Introduction to the plasma spectroscopy

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- Einstein coefficients
- energy state designation under L-S coupling scheme
- population mechanism for excited states collisional-radiative model
- effect of external field perturbation theory

introduction

glow discharge in LHD



main discharge with helium gas





- plasma shows various colors with different working gas
- quantitative treatment of color is, however, difficult
- spectrum is used for quantitative analysis instead

emission lines

properties of emission line



what can be known?

obser	vable	obtainable	
shift		ion velocity	
hunn danin a	Doppler	T_{i}	
broadening	Stark	n _e	}
splitting	Zeeman	magnetic field	
	Stark	electric field	
intensit intensity d	y ratios istribution	$T_{\rm e}$, $n_{\rm e}$ ionizing or recombining	
inte	nsity	$n_{\rm i}$	J

high resolution measurement

measurement

line intensity

 intensity is the product of population density and spontaneous transition probability or Einstein A coefficient





detailed balance



under thermodynamic equilibrium

$$n(p)X(p,q) = n(q)X(q,p)$$

n(q) and n(p) should obey Boltzmann distribution $\frac{n(p)}{n(q)} = \frac{g(p)}{g(q)} \exp\left[\frac{E_{pq}}{kT}\right]$

X(q, p) must be

$$X(q,p) = X(p,q)\frac{g(p)}{g(q)}\exp\left[\frac{E_{qp}}{kT}\right]$$

Einstein coefficients



B(p, q) can be calculated, then how A(q, p) and B(q, p) are derived?

 $A(q,p)n(q) + B(q,p)n(q)I_{\nu} = B(p,q)n(p)I_{\nu}$

under thermodynamic equilibrium

population ratio is subject to Boltzmann distribution

$$\frac{n(q)}{n(p)} = \frac{g(q)}{g(p)} \exp\left[-\frac{h\nu}{kT}\right]$$

the balance equation is rewritten as



this should be equivalent to Planck's black-body equation

$$I_{\nu} = \frac{2h\nu^{3}}{c^{2}} \frac{1}{\exp(h\nu/kT) - 1}$$

finally, interrelationships among Einstein coefficients are derived as

$$B(q,p) = \frac{g(p)}{g(q)}B(p,q)$$

$$A(q,p) = \frac{2hv^3}{c^2}B(q,p) = \frac{2hv^3}{c^2}\frac{g(p)}{g(q)}B(p,q)$$

level notations (angular momentum theory)

electron states for hydrogen

orbital angular momentum quantum number

mber	n	0 s (2)	1 p (6)	2 d (10)	3 f (14)	4 g (18)	5 h (22)
Inu c	1 (2)	1s					
ntun	2 (8)	2s	2p			$m_l =$	$-l,\ldots,l$
qual	3 (18)	3s	3р	3d		$m_s =$	$\pm 1/2$
cipal	4 (32)	4s	4p	4d	4f		
oring	5 (50)	5s	5p	5d	5f	5g	
	6 (72)	6s	6p	6d	6f	6g	6h

spin quantum number s = 1/2

() indicates statistical weight



NIST SP 966 (September 2003)

coupling of angular momentum

 j^* j = l + s (|s| = 1/2)

 $j = \begin{cases} l \pm \frac{1}{2} & \text{for } l \ge 1\\ \frac{1}{2} & \text{for } l = 0 \end{cases}$

total angular momentum quantum number

each
$$j$$
 state has $2j+1$ magnetic substates $m (= -j, -j+1, ..., j)$

(H. E. White, Introduction to Atomic Spectra)



(H. E. White, Introduction to Atomic Spectra)

quantum numbers

variables	meanings	values			
п	principal	0, 1, 2,			
S	anin]	1/2		
S	spin	0, 1/2, 1	, 3/2, 2,		
1	orbital	0 1 2	s, p, d, f,		
L	orditai	0, 1, 2,	S, P, D, F,		
j	total	0 1/2 1	3/2 2		
J	cotai	U , 1 / 2 , 1 ,	, 0, 2, 2,		
т	magnotic	0 +1/2 +1	⊥2/ <u>7</u> ⊥7		
M	magnetic	$0, \pm 1/2, \pm 1, \pm 3/2, \pm 2, \dots$			

term designation

$nl^k n'l'^{k'} \dots {}^{2S+1}L_J$

configuration	possible terms	isoelectronic sequence
3d	² D _{3/2,5/2}	H-like
1s4f	${}^{1}F_{3} \; {}^{3}F_{2, 3, 4}$	He-like
1s²2p	$^{2}P_{1/2, 3/2}$	Li-like
$1s^{2}2s^{2}$	${}^{1}S_{0}$	Be-like
1s ² 2s2p(³ P°)3p	$\begin{array}{cccc} {}^2S_{1/2} & {}^2P_{1/2,3/2} & {}^2D_{3/2,5/2} \\ {}^4S_{3/2} & {}^4P_{1/2,3/2,5/2} \\ {}^4D_{1/2,3/2,5/2,7/2} \end{array}$	B-like

one electronic configuration could have several terms

selection rules for transition

$$^{2S+1}L_J$$
 - $^{2S'+1}L'_{J'}$

 $\Delta S = 0$ $\Delta L = 0, \pm 1 \ (0 \rightarrow 0 \text{ excluded})$ $\Delta J = 0, \pm 1 \ (0 \rightarrow 0 \text{ excluded})$

besides the rules for total quantum numbers, $\Delta l = \pm 1$ is always required



FIG. 11.4.—Triplet-triplet transitions showing selection rules and relative intensities. (H. E. White, Introduction to Atomic Spectra)

$$I \propto \langle J_i ||D||J_k \rangle = (-1)^{S+1+L_i+J_k} \sqrt{g_i g_k} \left\{ \begin{array}{cc} L_i & J_i & S \\ J_k & L_k & 1 \end{array} \right\} \langle L_i ||D||L_k \rangle$$



(H. E. White, Introduction to Atomic Spectra)



population mechanisms

corona equilibrium



collisional excitation

 $C(q,p)n_{\rm e}n(1)$ [m⁻³s⁻¹]

rate coefficients are obtained from cross section

$$C(q,p) = \int_0^\infty \sigma_{qp}(v) f(v) v \mathrm{d}v$$

C(q, p) depends on T_e







corona model does not explain observed spectrum

atomic processes



collisional-radiative model



population consists of two independent components

$$n(p) = r_0(p)n_en_z + r_1(p)n_en(1)$$

= $n_0(p) + n_1(p)$





ionizing plasma



 $\frac{n(p)}{g(p)} \propto \begin{cases} p^{-0.5} & \text{for low } n_{\text{e}} \\ p^{-6} & \text{for high } n_{\text{e}} \end{cases}$

 $T_{\rm e}$ dependence on n(p)distribution is small

population flows (ionizing plasma)

low $n_{\rm e}$ case

high $n_{\rm e}$ case





close to corona equilibrium

(T. Fujimoto, *Plasma Spectroscopy*)

recombining plasma



when n_e is high, n(p) is expressed with Saha-Boltzmann equation

$$n(p) = \frac{g(p)}{2g_z(1)} \left(\frac{h^2}{2\pi m k T_e}\right)^{3/2}$$
$$\exp\left[\frac{\chi(p)}{kT_e}\right] n_e n_z(1)$$

(T. Fujimoto, *Plasma Spectroscopy*)

population flows (recombining plasma)

low $n_{\rm e}$ case

high $n_{\rm e}$ case



(T. Fujimoto, *Plasma Spectroscopy*)

ionizing plasma (I)



 $n(p) = r_1(p)n_en(1)$





recombining plasma (III)



recombining plasma (II)



- recombining plasma of Hell appears earlier than Hel
- derived T_e is higher

effect of external fields

splitting, shift, broadening, etc

- Zeeman effect magnetic field
- Stark effect electric field
- Stark broadening electric micro fields



. Zeeman eneer of a principal-series doublet.

(H. E. White, Introduction to Atomic Spectra)

polarization

 $\Delta M = \pm 1 \rightarrow \text{polarization perpendicular to } B (\sigma \text{-polarization})$ $\Delta M = 0 \rightarrow \text{polarization parallel to } B (\pi \text{-polarization})$

circularly polarized light (σ -polarization)



Fig. 10.2. Superposition of two linear-polarized phase-shifted waves (left-hand figure) into a circularly-polarized wave (right-hand figure). The sense of rotation is defined in the text.

(P. H. Heckmann, Introduction to the Spectroscopy of Atoms)

π -component is not seen for // B observation

 π and σ have the same intensity for $\perp B$ observation

perturbation theory (eigensystems)

$$H\psi = E\psi$$

$$H = H^{0} + V$$

$$= \begin{pmatrix} E_{1}^{0} + V_{11} & V_{12} & \cdots & V_{1n} \\ V_{21} & E_{2}^{0} + V_{22} & \cdots & V_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ V_{n1} & V_{n2} & \cdots & E_{n}^{0} + V_{nn} \end{pmatrix}$$

perturbation of magnetic field $|LSJM\rangle$ is taken as base function $\langle JM|V|J'M'\rangle$

$$= - \mu_{\rm B} B \langle JM | (g_L L_z + g_S S_z) | J'M' \rangle$$

$$= - \mu_{\rm B} B \sum_{M_L M_S} \langle JM | M_L M_S \rangle \langle J'M | M_L M_S \rangle (g_L M_L + g_S M_S)$$

$$= - \mu_{B}B \sqrt{2J+1} \sqrt{2J'+1}$$

$$\sum_{M_{L}M_{S}} \begin{pmatrix} 1 & 1 & J \\ M_{L} & M_{S} & -M \end{pmatrix} \begin{pmatrix} 1 & 1 & J' \\ M_{L} & M_{S} & -M \end{pmatrix} (g_{L}M_{L} + g_{S}M_{S})$$

$$(M = M_{L} + M_{S})$$

1s2p ³ P _{0,1,2}	$\langle JM V J'M'\rangle$	$= -\mu_{\rm B} B \langle JM $	$(g_{\rm L}L_z +$	$g_{\rm S}S_z) J'M'\rangle$
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	J	0		1				2		
J′	M	0	-1	0	1	-2	-1	0	1	2
0	0			-0.8165						
	-1		-1.5000				-0.5000			
1	0	-0.8165						-0.5774		
	1				1.5000				-0.5000	
	-2					-3.0000				
	-1		-0.5000				-1.5000			
2	0			-0.5774						
	1				-0.5000				1.5000	
	2									3.0000

 $\langle JM|V|J'M'\rangle = -\mu_{\rm B}B\langle JM|(g_{\rm L}L_z + g_{\rm S}S_z)|J'M'\rangle$

	J	0	1	2	1	2	1	2	2	2
J′	M	0		_	-1		1		2	
0		0	-0.8165							
1	0	-0.8165	0	-0.5774						
2			-0.5774	0						
1	1				-1.5000	-0.5000				
2	-1				-0.5000	-1.5000				
1	1						1.5000	-0.5000		
2	1						-0.5000	1.5000		
2	-2								-3.0000	
2	2									3.0000

perturbed eigenstate is expressed with base functions $|\psi_m\rangle = \sum C_i^m |\psi_i^0\rangle$

m

transition probability is written as

$$A^{q}_{\psi_{m}\to\varphi_{n}} \propto \left|\langle\varphi_{n}|D_{q}|\psi_{m}\rangle\right|^{2} = \left|\sum_{i,j} C^{n}_{j}C^{m}_{i}\langle\varphi_{j}^{0}|D_{q}|\psi_{i}^{0}\rangle\right|^{2}$$

each term is calculated as

$$\begin{aligned} |\psi_i^0\rangle &= |L_1 S_1 J_1 M_1\rangle \\ |\phi_j^0\rangle &= |L_2 S_2 J_2 M_2\rangle \\ \langle \phi_j^0 | D_q | \psi_i^0\rangle &= (-1)^{(J_1 - M_1) + (S + 1 + L_1 + J_2)} \sqrt{(2J_1 + 1)(2J_2 + 1)} \\ & \left(\begin{array}{cc} J_1 & 1 & J_2 \\ -M_1 & q & M_2 \end{array} \right) \left\{ \begin{array}{cc} L_1 & J_1 & S \\ J_2 & L_2 & 1 \end{array} \right\} \langle L_1 ||D|| L_2 \rangle \end{aligned}$$





application to fusion plasma





(M. Goto et al., Phys. Rev. E 65, 026401 (2002))