>10</sup>B, nuclear properties of 12  
 spin of 14
- <sup>11</sup>B 334
- <sup>11</sup>B, nuclear properties of 12, 12  
 quadrupole moment 207
- ball, notation for population 262
- bandwidth, pulse 256  
 sampling 75
- Barnett effect 20
- baseline distortions 104
- basis, singlet-triplet 359  
 Zeeman 153
- Bax, Ad 418
- benzene, chemical equivalence in 456  
 magnetic equivalence in 458, 460
- beta-decay 10
- B** field 37
- <sup>209</sup>Bi 350
- biaxiality 224, 225, 319, 614
- biaxiality, of CSA tensor 199, 225  
 of electric field gradient tensor 208
- bicelles 444, 450
- bicycle 28, 36, 38, 241
- bilayers 445
- binomial coefficients 57
- bismuth *see* <sup>209</sup>Bi
- Bloch equations 292, 653ff
- Bloch, Felix 1, 281, 653
- block diagonal matrix 129, 612
- blood 315, 513
- Boltzmann constant 267

- Boltzmann distribution 551, 267, 292, 326, 389, 526  
 Boltzmann factor 267, 326, 390, 438, 481, 552  
 Boltzmann, Ludwig 267  
 bore of magnet 66  
 boron *see*  $^{10}\text{B}$  and  $^{11}\text{B}$   
 Bose, S. N. 20  
 boson 7  
 boson, spin-pair 527  
   vector 10  
 bounds on operator transformations 491  
 box notation, for 5-spin-1/2 system 473  
   for AMX system 470  
   for AX systems 371  
   for quadrupolar nuclei 323  
   for single spins-1/2 261  
   frequency calculation using 472  
 $^{79}\text{Br}$  334  
 $^{81}\text{Br}$  334  
 bra state 122  
 brain 315, Plates 1, 3 and 4  
 bra-ket 123, 162  
 broadening, homogeneous 298  
   induced by cross-correlation 588ff  
   inhomogeneous 48ff, 204, 298  
   motional 518ff  
 bromine *see*  $^{79}\text{Br}$  and  $^{81}\text{Br}$   
 $^{12}\text{C}$ , abundance of 418  
   composition of nucleus 11  
   mass of 17  
   nuclear properties of 12  
 $^{13}\text{C}$ , abundance of 418  
   composition of nucleus 11  
   nuclear properties of 12  
   spin of 13  
 $^{13}\text{C}$ , spin of 15  
   typical chemical shifts of 55  
 $^{14}\text{C}$ , composition of nucleus 11  
 $\text{C}_{60}$  *see* fullerene  
 caesium *see*  $^{133}\text{Cs}$   
 calcium sulfate dihydrate *see* gypsum  
 CAMELSPIN 594  
 capacitors, matching and tuning 72  
 carbon *see*  $^{12}\text{C}$ ,  $^{13}\text{C}$  and  $^{14}\text{C}$   
 Carr-Purcell echo 316  
 central transition, echo of 345  
   excitation of 343ff  
   flip angle of 344  
   for spin-3/2 337, 340  
   for spin-5/2 348  
   for spin-7/2 349  
   signal enhancement techniques 351  
 cesium *see* caesium  
 $\text{CH}_2$  protons, chemically inequivalent 457, 458, 467  
   magnetically equivalent 458  
 $\text{CH}_3$  group *see* methyl group  
 $\text{CH}_3$  protons, magnetically equivalent 458  
 channels, spectrometer 44  
 chemical bond 218  
 chemical equivalence 455ff  
 chemical equivalence, and chirality 458  
   definition of 455  
 chemical exchange 510, 516ff  
 chemical exchange, and chemical shift 203  
   and NOESY 575  
   and ROESY 582  
   coalescence point 541  
   crossover point 517  
   effect on J-couplings 59  
   experimental example 523  
   fast intermediate 520ff  
   lineshape formulae 519, 520  
   slow intermediate 518ff  
   theory 654ff  
   timescale of 511  
 chemical shift 50ff, 182, 195ff  
 chemical shift, and electronegativity 202  
   and phase transition 204  
   and secular approximation 612  
   anisotropy of *see* CSA  
   antisymmetric component 293  
   chemical exchange and 203  
   definition of 53  
   direction of scale 54  
   evolution induced by 280, 399ff, 482ff  
   field dependence 53  
   for general molecular orientation 200  
   full form of interaction 201  
   in anisotropic liquid 203  
   in isotropic liquid 201  
   in solid 204  
   influences on 202  
   isotope effects 203  
   isotropic 198  
   mechanism of 195  
   of reference frequency 54  
   ring current mechanism 203  
   temperature dependence of 525, 541  
   typical ranges 55

- chemical shift anisotropy *see* CSA
- chemical shift frequency 201
- chemical shift tensor 196
- chemical shift tensor,  
ellipsoidal representation 199
- principal axes 197, 198
- principal values 198, 224
- uniaxial 199
- chirality 458
- citric acid 458
- <sup>35</sup>Cl 334
- <sup>35</sup>Cl, J-coupling to 364, 455
- nuclear properties of 12
- <sup>37</sup>Cl 334
- <sup>37</sup>Cl, J-coupling to 364, 455
- nuclear properties of 12
- <sup>59</sup>Co, quadrupole moment 207
- <sup>59</sup>Co 349
- coalescence point 541
- cobalt *see* <sup>59</sup>Co
- cogwheel phase cycle 648
- coherence, arrow notation for 263
- assignments in AX system 380
- calculation of frequency 472
- combination 471
- decay rate constant 40
- decay time constant *see* T<sub>2</sub>
- definition of 261
- dephasing time constant *see* T<sub>2</sub>
- double-quantum *see* double-quantum coherence
- evolution of 377
- excitation of 271, 328
- helical phase pattern induced by field gradient 651
- in multiple spin-1/2 systems 471
- in rotating frame 269
- in spin-1/2 ensemble 261
- multiple-quantum *see* multiple-quantum coherence
- observable 473
- phase of 266
- physical interpretation 265
- relationship to NMR signal 287, 293, 608ff
- simple 471, 503
- single-quantum *see* single-quantum coherence
- triple-quantum 337
- zero-quantum *see* zero-quantum coherence
- coherence decay time constant 35
- coherence dephasing time constant 35
- coherence order 323, 336, 371, 632
- coherence order, change in 632
- definition of 263
- from box notation 471
- inversion by  $\pi$  pulse 303
- coherence transfer 332, 413
- coherence transfer amplitude, definition 630
- dependence on phase 631
- coherence transfer echo 652
- coherence transfer pathway 305ff, 629ff
- coherence transfer pathway, phase of 633, 651
- selection by magnetic field gradients 640, 649ff
- selection by phase cycling 634ff
- coherence transfer pathway diagram,  
for 2D exchange 529
- for COSY 629
- for double-quantum-filtered COSY 644
- for INADEQUATE 429, 630, 643, 646
- for quadrupolar echo 334
- for spin echo 305
- coherences, degenerate 473, 503
- number of 471
- coil, field gradient 79ff
- oriented at magic angle 529
- receiver/transmitter 71
- coil reaction 292
- combination coherence 471
- commutation, definition of 126
- commutation, cyclic *see* cyclic commutation
- commutator, definition of 126
- compass 27, 30, 37, 176
- complex amplitude *see* amplitude, complex
- complex conjugate 122
- complex Lorentzian *see* Lorentzian, complex
- composite pulse *see* pulse, composite
- conservation laws 148, 500
- continuous wave method 653
- contour plot 107
- Cooley, James 116
- copper *see* <sup>63</sup>Cu and <sup>65</sup>Cu
- Coriolis force 244
- correlation of spin polarizations *see* spin correlation
- correlation spectroscopy *see* COSY
- correlation time 545ff
- correlation time, critical 564, 575
- definition of 548
- rotational 556
- temperature dependence 548
- cosh function 531

- COSY, ambiguity of spectra 497  
   coherence theory 411  
   coherence transfer pathway diagram 629  
   cross peaks 414, 494  
   diagonal peaks 414, 496  
   double-quantum filtered *see* double-quantum-filtered COSY  
   experimental examples 418, 419, 420  
   in AMX systems 492  
   in AX systems 409ff  
   in multiple-spin systems 491ff  
   peakshapes in 416ff  
   product operator theory 415ff, 491ff  
   pulse sequence 411, 491  
   States procedure for 411, 417  
   unexpected cross peaks in 503  
   vanishing cross peaks in 497
- counter, cycle 90  
   transient 90
- coupling, direct dipole-dipole *see* DD coupling  
   hyperfine *see* hyperfine coupling  
   indirect dipole-dipole coupling *see* J-coupling  
   scalar *see* J-coupling, isotropic  
   strong *see* strong coupling  
   through-space dipole-dipole *see* DD coupling  
   weak *see* weak coupling
- critical correlation time 564, 575
- cross peak, definition of 414  
   in 2D exchange 530, 537  
   in COSY 414, 493  
   in NOESY 573  
   in ROESY 582  
   in TOCSY 502
- cross-correlated relaxation 584ff
- cross-correlated relaxation,  
   and product operators 405, 407  
   and unexpected COSY peaks 503  
   experimental examples 588, 589  
   linewidth effects 588ff
- cross-correlation, and Solomon equations 662  
   and transition probability 586  
   between DD couplings 585  
   DD-CSA 590ff
- cross-correlation function,  
   and interbond angle 586  
   definition 585
- crossover point 517, 520
- cross-relaxation 662
- cross-relaxation, in NOESY 573  
   longitudinal 564  
   transverse 577
- cross-relaxation rate constant, longitudinal 563  
   sign convention 594  
   transverse 579
- cryoprobe 70, 115
- crystal 19
- crystal, asymmetric unit of 203, 225  
   chemical shift in 203  
   unit cell 225
- <sup>133</sup>Cs 342, 349
- CSA 198ff, 590
- CSA, antisymmetric component 224  
   as relaxation mechanism 544  
   biaxiality of 199  
   definition of 199  
   for quadrupolar nuclei 350  
   in gas 194
- CSA-DD cross correlation, in TOCSY 497ff
- CTP diagram *see* coherence  
   transfer pathway diagram
- <sup>63</sup>Cu 334
- <sup>63</sup>Cu, nuclear properties of 12  
   quadrupole moment 207
- <sup>65</sup>Cu 334
- <sup>65</sup>Cu, nuclear properties of 12  
   quadrupole moment 207
- cycle counter 90
- cyclic commutation, and 3D rotations 138ff, 604ff  
   of angular momentum operators 143, 395, 484, 604ff  
   of product operators 401, 484
- cyclosporin 528
- DAC 79
- Dalton (Da) 17
- DAS 342, 348, 351
- data matrix 92
- DD coupling 183, 211ff, 556ff
- DD coupling, and AB spectra 620  
   and motional averaging 541  
   and relaxation 216  
   angle between pair of 586  
   between <sup>13</sup>C and <sup>1</sup>H 515  
   cross-correlated 585  
   full form of interaction 212  
   heteronuclear secular form 214, 443  
   homonuclear secular form 213, 357  
   in anisotropic liquid 216  
   in isotropic liquid 215  
   in solid 216

- DD coupling (*Continued*)  
 and AB spectra 620  
 long-range 215, 453  
 residual 443ff  
 short-range 215  
 splitting caused by 620  
 vibrationally averaged 515
- DD coupling constant 212, 362, 444, 558
- DD coupling constant, sign of 212
- DD relaxation 544, 556ff
- DD-CSA cross correlation 586  
 linewidth effects 592
- DD-DD cross correlation 585
- decay, homogeneous 35
- decoupling, heteronuclear 59ff, 91
- degeneracy 7, 131
- degeneracy, of coherences 473, 503
- demagnetizing field, nuclear 115
- density matrix *see* density operator
- density operator 259ff
- density operator, and density matrix 261  
 definition of 261  
 for AMX ensemble 470ff  
 for AX ensemble 370ff  
 for quadrupolar nuclei 321ff, 336, 347  
 in rotating frame 268  
 microscopic ambiguity of 292  
 thermal equilibrium 268, 326, 389, 481,  
 543, 551
- DEPT 504
- deshielding convention, for chemical shifts 224
- deuteration 593
- deuterium *see*  $^2\text{H}$
- diagonal, double-quantum 434
- diagonal matrix 129
- diagonal peak, definition of 414  
 in 2D exchange 530, 537  
 in COSY 414, 493, 496  
 in NOESY 573  
 in ROESY 582  
 in TOCSY 502
- diagonalization, of matrix 134ff
- diamagnetism 24, 36
- diastereotopic protons 457, 458, 467
- diffusion 77, 187ff, 512, 539ff
- diffusion, and gradient echoes 307  
 coefficient of 540  
 estimation by spin echo 303
- diffusion tensor 540
- diffusion tensor imaging *see* DTI
- digital-to-analogue converter *see* DAC
- digitization 75
- digitizer phase 76
- dihydrogen 226
- dipolar echo 363, 367
- dipole-dipole coupling 56
- Dirac notation 122
- Dirac, Paul 7, 26, 122
- direct dipole-dipole coupling *see* DD coupling
- direct product of matrices 382
- director 18, 187, 445, 446
- dispersion Lorentzian *see* Lorentzian, dispersion
- DNP 81
- DOR 342, 348, 351, 529
- double rotation *see* DOR
- double-quantum coherence 587
- double-quantum coherence, and phase shifts 449  
 evolution of 403, 433  
 for quadrupolar nuclei 323, 337  
 in AX system 371, 386  
 in INADEQUATE 427ff  
 physical interpretation 389
- double-quantum diagonal 434
- double-quantum-filtered COSY 418, 451, 497
- double-quantum-filtered COSY, coherence transfer  
 pathway diagram 644  
 phase cycle 451, 645  
 pulse sequence 451
- doublet (J-multiplet) 56, 476
- DTI 540, Plate 4
- duplexer 69
- dwelt time 75
- dynamic frequency shift 194, 225, 351
- dynamic nuclear polarization *see* DNP
- dynamic-angle spinning 342
- echo, spin *see* spin echo
- effective rotation axis, for off-resonance pulse 254
- eigenbasis, Zeeman 153
- eigenequation 131ff
- eigenfunction 131ff
- eigenfunctions, of commuting operators 132  
 of hermitian operator 132
- eigenvalue 131ff
- eigenvalues, of hermitian operator 132
- eigenvector 134
- Einstein, Albert 20, 233
- Einstein-de Haas effect 20
- electric charge, nuclear 5, 172
- electric dipole moment, vanishes for nucleus 174

- electric field 23  
 electric field gradient 175  
 electric field gradient tensor, biaxiality of 208  
     principal axes 207, 614  
     principal values 207, 225, 614  
 electric multipole moments, nuclear 173, 615  
 electric potential 173  
 electric quadrupole coupling  
     *see* quadrupole interaction  
 electric quadrupole moment, nuclear 173, 175  
     table of values 207  
     vanishes for spin-1/2 174  
 electromagnetic interaction, high-order 615  
 electron, charge of 9  
     mass of 11  
     spin of 9, 11, 16  
 electron magnetic resonance *see* EPR  
 electron paramagnetic resonance *see* EPR  
 electron spin resonance *see* EPR  
 electronic structure calculations 225  
 emission, stimulated 275  
 emission peak, discouraged nomenclature 116  
 EMR *see* EPR  
 energy, activation 523  
     conservation of 148  
     in natural units 146  
     magnetic 24, 176  
     rotational 7  
     thermal 267  
     transport in an NMR experiment 284  
 energy levels, as eigenvalues of  
     Hamiltonian 145  
     for particle in a box 145  
     for quadrupolar nuclei 321, 335, 347  
     for spin-1/2 233  
     of AMX system 468  
     of AX system 364  
     of magnetically-equivalent spin pair 360  
     of multiple spin-1/2 systems 469  
 ensemble, definition 259  
     of isolated spins-1/2 259ff  
     of multiple spin-1/2 systems 470  
     of quadrupolar nuclei 321  
     of spin pairs 355  
 entropy 283  
 EPR 37  
 equilibrium constant 525  
 equilibrium, thermal *see* thermal equilibrium  
 equivalence, chemical *see* chemical equivalence  
     magnetic *see* magnetic equivalence  
 ergodic hypothesis 186, 546  
 Ernst, Richard R. 411  
 ESR 37  
 ethanol 476, 486  
 ethanol, <sup>1</sup>H spectrum of 58  
     <sup>13</sup>C spectrum of 52, 53, 54, 58, 60, 422  
     chemical exchange in 455  
     isotopomers of 52, 418ff  
     proton spin system 468  
 ethyl chloride, chemical equivalence in 456  
     J-couplings in 455  
     magnetic equivalence in 458  
 Euler angles 599ff  
 Euler rotation matrix 601  
 evolution, free *see* free evolution  
 evolution operator *see* propagator  
 exchange, chemical *see* chemical exchange  
 excitation of coherence 328  
 expectation value 145, 260  
 exponential operator 135ff  
 exponential operator, inverse of 137  
     matrix representation of 138  
     products of 137  
 extreme narrowing 566  
  
<sup>19</sup>F, nuclear properties of 12  
     spin of 15  
 fast Fourier transform *see* FFT  
<sup>56</sup>Fe, spin of 13  
 fermion 7, 9  
 ferromagnetism 8, 26, 37  
 FFT 102, 116  
 fid 36  
 field, electric 23  
     electromagnetic 23  
     gradient *see* pulsed field gradient  
     induced *see* magnetic field, induced  
     magnetic *see* magnetic field  
     magnetic flux density *see* magnetic field  
     magnetic induction *see* magnetic field  
     radiofrequency *see* r.f. field  
 field gradient coil 79ff  
 field-frequency lock *see* lock  
 fine structure 16  
 first-order quadrupolar Hamiltonian  
     *see* quadrupolar coupling, first order  
 first-order spectra 620  
 flip angle 89, 249, 270, 327, 339, 343, 391  
 flip-flop term 358, 364  
 floor function 644  
 flow 77, 187, 303, 315, 317, 512  
 fluorine *see* <sup>19</sup>F

- flux density *see* magnetic field
- fluxional compound 538
- fMRI 315, Plate 1
- folding 116
- force particle 9
- Fourier transformation *see* FT *see* FT
- Fourier transformation, two-dimensional *see* 2D FT
- frame, rotating *see* rotating frame
- free evolution 376, 397ff, 472, 482
- free induction decay 36
- free precession, of single spin-1/2 240  
of spin-1/2 ensemble (with relaxation) 281ff  
of spin-1/2 ensemble (without relaxation) 276ff, 280  
propagator *see* propagator
- free radical 36
- frequency, angular *see* angular frequency
- chemical shift *see* chemical shift frequency
- Larmor 29ff
- nutaton *see* nutation frequency
- of rotating frame 242
- offset *see* resonance offset
- precession 29ff
- quadrupolar *see* quadrupolar coupling
- constant
- reference 45
- relative (for  $\gamma < 0$ ) 47
- relative (for  $\gamma > 0$ ) 45
- relative Larmor *see* resonance offset
- frequency axis, labelling of 46, 47, 60
- frequency labelling, of magnetization components 534
- frequency shift, dynamic 194, 351
- FT 86ff, 593
- FT, computer algorithm *see* FFT
- definition of 96
- discrete 116
- explanation of 100
- fast *see* FFT
- fullerene 19, 192, 513
- full-width-at-half-height *see* FWHH
- function, basis 124  
continuous 121  
state 143  
vector representation of 123
- functional magnetic resonance imaging *see* fMRI
- functional NMR imaging *see* fMRI
- functions, orthogonal 122  
orthonormal 122
- FWHH 98
- <sup>69</sup>Ga 334
- <sup>71</sup>Ga 334
- gallium *see* <sup>69</sup>Ga and <sup>71</sup>Ga
- gas 545
- gas, definition of 17  
diffusion in 188  
experimental spectra of 523  
motional averaging in 190  
noble, optical pumping in 81, 334  
orientational average in 187  
relaxation in 224  
spin-rotation interaction in 224
- Gauss 23
- gel 342, 444
- geology 19
- glass 19, 20
- glucose, anomers of 587  
cross-correlated relaxation in 587
- gluon 10, 20
- God 233
- gold *see* <sup>197</sup>Au
- Goudsmidt, Samuel 20
- gradient driver 79
- gradient echoes 306ff, 652ff
- gramicidin 442
- gypsum 367
- gyromagnetic ratio, definition of 26  
sign of 26  
table of values 12
- <sup>1</sup>H *see also* proton
- <sup>1</sup>H, typical chemical shifts of 55
- <sup>2</sup>H 319, 350, 351
- <sup>2</sup>H, and molecular motion 319  
as quadrupolar nucleus 175  
composition of nucleus 13  
experimental spectrum 334  
J-coupling to 455  
nuclear properties of 12  
quadrupole moment 207  
spin of 13, 13, 15  
used for lock 82
- <sup>3</sup>H, composition of nucleus 11, 11  
nuclear properties of 12
- H<sub>2</sub>O *see* water
- Hahn echo 316, 334
- Hahn, Erwin 302, 504
- halogen 334
- Hamiltonian 144

- Hamiltonian, eigenvalues of *see* energy levels  
 Hamiltonian, for particle in box 144  
   spin *see* spin Hamiltonian  
 Hartmann-Hahn transfer 504  
<sup>3</sup>He, spin of 15  
 helium, liquid 66  
 hermitian operator 131  
 hermitian operator, complex exponential of 137  
   eigenvalues of 132  
 hertz (Hz), conversion to  $\text{rads}^{-1}$  29  
   definition of 29  
 heteronuclear AX system 438ff, 443ff  
 heteronuclear decoupling 59ff, 463, 463, 465  
 heteronuclear experiments 90  
 heteronuclear multiple-quantum coherence  
   *see* HMQC  
 heteronuclear spin system 462  
**H** field 37  
 high-field approximation 390  
 high-temperature approximation 268, 389  
 HMQC 450  
 HMQC, pulse sequence 451  
<sup>165</sup>Ho 349  
 HOHAHA *see* TOCSY, *see* TOCSY  
 holmium *see* <sup>165</sup>Ho  
 homogeneous broadening  
   *see* broadening, homogeneous  
 homogeneous decay *see* decay, homogeneous  
 homonuclear AX system 369ff  
 homonuclear spin system *see* spin system, homonuclear  
 hydride, metal 226  
 hydrogen, isotopes of *see* proton, deuterium  
   and tritium  
   molecular *see* dihydrogen  
 hydrogen bond 218  
 hydrogen molecule 226  
 hyperfine coupling 16, 222, 525  
 hyperfine structure 16  
<sup>127</sup>I 345  
 imaging, NMR *see* MRI  
<sup>115</sup>In 350  
 INADEQUATE 418ff  
 INADEQUATE, 2D *see* 2D INADEQUATE  
   acronym 418  
   coherence transfer pathway 429ff  
   coherence transfer pathway diagram 630, 643,  
   646  
   experimental example 422  
   in cross-correlated relaxation experiment 587  
   low sensitivity of 436  
   phase cycle 424, 643, 648  
   product operator theory 424ff  
   pulse sequence 423  
   spectral appearance 429  
 indeterminacy, quantum 145, 232  
 indirect dipole-dipole coupling *see* J-coupling  
 indium *see* <sup>115</sup>In  
 INEPT 436ff, 488ff, 570  
 INEPT, acronym 437  
   experimental example 440  
   in I<sub>2</sub>S systems 488ff  
   in I<sub>3</sub>S systems 490  
   meaning of word 449  
   product operator theory for 438ff  
   pulse sequence 437  
   refocussed *see* refocussed INEPT  
   spectral appearance 439  
 inhomogeneous broadening 48ff, 204, 345  
 initial rate regime 532  
 in-phase multiplet 385  
 insulator, electric 19  
 interaction, cross-correlated 585  
   electromagnetic 172  
   intermolecular 189  
   intramolecular 189  
   long-range intermolecular 189, 291  
   non-secular *see* spin Hamiltonian, non-secular  
   nuclear exchange 226  
   quadrupolar *see* quadrupolar coupling  
   short-range intermolecular 189  
   spin-rotation 183  
   Zeeman 179  
 interbond angle, and cross-correlated relaxation  
   590  
   and J-coupling 221  
 intermolecular interaction  
   *see* interaction, intermolecular  
 internal molecular motion  
   *see* molecular motion, internal  
 interval, mixing *see* mixing interval  
   sampling *see* sampling interval  
   waiting *see* waiting interval  
 intramolecular interaction  
   *see* interaction, intramolecular  
 intrinsic quadrupole moment 193  
 inverse of operator 130  
 inversion-recovery 295ff  
 iodine *see* <sup>127</sup>I

- ion 16
- $^{191}\text{Ir}$  334
- $^{193}\text{Ir}$  334
- iridium *see*  $^{191}\text{Ir}$  and  $^{193}\text{Ir}$
- iron 37
- iron *see*  $^{56}\text{Fe}$
- isotope shift, primary 225
  - secondary 203
- isotopes, 11ff
  - abundance of 11
  - radioactive 11
  - stable 11
  - table of properties 12
- isotopic enrichment 17
- isotopomers 16, 42ff, 418ff, 454
- isotopomers, abundance calculation 43, 421
  - number of 423
  - separation of 17
- isotropic average 187, 201
- isotropic chemical shift *see* chemical shift, isotropic
- isotropic J-coupling *see* J-coupling, isotropic
- isotropic liquid 18
- isotropic liquid, chemical shift in 201
  - DD coupling in 215
  - J-coupling in 219
  - motional averaging in 190
  - orientational average in 187
  - quadrupolar relaxation in 209
  - quadrupole coupling in 209
  - spectrum of magnetically-equivalent spin pairs
    - 362
    - spin-1 spectrum 329
    - spin-3/2 spectrum 341
    - spin-5/2 spectrum 348
  - spin-rotation interaction in 223
- J-anisotropy 221, 226
- J-coupling 51, 183, 217ff, 523
- J-coupling, and hydrogen bond 218
  - and interbond angle 221
  - and magnetic equivalence 621ff
  - and multiple-quantum evolution 403
  - and peak assignment 380
  - and quadrupolar nuclei 364
  - and secular approximation 613
  - and torsional angle 220
  - $^{13}\text{C} - ^{13}\text{C}$  221, 421, 423
  - $^{13}\text{C} - ^1\text{H}$  221, 406
  - evolution caused by 483
  - evolution induced by 400ff
  - exchange contribution 226
  - full form of interaction 218
  - $^1\text{H} - ^1\text{H}$  221, 406
  - heteronuclear secular form 219
  - homonuclear secular form 219
  - in anisotropic liquid 221
  - in isotropic liquid 219
  - in solid 221
  - isotropic 219
  - Karplus relationship 221
  - long-range 55
  - mechanism of 222ff
  - motinally suppressed 364, 454ff
  - multiplets caused by 56ff
  - $^{15}\text{C} - ^1\text{H}$  437
  - notation 55
  - sign of 220
  - tensor 218
- Jeener, Jean 411
- $^{39}\text{K}$  334
- $^{40}\text{K}$  14
- Karplus relationship 221
- ket state 122
- ket-bra 162
- kilodalton (kDa) 17
- kinetic energy operator 144
- k-jargon 75
- Knight shift 51, 525
- $^{83}\text{Kr}$  350
- Kronecker delta 122
- krypton *see*  $^{83}\text{Kr}$
- $^{139}\text{La}$  349
- laboratory frame 179, 603
- lanthanum *see*  $^{139}\text{La}$
- Larmor frequency 29ff, 201, 453
- Larmor timescale 513
- laser 275
- Lauterbur, Paul 49, 309
- lead *see*  $^{207}\text{Pb}$
- leakage rate constant
  - see* auto-relaxation rate constant
- lepton 9
- $^6\text{Li}$  319
- $^6\text{Li}$ , quadrupole moment 207
  - spin of 13
- $^7\text{Li}$  319, 334
- $^7\text{Li}$ , quadrupole moment 207

- libration 509, 541
- linear prediction 102
- linear regime 257
- linear spin system 464, 476, 497, 498
- lineshape, motional *see* motional lineshape
- linewidth 98
- linewidth, cross-correlation effects 497ff, 590ff
  - definition 40
  - relationship to  $T_2$  40, 288
- lipids 445, 450
- liquid, anisotropic *see* anisotropic liquid
  - definition of 17
  - isotropic *see* isotropic liquid
  - weakly oriented 443ff
- liquid crystal, *see* anisotropic liquid
- lithium *see*  $^6\text{Li}$  and  $^7\text{Li}$
- lock, field-frequency 82, 350
- longitudinal, meaning of 32
- longitudinal cross-relaxation *see* cross-relaxation, longitudinal
- longitudinal magnetization *see* magnetization, longitudinal
- longitudinal magnetization, exchange of 529ff
- longitudinal relaxation 30ff, 283, 543, 552, 564ff
- long-lived spin states 540, 593
- Lorentzian, absorption (1D) 40, 97
  - absorption (2D) 109
  - complex (1D) 97
  - complex (2D) 107
  - dispersion (1D) 97, 116
- low-field/high-field notation, recommendation
  - against 56, 60
- $^{176}\text{Lu}$ , spin of 15
- lungs 513
  
- magic angle 214, 527
- magic-angle spinning *see* MAS
- magnesium *see*  $^{25}\text{Mg}$
- magnet 65ff
- magnet, bore of 66
  - physical construction 65
  - superconducting 65
- magnetic constant 24
- magnetic equivalence 366, 458ff, 619, 621ff
- magnetic equivalence, and degeneracy 476
  - and J-coupling 459
  - and multiplet structure 59
  - consequences of 459
  - definition 458
- magnetic field 23
  - magnetic field, external 177
    - gradient *see* pulsed field gradient
    - induced 195
    - radiofrequency 178
    - static 177
  - magnetic field gradient *see* pulsed field gradient
  - magnetic field homogeneity 65
  - magnetic flux density field 37
  - magnetic induction field 37
  - magnetic moment 23
  - magnetic resonance imaging *see* MRI
  - magnetic susceptibility *see* susceptibility, magnetic
  - magnetism, electronic 36ff
    - induced 24
    - intrinsic 25
    - macroscopic 23
    - microscopic 25
    - permanent 24
  - magnetization, longitudinal 32, 270
    - steady state 653
    - transverse 33ff, 270
  - magnetization exchange, longitudinal 529ff, 658
  - magnetization helix 307
  - magnetization vector 269ff
  - magnetization vector, relaxation of 285
    - trajectory of 285
  - magnetoencephalography Plate 3
  - magnetogyric ratio *see* gyromagnetic ratio
  - manganese *see*  $^{55}\text{Mn}$  and  $^{57}\text{Mn}$
  - Mansfield, Peter 49, 309
  - Markov process 655
  - married couples 388, 389
  - MAS 178, 226, 527ff
  - MAS, experimental example 528
    - multiple-quantum *see* MQ-MAS
    - satellite transition *see* ST-MAS
  - mass, molecular 17
  - mass number 11
  - mass of nucleus 5
  - matched weighting 115
  - matrix, block diagonal 129, 612
    - diagonal 129
    - trace of 159
    - traceless 159
  - matrix element 127
  - matrix representation 127
  - matter, states of 17ff
  - maximum entropy 102
  - Maxwell equations 23, 36, 38
  - mechanical detection of NMR 82

- megahertz (MHz) 29  
 Meissner effect 541  
 meson 20  
 metabolites 315  
 metal 19, 526  
 metal, alkali 334  
 metal hydride 226  
 meteorite 37  
 methyl group, rotation of 19, 510  
 $^{25}\text{Mg}$  345  
 microwave 81  
 mineral 513  
 mixer, r.f. 609  
 mixing interval, in 2D exchange 530  
   in NOESY 571  
   in ROESY 580  
   in TOCSY 499  
 mixing time *see* mixing interval  
 $^{55}\text{Mn}$  345  
 $^{55}\text{Mn}$ , quadrupole moment 207  
 molecular motion 186, 509ff  
 molecular motion, in anisotropic liquid 18, 187  
   in gas 187  
   in isotropic liquid 18, 187  
   in polymers 306  
   in proteins 510, Plate 2  
   in solid 19, 187  
   internal 19, 186, 331, 331  
   translational 512  
 molecular rotation 18, 186, 511  
 molecular rotation, and DD relaxation 556ff  
   effect of temperature 511  
   effect of viscosity 511  
   rough estimate of timescale 511  
 molecular spin system *see* spin system  
 molecular structure determination, by  
   cross-correlated relaxation 590  
   by NOESY 576, Plates 2 and 5  
   by residual DD couplings 443  
   by ROESY 582  
 molecular translation 186, 187, 512  
 molecule, structure of 16ff  
 Mössbauer spectroscopy 20  
 motion 509ff  
 motional averaging 71, 185, 186ff, 515ff  
 motional broadening 518ff  
 motional lineshapes 516ff, 516ff  
 motional narrowing 520ff  
 motional processes 509ff  
 motional regime 517, 522, 539  
 MQ-MAS 342, 348  
 MRI, basic explanation 50ff  
   functional *see* fMRI  
   image generated by Plates 1, 3 and 4  
   more detailed explanation 309ff  
   pulse sequence for 312, 313  
 multiple-quantum coherence, heteronuclear  
   *see* HMQC  
   in AX system 371  
 multiple-quantum MAS *see* MQ-MAS  
 multiplet, antiphase 386  
   cross-peak *see* cross-peak multiplet  
   in-phase 385  
   spectral 53ff  
 multipole, electric *see* electric multipole  
 $^{14}\text{N}$  319, 350  
 $^{14}\text{N}$ , difficulty of NMR 319  
   J-coupling to 455  
   nuclear properties of 12  
   quadrupole moment 207  
   spin of 14, 15  
 $^{15}\text{N}$ , nuclear properties of 12  
   sense of precession 29  
   sensitivity enhancement of 436ff  
   spin of 15  
   typical chemical shifts of 55  
   typical CSA of 594  
 $^{23}\text{Na}$  334  
 $^{23}\text{Na}$ , nuclear properties of 12  
   quadrupole moment 207  
   spectrum of 342  
 natural abundance, table of values 12  
 natural units 146  
 $^{93}\text{Nb}$ , magnetic moment 350  
   quadrupole moment 207  
   spin of 350  
 $^{21}\text{Ne}$  334  
 neon *see*  $^{21}\text{Ne}$   
 nerves, tracing by DTI 540  
 nested phase cycle 644  
 neutron, mass of 11  
   spin of 10, 11  
   structure of 10  
 Newman projection 456  
 $\text{NH}_3^+$ , rotation of 510  
 $\text{NH}_4^+$  *see* ammonium ion  
 niobium *see*  $^{93}\text{Nb}$   
 nitrogen, isotopes of *see*  $^{14}\text{N}$  and  $^{15}\text{N}$   
   liquid 66

- NMR, discovery of 1  
 Fourier transform 85ff  
 range of 1
- NMR imaging *see* MRI
- NMR imaging, functional *see* fMRI
- NMR quantum computing 503
- NMR signal 36ff
- NMR signal, and quadrature detection 287, 608ff  
 complex 74  
 factors influencing strength of 436  
 general form of 93  
 reasons for its weakness 65  
 relationship to coherence 287, 293, 608ff
- NMR spectrometer 65ff
- NMR spectrum 96ff
- NMR spectrum, first-order 620  
 second-order 620
- NMR tube 71
- NO (nitric oxide) 16
- Nobel prize 1, 49, 309, 411, 576
- noble gas 81, 194, 334
- NOE 60, 91, 423, 424
- NOE, enhancement factor 424, 427, 569, 594  
 for  $^{13}\text{C}$  569  
 for  $^{15}\text{N}$  569  
 theory of 566ff
- NOESY 443, 570ff
- NOESY, and chemical exchange 575  
 and molecular structure determination 576,  
 Plate 5  
 diagonal and cross peak amplitudes 572  
 distance dependence of cross peaks 576  
 experimental example 576, Plate 5  
 pulse sequence 570  
 sign of cross peaks 573, 594
- noise, frequency dependence of 436  
 origins of 86  
 root-mean-square (rms) 87  
 stationary 87  
 suppression of 87  
 uncorrelated 87
- non-linear regime 257
- normalization 122, 143
- northern lights 585
- nuclear demagnetizing field 115
- nuclear electric moment, high-order 193
- nuclear exchange interaction 226
- nuclear force, strong 10  
 weak 10
- nuclear magnetic resonance *see* NMR
- nuclear Overhauser effect *see* NOE
- nuclear spin 12ff
- nuclear spin, ground state 13  
 of all isotopes Plates A, B, C  
 table of values 12
- nucleon 11
- nucleus, properties of 5  
 quadrupolar *see* quadrupolar nucleus  
 structure of 11ff
- null operator 126  
 exponential of 136
- number of sampling points, jargon for 75
- notation, meaning of 251
- nutaton frequency 181, 248, 251, 256, 270, 327, 339,  
 343, 391, 578
- nutaton frequency, central-transition 344, 348,  
 349
- $^{16}\text{O}$ , nuclear properties of 12  
 spin of 13
- $^{17}\text{O}$  345
- $^{17}\text{O}$ , experimental example 349  
 nuclear properties of 12  
 quadrupole moment 207  
 spin of 15  
 typical chemical shifts of 55
- observation in quantum mechanics 144ff, 232
- ocean currents 244
- off-resonance effects 253
- offset, resonance *see* resonance offset
- oil 513
- operator 124ff  
 adjoint of 130
- operator, angular momentum *see* angular  
 momentum operator
- operator complex exponential of 137
- operator, density *see* density operator
- exponential 135ff  
 exponential of small 137  
 hermitian 131  
 inverse of 130  
 kinetic energy 144  
 magnetic moment 176  
 matrix representation of 127  
 null 126  
 polarization *see* projection operator  
 potential energy 144  
 power of 135  
 product *see* product operator

- operator, (*Continued*)  
 density *see* density operator  
 projection 165  
 rotation *see* rotation operator  
 shift *see* shift operator  
 statistical 292  
 trace of 159, 159  
 traceless 159  
 unitary 131  
 unity 126
- operator transformations, bounds on 491  
 for isolated spins-1/2 279ff
- optical detection 82
- optical pumping 20, 81
- orbital angular momentum *see* angular momentum, orbital
- orbitals, atomic *see* atomic orbitals
- order of coherence *see* coherence order
- orientation transfer 445
- orienting media 444
- orthogonal 122
- orthonormal 122
- oscillator, electromagnetic 72  
 mechanical 82
- Overhauser, Albert 566
- Overhauser effect, steady state 566ff
- oversampling 82
- overtone 193, 225, 350
- oxygen *see*  $^{16}\text{O}$  and  $^{17}\text{O}$
- oxygen, molecular 16
- $^{31}\text{P}$ , nuclear properties of 12  
 typical chemical shifts of 55
- Pake, George 329
- Pake pattern 329, 330, 341, 362, 367
- parahydrogen 81, 226
- paramagnetic shift 51, 527
- paramagnetism 32, 24, 37
- parity conservation 193
- parts per million *see* ppm
- passive rotations 602
- passive spin 470, 493
- pathway phase, for coherence transfer 632
- Pauli principle 9, 16, 20, 36, 222
- Pauli, Wolfgang 20
- $^{207}\text{Pb}$ , nuclear properties of 12  
 typical chemical shift range of 202
- peak amplitude, general formula 618, 620
- peakwidth *see* linewidth
- Penrose, Roger 350
- perturbation theory, time-independent 613
- phase, digitizer 76, *see* digitizer phase  
 jargon for 69  
 of coherence transfer pathway 633, 651  
 of quantum state 147  
 of signal component 94  
 post-digitization 76  
 radiofrequency 68  
 receiver 76
- phase correction, frequency-dependent 103
- phase cycle, cogwheel 648  
 counter for 90  
 for 2D exchange 530  
 for 2D INADEQUATE 433  
 for double-quantum-filtered COSY, 645  
 for INADEQUATE 424, 643, 648  
 for ROESY 581  
 for spin echo 90  
 general construction procedure 637  
 nested 644
- phase cycling 629ff
- phase cycling, and States procedure 640  
 and thermal equilibrium terms 571  
 introduction 89
- phase factor 236
- phase of matter 17ff
- phase shift, radio-frequency 67  
 sign of 82, 450  
 signal 76, 82  
 spectral 102
- phase transition, and chemical shift 204  
 and quadrupolar coupling 210
- phase twist 107
- phosphorus *see*  $^{31}\text{P}$
- photon 10  
 spin of 11
- Planck constant 6, 144
- plastic crystal 192, 204, 217
- plot, contour 107  
 surface 107
- polarization operator 162, 166
- polarization transfer 437
- polarized light, rotation of 82
- poly(methylmethacrylate) 334
- polymers 306
- population, definition of 261  
 for spin-1 322  
 for spin-3/2 336  
 fractional 292  
 in rotating frame 269

- population, (*Continued*)  
  in thermal equilibrium 267  
  of multiple spin-1/2 systems 471  
  of spin-1/2 ensemble 261  
  physical interpretation 264  
population inversion 273  
population vector 660  
post-digitization phase 76  
potassium *see*  $^{39}\text{K}$  and  $^{40}\text{K}$   
potential energy operator 144  
powder 204  
powder, spectrum of magnetically-equivalent spin pairs 362  
  spin-1 spectrum 329  
  spin-3/2 spectrum 341  
  spin-5/2 spectrum 348  
powder pattern 204  
powder pattern, experimental example 206  
  for spin-1 329, 330  
ppm, meaning of 54, 60  
preamplifier, signal 73  
precession, qualitative picture 26ff  
  quantum derivation 240  
  sense of 29, 38, 41  
precession frequency 29ff  
precession in rotating frame 245  
  sense of 246  
pre-exponential factor, in Arrhenius equation 523  
principal axes 197, 614  
principal values 198, 614  
probability density 187  
probe 70ff  
probe, tuning the 72  
product, direct *see* direct product  
product operator 381ff, 477  
product operator, and cyclic commutation 401  
  and populations/coherences 383  
  and spectral appearance 479  
  and spin correlations 389  
  chemical shift evolution 399ff, 482  
  commutation 403  
  construction of 382, 477  
  free evolution of 397ff  
  J-coupling evolution 400ff, 483  
  physical interpretation 386ff, 480  
  relaxation of 405  
  rotation of 391ff, 481  
product state, Zeeman 356, 370  
projection operator, ket-bra notation 162  
  meaning of 165  
  spin-1/2 162  
propagator, chemical shift 398  
  for off-resonance pulse 255  
  for on-resonance pulse 252  
  free evolution 377  
  J-coupling 398  
  pulse 249  
  spin echo sandwich 406  
protein, COSY spectrum of 420  
  degeneracy of coherences 473  
  molecular motion in 510, Plate 2  
  NOESY spectrum of 576  
  residual dipolar couplings in 448  
  rotational diffusion of 17  
  spectrum of 448  
  structure of 2, Plates 2 and 5  
  typical 1D spectrum 95  
proton *see also*  $^1\text{H}$   
proton, charge of 10, 11  
  mass of 11  
  nuclear properties of 12, 12  
  spin of 10, 11  
  structure of 10  
protons, diastereotopic 457, 458, 467  
pulse, bandwidth of 256, 257  
  composite 294  
  duration of 89  
  flip angle 89  
  frequency-selective 257, 308  
  generation of 68  
  icon 39  
  notation for 89  
  of general phase 252  
  on AX ensemble 391ff  
  on quadrupolar nuclei 326ff, 339ff, 343ff, 348, 349  
  on single spin-1/2 247ff  
  on spin-1/2 ensemble 270, 279  
  phase of 68  
  propagator of 249  
  qualitative picture 34  
  rectangular 68, 257  
  shaped 257, 308  
  strong 256  
  weak 256, 257  
pulse flip angle *see* flip angle  
pulse gate 68  
pulse programmer 67  
pulse sequence, 2D 92  
  2D exchange 529  
  2D INADEQUATE 432  
  2QF-COSY 451

- pulse sequence (*Continued*)
- 3D 92
  - arrayed 91
  - COSY 91
  - DEPT 505
  - for COSY 411
  - for MRI 312, 315
  - for refocussed INEPT 488
  - gradient echo 306
  - heteronuclear 90
  - HMQC 451
  - INADEQUATE 423
  - INEPT 437
  - inversion-recovery 295
  - NOESY 570
  - pulsed field gradient 91
  - quadrupolar echo 331
  - refocussed INEPT 441
  - ROESY 580
  - slice selection 308
  - spin echo 89, 299
  - spin-locking 305
  - stimulated echo 91
  - TOCSY 499
  - two-dimensional 92
- pulse width 68
- pulsed field gradient, and coherence transfer
- pathway selection 649ff
  - hardware 77ff
  - in diffusion experiments 540
  - in MRI 309ff
- Purcell, Edward 1, 316
- pure absorption 2D spectroscopy 109
- quadrature detection 74, 287ff, 608ff
- quadrature detection, in the second dimension 114
- quadrature image 292
- quadrature receiver *see* receiver, quadrature
- quadrupolar coupling 182, 206ff, 319, 614ff
- quadrupolar coupling, biaxiality of tensor 319, 331
- first-order *see* quadrupolar interaction, first order
  - for spin-1 321
  - for spin-3/2 335
  - for spin-5/2 346
  - in anisotropic liquid 209
  - in isotropic liquid 209
  - in solid 210
  - second-order *see* quadrupolar interaction, second order
- quadrupolar coupling constant 210, 225, 321, 346
- quadrupolar echo 331ff, 351
- quadrupolar interaction, first-order 321, 335, 346, 361, 615
- full form 208, 614
  - second-order 208, 225, 348, 615
  - third-order 208
- quadrupolar nuclei 175, 319ff
- quadrupolar nuclei, half-integer spin 15, Plate C
- integer spin 15, Plate B
- J-couplings involving 364, 455
  - relaxation 455
- quadrupolar relaxation 364, 545
- quadrupolar shift, second-order 351
- quadrupole moment, nuclear 193, 614
- quantum chemistry 225
- quantum computing, by NMR 503
- quantum electrodynamics 26
- quantum indeterminacy 145, 232
- quantum mechanics, relativistic 7
- spinless 143ff
  - statistical 267
- quantum number, azimuthal 7, 153, 158
- nuclear spin 11
  - projection 153
- quark 10, 20
- quartet (J-multiplet) 56, 477
- quintet (J-multiplet) 56
- r.f. field 179
- r.f. field, inhomogeneity of 294
- longitudinal component 180, 193
  - non-resonant component 180, 193, 257
  - resonant component 180
  - rotating 180, 194
- r.f. phase 68
- r.f. pulse *see* pulse
- r.f. synthesizer *see* synthesizer
- radiation damping 115, 292
- radical, free 36
- radical pairs, photoinduced 81
- radio receiver 74
- radio-frequency *see* r.f.
- rad  $s^{-1}$ , conversion to Hz 29
- random field, spin-dependent 552
- spin-independent 547
  - stationary 547
- random field relaxation *see* relaxation, random field

- rate constant, auto-relaxation *see*
  - auto-relaxation rate constant
  - coherence decay *see*
  - coherence decay rate constant
  - cross-relaxation *see*
  - cross-relaxation rate constant
  - for chemical exchange 516
  - leakage *see* auto-relaxation rate constant
- <sup>87</sup>Rb 334
- <sup>87</sup>Rb, quadrupole moment 207
- <sup>185</sup>Re 345
- <sup>187</sup>Re 345
- receiver, quadrature 73
- receiver artefact *see* quadrature image
- receiver phase *see* phase, receiver
- receiver phase, hardware limitations 640
- receiver section 72
- reference frame, laboratory *see* laboratory frame
  - orientation of 601
  - rotating *see* rotating frame
  - transformations of 599ff
- reference frequency 45
- reference frequency, chemical shift of 54
- refocussed INEPT 440
- refocussed INEPT, experimental example 440, 442
  - pulse sequence 441
- refocussing 302ff
- relative frequency *see* frequency, relative
- relative Larmor frequency 245
- relative Larmor frequency, definition of 46
  - generation in receiver 73
- relaxation 185, 543ff
- relaxation, and spin Hamiltonian hypothesis 193
  - by CSA 544
  - by DD coupling 544, 556ff
  - by quadrupole coupling *see*
    - quadrupolar relaxation
  - by spin-rotation interaction *see*
    - spin-rotation relaxation
  - cross-correlated *see* cross-correlated relaxation
  - longitudinal *see* longitudinal relaxation
  - mechanisms of 543
  - of heteronuclear systems 449
  - of many-spin systems 485
  - quadrupolar *see* quadrupolar relaxation
  - random field 545ff
  - spin-lattice *see* longitudinal relaxation
  - spin-rotation 545
  - spin-spin *see* transverse relaxation
  - transverse *see* transverse relaxation
- relaxation agent, paramagnetic 422
- relaxation time constant, for coherence decay 35
  - longitudinal *see* T<sub>1</sub>
  - spin-lattice *see* T<sub>1</sub>
  - spin-spin *see* T<sub>2</sub>
  - transverse *see* T<sub>2</sub>
- relaxation timescale 514
- residual DD coupling 443ff
- residual DD coupling, experimental example 448
- resonance offset 46, 245
- rest mass 11
- rhenium *see* <sup>185</sup>Re and <sup>187</sup>Re
- rhombicity *see* biaxiality
- ring-current shift 203
- ROESY 443, 577ff
- ROESY, and chemical exchange 582
  - and molecular structure determination 582
  - and TOCSY 583
  - diagonal and cross peak amplitudes 582
  - pulse sequence 580
  - sign of cross peaks 582
- rotating frame 241, 375ff
- rotating frame, experiment in 594
  - phase convention 244
  - phase of 244
  - precession in 245
  - spin Hamiltonian in 244
  - spin state in 243
- rotation, hindered 510
  - mechanical 70, *see also* MAS, DOR
  - molecular *see* molecular rotation
  - of the earth 244
  - passive 602
- rotation axis, effective 254
- rotation operator, definition 150
  - spin *see* spin rotation operator
- rotation sandwich 151, 605ff
- rotational constant, molecular 7
- rotational correlation time 556, 593
- rotational energy 7
- rubidium *see* <sup>87</sup>Rb
- <sup>32</sup>S, spin of 14
- sampling bandwidth 75
- sampling interval 75
- sampling points, jargon for 75
- sandwich formula *see* cyclic commutation
- satellite order 323, 332, 334, 336, 347, 350, 351
- satellite peak 367, 422
- satellite transition 340, 351

- satellite-transition MAS *see* ST-MAS
- saturation 567, 594, 653
- $^{121}\text{Sb}$  345
- $^{45}\text{Sc}$ , quadrupole moment 207
- $^{45}\text{Sc}$  349
- scalar coupling *see* J-coupling, isotropic
- scandium *see*  $^{45}\text{Sc}$
- Schrödinger equation in rotating frame 243
- Schrödinger equation, time-dependent 144, 238  
time-independent 146
- second-order quadrupolar coupling *see* quadrupolar interaction, second order
- second-order spectra 620
- secular approximation 185, 462, 611ff
- semiconductor 334, 526
- semi-metal 334
- sense of precession 30, 38
- sensitivity, field dependence of 436  
isotope dependence of 436  
methods for enhancing 81  
of INADEQUATE 436
- SES *see* spin echo sandwich
- shielding, chemical *see* chemical shift
- shielding convention 224
- shift, chemical *see* chemical shift  
Knight *see* Knight shift  
paramagnetic *see* paramagnetic shift  
ring current *see* ring current shift
- shift operator, definition 154  
ket-bra notation 162  
matrix representation 154  
spin-1/2 161
- shift reagent, paramagnetic 527
- shim, meaning of word 82  
room-temperature 66  
superconducting 66
- shoe 167
- $^{28}\text{Si}$ , natural abundance of 43
- $^{29}\text{Si}$ , natural abundance of 43  
nuclear properties of 12  
sense of precession 29
- $^{30}\text{Si}$ , natural abundance of 43
- signal amplitude, and (-1)-quantum coherence 288
- signal averaging 86
- signal pathway *see* coherence transfer pathway
- signal surface, two-dimensional 105
- signal-to-noise ratio 88
- silicon *see*  $^{28}\text{Si}$ ,  $^{29}\text{Si}$  and  $^{30}\text{Si}$
- silver *see*  $^{107}\text{Ag}$  and  $^{109}\text{Ag}$
- simple coherence 471, 503
- singlet (non-split peak) 56
- singlet state 366, 9, 359
- singlet-triplet basis 359
- sinh function 531
- slice selection 307ff
- soap film 18
- sodium *see*  $^{23}\text{Na}$
- solid, amorphous 19  
chemical shift in 204  
DD coupling 216  
definition of 19  
diffusion in 188  
J-coupling 221  
mechanical rotation of 513  
molecular 19  
motional averaging in 191  
non-molecular 19  
quadrupole coupling in 210  
spin-rotation interaction in 224
- solid echo 367
- Solomon equations 660ff
- Solomon equations, and cross-correlation 662  
generalized 662  
longitudinal 561ff  
transverse 578
- spectral density 548ff
- spectral density, at the Larmor frequency 558  
at twice the Larmor frequency 558, 560ff  
at zero frequency 559  
normalized 549
- spectral timescale 514
- spectral width *see* bandwidth, sampling
- spectrometer, NMR 65ff
- spectrometer channels 44
- spectroscopy, three-dimensional *see* 3D spectroscopy  
two-dimensional *see* 2D spectroscopy
- spectrum, definition of 97  
of AX system 365  
phase-corrected 104  
simple example 40  
two-dimensional 106, *see* 2D spectroscopy
- spherical harmonic 154, 593
- spherical tensor operator, irreducible 615
- spin 157ff
- spin, active *see* active spin  
concept of 5ff  
nuclear 11, Plates A, B, C  
passive *see* passive spin
- spin angular momentum operator 157

- spin angular momentum operator,
  - cyclic commutation of 157
  - eigenequation of 158
  - matrix representation of 160
- spin correlation, and product operators 387, 480
  - creation and destruction 389, 401, 407
- spin coupling topology 464
- spin density distribution 50, 311
- spin density matrix *see* density matrix
- spin density operator *see* density operator
- spin echo 298ff
- spin echo, Carr-Purcell type 316
  - coherence interpretation 303
  - coherence transfer 652
  - coherence transfer pathway 305
  - dipolar 363, 367
  - Hahn type 316, 334, 345
  - induced by gradient reversal 306
  - of central transition 345
  - phase cycle 90
  - pulse sequence 89, 299
  - quadrupolar 331ff, 351
  - solid 367
  - stimulated 91, 539
  - Zeeman 351
- spin echo sandwich 405ff, 485, 623ff
- spin echo sandwich, heteronuclear 437, 627
  - in INADEQUATE 424
  - in INEPT 437
  - in refocussed INEPT 441
  - long duration limit 625
  - short duration limit 625
- spin ensemble 454, *see* ensemble
- spin Hamiltonian 171ff
- spin Hamiltonian, diagonal part 358
  - during pulse 248
  - electric 173
  - flip-flop term 358
  - for gradient field 181
  - hypothesis 171, 193
  - in rotating frame 244, 247
  - internal 182ff
  - magnetic 173
  - motional averaging of 516
  - of AB system 615
  - of AX system 369
  - off-diagonal part 358
  - secular 185
  - transverse part 181
  - with heteronuclear decoupling 463, 465
- spin interaction, external 177
  - internal 177
- spin locking 305ff, 316, 578, 581
- spin pair, Hamiltonian of 357, 615
  - heteronuclear 355, 366
  - homonuclear 355, 615
  - magnetically equivalent 359ff, 619
  - rotations of 392
  - strongly-coupled 356, 615ff
  - superposition state of 356
  - weakly-coupled 356, 363ff, 619ff
- spin polarization, arrow symbol 231, 238
  - axis of 26
- spin precession *see* precession
- spin quantum number 11
- spin rotation operator 158, 606ff
- spin rotation operator, sandwich formula 158
- spin state, in rotating frame 243
  - long-lived 366, 540, 593
- spin state, arrow symbol 231, 238
- spin system, heteronuclear 453, 462
  - homonuclear 453
  - linear 464, 476, 497, 498
  - molecular 453
- spin-1 319ff
- spin-1, angular momentum operator 163
  - coherence 322
  - density matrix of 321
  - eigenstates of 319
  - energy levels 320
  - method of depicting state 350
  - population 322
  - rotation operator 163
  - superposition state of 320
- spin-1/2 15, 231ff, Plate A
- spin-1/2, angular momentum operator 160
  - ensemble 259ff
  - general state of 234
  - pairs of 355ff
  - polarization operator 162
  - projection operator 162
  - rotation operator 160, 606ff
  - shift operator 161
  - superposition state of 234
  - unity operator 161
  - Zeeman eigenstate of 160
- spin-3/2 334ff
- spin-3/2, angular momentum operator 163
  - arrow notation for state 350
  - coherence 336

- spin-3/2, (*Continued*)  
 density matrix of 336  
 eigenstates of 335  
 energy levels 335  
 population 336  
 spectrum of 340
- spin-5/2 345ff  
 spin-5/2, angular momentum operator 165  
 density matrix of 347  
 eigenstates of 346  
 energy levels 346  
 spectrum of 348
- spin-7/2, energy levels 349  
 spectrum of 349
- spin-7/2 349ff  
 spin-9/2 350  
 spin-down 232  
 spin-lattice relaxation 543, 552ff  
 spin-lattice relaxation, in rotating frame 306, 316  
 spin-lattice relaxation time constant *see*  $T_1$   
 spinning sideband 528  
 spinor 165  
 spin-rotation interaction 183, 223, 226, 545  
 spin-rotation relaxation 545  
 spin-spin coupling 51  
 spin-spin relaxation *see* transverse relaxation  
 spin-spin relaxation time constant *see*  $T_2$   
 spin-up 232  
 SQUID 38, 82  
 standard model 193  
 state function, quantum 143  
 state of matter 17ff  
 States procedure 109ff, 450  
 States procedure, comparison with TPPI 116  
 for 2D exchange 530, 536  
 for 2D INADEQUATE 432  
 for COSY 411, 491, 495, 496  
 for NOESY 572  
 for ROESY 581  
 for TOCSY 502  
 sign convention 116, 503  
 stationary random field 547  
 stationary state 145, 147ff, 240  
 statistical operator 292  
 statistical quantum mechanics 267  
 steady state NOE *see* NOE  
 steady-state magnetization 653  
 Stern-Gerlach experiment 257  
 stimulated absorption 275  
 stimulated echo 91, 539  
 stimulated emission 275  
 ST-MAS 343, 348  
 strong coupling 449, 462, 613, 615ff  
 strong nuclear force 10  
 strong pulse limit, for quadrupolar nuclei 327, 339, 347  
 sucrose 435  
 sulfur *see*  $^{32}\text{S}$   
 sum theorem for phase cycling 633  
 sunspots 585  
 superconducting quantum interference device *see* SQUID  
 superconductor 19, 66  
 superconductor, high- $T_c$  82  
 Knight shift in 527  
 Meissner effect in 541  
 NMR in 541  
 superposition state 147ff  
 superposition state, dynamics of 240  
 for spin-1 321  
 of AMX system 469  
 of AX system 370  
 of spin-1/2 234  
 superstring 10  
 surface plot 107  
 susceptibility, magnetic 24, 32, 315, 445, 449  
 tensor of 37  
 swing, child's 72, 247, 256  
 synthesizer, radio-frequency 67
- $T_1$  33, 283, 543, 564  
 $T_1$ , and transition probability 553  
 field-dependence 556  
 in heteronuclear systems 449  
 in spin-pair systems 564  
 measurement of 295  
 mechanism of *see* longitudinal relaxation  
 minimum of 554, 565  
 of electrons 526  
 of quadrupolar nuclei 455  
 relationship with  $T_2$  284, 292  
 temperature-dependence 555, 556  
 $T_{1\rho}$  305, 316  
 $T_2$  35, 281, 543, 565  
 $T_2$ , adiabatic contribution to 292  
 in homonuclear AX system 565  
 measurement of 298  
 mechanism of 282  
 non-adiabatic contribution to 292  
 relationship with  $T_1$  284, 292

- $T_2^*$  316  
 tanh function 532  
 tensor, antisymmetric part 224  
     chemical shift 603, *see* CSA  
     diffusion 540  
     electric field gradient 207, 614  
     J-coupling 218  
     susceptibility 37  
     symmetric *see* tensor, uniaxial  
     transformations of 603  
     uniaxial 225  
 tesla 23  
 thermal energy 267  
 thermal equilibrium 31, 32, 266ff, 292, 326, 389, 481, 543, 551  
 thermodynamics, first law of 148  
 three-dimensional *see* 3D  
 through-space dipole-dipole coupling *see* DD coupling  
 time-dependent Schrödinger equation  
     *see* Schrödinger equation  
 time-proportional phase incrementation *see* TPPI  
 timescale, Larmor 513  
     of chemical exchange 511  
     of diffusion 513  
     of flow 513  
     of vibration 509  
     relaxation 514  
     spectral 514  
 TMS, isotopomers of 44  
 TOCSY 497ff, 627  
 TOCSY, and ROESY 583  
     pulse sequence 499  
     simulation of 502  
     theory of 499ff  
 top (child's toy) 28  
 torsional angle 221  
 TPPI 116  
 trace, of a matrix 159  
     of an operator 159  
     properties of 159  
 traceless matrix 159  
 transformation, Fourier *see* FT  
 transient 88  
 transient counter 90  
 transient NOE experiment 594  
 transition probability 550ff  
 transition probability, and cross correlation 586  
     arrow notation 550  
     distance dependence 559  
     double-quantum 558  
     for DD relaxation 557ff  
     for pulse 255  
     for random field relaxation 552  
     heteronuclear 566, 567  
     homonuclear 558  
     of relaxation process 292  
     per unit time 517, 550  
     single-quantum 558  
     thermally corrected 551  
     zero-quantum 559  
 translation, molecular *see* molecular translation  
 transmitter section 66ff  
 transverse, definition of 34  
 transverse cross-relaxation 577  
 transverse magnetization 33ff, 270  
 transverse magnetization, steady state 654  
 transverse relaxation 33ff, 281, 543  
 transverse relaxation, adiabatic contribution 292  
     non-adiabatic contribution 292  
 transverse Solomon equations 578  
 triple-quantum coherence, for spin-3/2 337  
     in multiple spin-1/2 systems 471  
 triplet (J-multiplet) 56, 476, 476  
 triplet state 9, 359  
 tritium *see*  $^3\text{H}$   
 TROSY 566, 590ff  
 TROSY, experimental example 593  
     meaning of acronym 593  
 truncation of signal 116  
 Tukey, John 116  
 tuning 72  
 two-dimensional *see* 2D  
 two-site exchange, asymmetric 524  
     symmetric 516ff, 529  
 two-spin order 384  
  
 Uhlenbeck, George 20  
 unit cell 225  
 unitary operator 131  
 units, natural 146  
 unity operator 126, 136  
  
 $^{51}\text{V}$ , quadrupole moment 207  
 $^{51}\text{V}$  349  
 vacuum permeability 24  
 vanadium *see*  $^{51}\text{V}$   
 vector, column 124  
     row 124

- vector representation 123
- vibration, molecular 509, 515, 541
- virus 444
  
- Wüthrich, Kurt 576
- waiting interval 295
- water, chemical equivalence in 456
  - DD coupling in 367
  - diffusion in 17
  - isotopomers of 16
  - magnetic equivalence in 458, 460
  - molecular structure of 16
  - $^{17}\text{O}$  spectrum of 348
  - spin system of 259, 291
  - susceptibility of 24
- wavefunction 143
- wavelength, electromagnetic 23
- weak coupling 363ff, 461ff, 613, 619ff
- weak coupling, breakdown of 465, 500
  - condition in isotropic liquids 364, 461
  - general condition 363
- weak nuclear force 10
- weak pulse limit, for quadrupolar nuclei 343, 348, 349
  
- Wigner-Eckart theorem 37, 193
- wind, and Coriolis force 244
  
- $^{129}\text{Xe}$ , chemical shift 194
- $^{129}\text{Xe}$ , nuclear properties of 12
- $^{129}\text{Xe}$ , optical pumping of 20, 81
- $^{129}\text{Xe}$ , spin of 15
- $^{131}\text{Xe}$  334
- xenon *see*  $^{129}\text{Xe}$  and  $^{131}\text{Xe}$
  
- Zeeman echo 351
- Zeeman effect 7
- Zeeman eigenbasis 153
- Zeeman eigenstate 160, 231
- Zeeman order vector 660
- Zeeman product state 356, 370
- Zeeman splitting 7, 14ff, 233
- zero-quantum coherence 471
- zero-quantum coherence, evolution of 403
  - in AX system 371, 386
  - physical interpretation 389
- zero-spin nuclei 14