

Table of contents

Atomic Properties in Hot Plasmas

From Levels to Superconfigurations

Jacques Bauche, Claire Bauche-Arnoult,
Olivier Peyrusse

Contents

Chapter 1 – Introduction	1
Chapter 2 – The central-field configurational model	7
2.1. The central-field model	8
2.2. The spin and the antisymmetry principle.....	9
2.3. The perturbation procedure	11
2.3.1. The perturbing operator	11
2.3.2. The LS coupling	12
2.3.3. The spin-orbit operator	13
2.4. The intermediate coupling	14
2.4.1. The αJ levels	14
2.4.2. Selection rules	15
2.4.3. The energy radial integrals	15
2.4.4. The energy angular coefficients	16
2.4.5. Examples of intermediate coupling: the $3d^2$ and $3p^2$ configurations	16
2.4.6. Other couplings	18
2.5. Configuration interaction. The parity quantum number	18
2.5.1. Configuration interaction. Selection rules	18
2.5.2. The parity quantum number	19
2.6. Determination of the radial integrals	20
2.6.1. The Thomas-Fermi potential	20
2.6.2. Hartree-Fock calculations	20
2.6.3. Parametric potentials	22
2.7. The relativistic central-field model	24
2.7.1. Hydrogenic ions	24

2.7.2.	<i>N</i> -electron ions	26
2.7.3.	The Breit operator	28
2.7.4.	Other relativistic approaches	29
2.8.	From detailed calculations to statistical methods	30
2.8.1.	Successes and lacks of the detailed methods	30
2.8.2.	Advantages and failures of the statistical methods	31
	References	32
	Chapter 3 – Distribution functions. Energy levels	37
3.1.	Distribution functions and moments	37
3.2.	Computation of the distribution moments	39
3.2.1.	Tensor-operator formalism	39
3.2.2.	Graphical methods	39
3.2.3.	Second-quantization method	40
3.2.4.	Complementarity and anticomplementarity	40
3.3.	Choice of the distribution function	41
3.4.	<i>J</i> statistics. Number of levels	41
3.4.1.	The distribution moments	41
3.4.2.	The Gram-Charlier distribution function	43
3.4.3.	Other distribution functions	44
3.5.	Statistics of level energies	46
3.5.1.	The distribution moments	46
3.5.2.	The distribution function	47
	References	50
	Chapter 4 – Statistical properties of transition arrays	53
4.1.	Definition of the transition arrays	54
4.2.	Number of lines in transition arrays	57
4.2.1.	Number of lines in E1 transition arrays	57
4.2.2.	Number of lines in singular E1 transition arrays	60
4.2.3.	Numbers of lines in M1 and E2 transition arrays	61
4.3.	Total strengths	64
4.3.1.	Definitions	64
4.3.2.	Total strength of E1 transition arrays	65
4.3.3.	Total strength of E2 transition arrays	66

Contents	IX
4.4. Strength-weighted distribution of line wavenumbers	66
4.4.1. Average wavenumber of the arrays	67
4.4.2. Array width	68
4.4.3. Asymmetrical arrays	74
4.4.4. Emissive and absorption zones	78
4.5. Configuration interaction	81
4.6. Relativistic effects. Spin-orbit interaction	86
4.6.1. Configurations and arrays in $j-j$ coupling	88
4.6.2. Average energies and widths of the subarrays	90
4.6.3. Breakdown of $j-j$ coupling	98
4.6.4. Interpretation of experimental spectra	102
4.7. Correlations	108
4.7.1. Propensity law for the upper and lower energies of the lines	108
4.7.2. Correlation between the strengths and wavenumbers of the radiative lines	111
4.8. Line-strength statistics	113
4.8.1. The J -file sum rule	113
4.8.2. The extended J -file sum rule	114
4.8.3. The GOE approach	118
4.8.4. The scars of symmetries	123
4.8.5. A fractal structure	125
4.9. Plasmas in strong magnetic fields	127
References	128
Chapter 5 – Modeling of ionic spectra	135
5.1. Emission and absorption spectra	136
5.1.1. Line widths	138
5.2. The Unresolved Transition Arrays	140
5.2.1. Representation by continuous curves	140
5.2.2. Impact of higher-order moments on the shape of a transition array	143
5.3. Simulation of resolved transition arrays	146
5.3.1. The Monte Carlo simulation of a transition array	146
5.3.2. The Planck and Rosseland mean absorption coefficients ..	153
References	156

Chapter 6 – Static and dynamical equilibrium in plasmas	161
6.1. General remarks	162
6.2. Local Thermodynamical Equilibrium. Overview and fundamental laws	164
6.3. Statistical mechanics of LTE. Partition functions. Saha-Boltzmann equilibrium	165
6.3.1. Grand Canonical and Canonical partition functions	166
6.3.2. Partition function for N corpuscles having a kinetic energy and an internal structure	168
6.3.3. Ionization equilibrium within the Maxwell-Boltzmann equilibrium	169
6.3.4. Equation of State and LTE ionization equilibrium	172
6.3.5. The LTE Average Atom model	173
6.3.6. LTE detailed level accounting	174
6.3.7. LTE detailed configuration accounting	174
6.3.8. LTE detailed balance and microreversibility	176
6.4. Coronal equilibrium	182
6.5. Collisional-Radiative equilibrium	183
6.5.1. Detailed level accounting and major simplifications	183
6.5.2. NLTE detailed configuration accounting	185
6.6. Level to level rate calculations	186
6.6.1. Radiative transition rates	186
6.6.2. Autoionization / resonant capture rates	187
6.6.3. Collisional excitation / de-excitation strengths	188
6.6.4. Collisional ionization / 3-body recombination strengths ..	189
6.6.5. Photoionization / radiative recombination cross sections ..	190
6.6.6. Non-Maxwellian effects	191
6.7. Configuration to configuration rate calculations	192
6.7.1. Radiative transition rates	192
6.7.2. Collisional excitation strengths	193
6.7.3. Collisional ionization strengths	195
6.7.4. Autoionization rates	195
6.7.5. Photoionization cross sections	196
6.8. Emissivity and opacity	197
References	199

Chapter 7 – Superconfigurations and Super Transition Arrays	203
7.1. Definitions and theoretical background	203
7.2. LTE Superconfiguration Accounting (LTE SCA)	206
7.2.1. Basics	206
7.2.2. Superconfiguration average energies	207
7.3. NLTE Superconfiguration Accounting (NLTE SCA)	210
7.3.1. Superconfiguration collisional-radiative model	210
7.3.2. Superconfiguration-average transition rates	211
7.4. Super Transition Arrays	215
7.5. Photon emission and absorption between superconfigurations ...	219
7.5.1. Bound–bound transitions	219
7.5.2. Bound–free transitions	221
References	222
Chapter 8 – Global approach to plasmas in LTE equilibrium	225
8.1. Detailed configuration accounting	226
8.1.1. Experimental examples in absorption	226
8.1.2. Temperature corrections in absorption calculations	228
8.1.3. Temperature corrections in emissivity calculations	231
8.2. Superconfiguration approach. Opacity experiments	232
References	239
Chapter 9 – Global approaches to Non-LTE hot dense plasmas. Effective temperatures	243
9.1. Results obtained using global approaches	244
9.1.1. Superlevel accounting	244
9.1.2. Importance of the dielectronic recombination	248
9.2. Definition of effective temperatures	252
9.2.1. Evidence of configuration temperatures $T(C)$	252
9.2.2. Evidence of superconfiguration temperatures $T(SC)$, and of ionic-excitation temperatures $T(I)$	255
9.2.3. Definitions of other effective temperatures	257
9.3. Analytical computation of effective temperatures. Applications .	259
9.3.1. Computation of $T(SC)$	259
9.3.2. Examples and use of $T(SC)$	265
9.3.3. Derivation of $T(I)$ from SC results	269
9.3.4. Remark on the definitions of the average-state population	272

9.3.5. Direct computation of $T(I)$	272
9.3.6. Calculation of the charge-state distribution using $T(I)$..	274
9.4. Discussion of the validity of global approaches	276
References	279
Chapter 10 – Hybrid models	283
10.1. Hybrid models for plasmas in LTE	283
10.2. Hybrid models in Non-LTE cases. Levels, configurations and superconfigurations	286
10.3. Another global approach: RDCA	289
10.4. Simplified models	292
References	293
Chapter 11 – Plasma simulations	297
11.1. Local time-dependent population kinetics	297
11.1.1. Steady-state solution	298
11.1.2. Time-dependent solution	299
11.2. Radiation energy transfer	299
11.3. Hydrodynamics calculations	304
References	307
Chapter 12 – Applications to hot-plasma radiation	311
12.1. Spectroscopic diagnostics for T_e , N_e , and $\langle Z \rangle$	312
12.2. Global characterizations of plasma radiation	314
12.2.1. Radiative power losses	315
12.2.2. Cooling coefficients	315
12.2.3. Rosseland mean	317
12.3. Specific experiments	318
12.3.1. X-ray production	318
12.3.2. Dielectronic recombination measurements	318
12.3.3. Hollow-atom physics	320
12.3.4. Precise evaluations of continuum lowering	322
References	325

Appendix A – The tensor-operator formalism	329
A.1. Definitions	329
A.2. The Wigner-Eckart theorem	330
A.3. Definition and properties of the 3- <i>j</i> coefficients	332
A.4. Reduced matrix elements	334
A.5. The Landé factor for the Zeeman effect	334
A.6. Definition and properties of the 6- <i>j</i> coefficients	335
A.7. Generalization: the 3 <i>n</i> - <i>j</i> coefficients	337
A.8. Coupled tensor operators	337
A.9. Some applications of the tensor-operator method	339
A.9.1. The Landé <i>g</i> -factor	339
A.9.2. Coefficients of the Slater integrals in the level energies of the $n\ell n'\ell'$ configuration	340
A.9.3. Total strength of the $n\ell n'\ell' - n\ell^2$ transition array	342
References	343
Appendix B – The second-quantization method for electrons in atoms	345
B.1. Definition of the operators	345
B.2. Examples of applications	347
B.2.1. Total strength of the $n\ell^{N+1} - n\ell^N n'\ell'$ transition array ..	347
B.2.2. Calculation of a distribution moment	349
B.3. Guide-line for a quick calculation of a sum over the states of a configuration	350
References	351
Appendix C – Partition function algebra	353
C.1. Recursion relations	353
C.2. Application: working formula for the superconfiguration average energy	356
C.3. Application: working formula for the average energy of a supertransition array	357
C.4. Application: working formula for the variance of a supertransition array	358
References	359

Appendix D – Analytical evaluation of the ionic-excitation temperature $T(I)$	361
References	366
Appendix E – Evaluation of the radiative power losses of a superconfiguration	367
E.1. Definitions	367
E.2. Use of the second-quantization formalism	368
E.3. Determination of the p_k parameters. Numerical applications	369
E.4. Generalization	372
References	374