Notes

These notes are designed to supplement the material in the textbook. They generally complement or elucidate a specific topic. References to individual chpaters, sections, equations, and figures are therefore explicitly made. The titles below are notes posted thus far on the following pages. Readers are advised to check this page periodically.
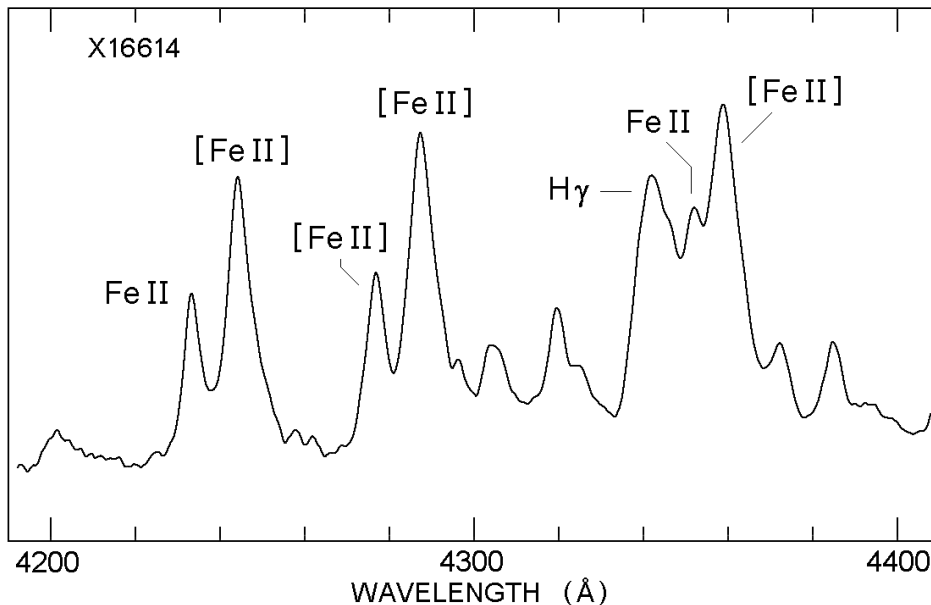
Figure 1: Singly ionized iron in Eta Carinae: allowed Fe II and forbidden [Fe II] lines

Cover: The Eta Carinae nebula and the central stellar system

We have referred to the image on the jacket cover several imes in the book. But it is worthwhile to begin this series of notes by summarizing a few salient features, ith additional details and references to relevant material in the text. specially so, since Eta Carinae displays the characterstics of several different types of astronomical objects: stars, nebulae, and (pre)supernovae. It is instructive to see how spectroscopy might reveal, or be complicated by, the dynamical nature of the source.

The Eta Carinae nebula is formed by one of the most massive and luminous stars known, more than 100 times the mass and over 5 million times more luminous than the Sun. It is almost 8000 light years away and is a **symbiotic star**: a binary system with two stars in different stages of evolution (Ch. 10). Since it is so massive, its inevitable end must be a **Type II supernova** explosion (Chs. 10 and 14). However, to avoid that fate the star is ejecting mass rapidly in a pre-supernova (hypernova?) phase. Owing to its immense brightness, it belongs to the class of stars known as Luminous Blue Variables (LBV). The LBVs are the most extreme class of stars in mass and luminosity, inhabiting the upper-left corner of the HR diagram (Fig. 10.2).

The nebula is also called the Homonculus nebula, and is unlike most nebulae in the variety of prevailing physical conditions and material constituents. It is ionized and neutral gas with dust. The dumb-bell shape is due to rapid rotation of the binary system at the core, surrounded by ejecta that dominates in the equatorial regions.

Eta Carinae is an ideal laboratory for multi-wavelength analysis. Spectroscopic observations range from typical nebular lines, forbidden and allowed, and up to X-ray spectra observed by the Chadra X-ray Observatory. Singly ionized iron, Fe II, is particularly interesting (Fig. 1). It has been shown that some transitions in Fe II could be pumped by the UV radiation background (Ch. 13) so as to emit laser-like radiation. Even more energetic are the X-rays produced by the star, with vastly anomalous intensities. Clearly, there is much to be learned about the dynamic coupling between the central star(s) and the huge volume of gas being ejected (Davidson and Humphreys 1997, Ref. [278]).

Ch. 1. Introduction

Fermion and Boson Wavefunctions:

Footnote 4. The 'proof' from Condon and Shortley [3] of the existence of two kinds of particles, fermions and bosons, rests on the fact that probabilities of real observable quantities are obtained from the square of the wavefunctions, and therefore there are two possible signs of the wavefunctions. Without loss of generality we consider a two-particle system with associated coordinates λ_1, λ_2. Indistinguishablity then implies

$$|\psi(\lambda_1, \lambda_2)|^2 = |\psi(\lambda_2, \lambda_1)|^2. \tag{1}$$

The interchange does not affect the system except possibly through a phase factor, i.e.

$$\psi(\lambda_2, \lambda_1) = exp(i\alpha)\psi(\lambda_1, \lambda_2). \tag{2}$$

Experimentally however the two states $\psi(\lambda_1, \lambda_2)$ and $\psi(\lambda_2, \lambda_1)$ can not be distinguished. Now if we define an *exchange* operator P_{12} such that

$$P_{12}\psi(\lambda_1, \lambda_2) = \psi(\lambda_2, \lambda_1). \tag{3}$$

If P_{12} operates on Eq. (0.2) then

$$P_{12}\psi(\lambda_2, \lambda_1) = exp(i\alpha)P_{12} = \psi(\lambda_1, \lambda_2), \tag{4}$$

$$\psi(\lambda_1, \lambda_2) = exp(2i\alpha)\psi(\lambda_1, \lambda_2). \tag{5}$$

It follows that

$$exp(2i\alpha) = 1 \tag{6}$$

or

$$exp(i\alpha) = \pm 1, \tag{7}$$

and

$$\psi(\lambda_2, \lambda_1) = \pm\psi(\lambda_1, \lambda_2). \tag{8}$$

Thus the wavefunction ψ is constrained to two kinds of functions with signs: '+' $\longrightarrow$ *symmetric*, and ' - ' $\longrightarrow$ *anti-symmetric* with respect to interchange of the two coordinates. The argument above may be generalized to any N-particle ensemble described by the wavefunction

$$\Psi(\lambda_1, \lambda_2, \ldots, \lambda_N).$$

The principle of indistinguishablity then divides all kinds of particles into two classes depending on whether the wavefunction is symmetric or antisymmetric. Those with anti-symmetric wavefunctions are *Fermions* with non-integral spin and obey *Fermi-Dirac* statistics (§1.6.2). The Fermion wavefunction for a two-particle system is written as:

$$\Psi_A(\lambda_1, \lambda_2) = \frac{1}{\sqrt{2}}[\psi_1(\lambda_1)\psi_2(\lambda_2) - \psi_1(\lambda_2)\psi_2(\lambda_1)]. \tag{9}$$

Note that the particles are labelled 1 and 2, and that interchange of coordinates changes the sign, i.e. $\Psi(\lambda_2, \lambda_1) = -\Psi(\lambda_1, \lambda_2)$. As discussed in Ch. 1, the *anti-symmetrization* property of an N-fermion system, such as an atom, manifests itself in *atomic structure* with quantized energy levels.

The second class of partcles with symmetric wavefunctions

$$\Psi_S(\lambda_1, \lambda_2) = \frac{1}{\sqrt{2}}[\psi_1(\lambda_1)\psi_2(\lambda_2) + \psi_1(\lambda_2)\psi_2(\lambda_1)] \tag{10}$$

are *Bosons*, have integral spin, and obey *Bose-Einstein* statistics (§1.6.3). The two-particle and N-particle wavefunctions are discussed in Ch. 2 on *Atomic Structure*.

Table 2. Fifteen possible distributions for the np^2 electrons.

M_S/ $M_L= 2$	1	0	-1	-2
0	1^+1^-	1^+0^-	1^+-1^-	-1^+0^-	-1^+-1^-
1		1^+0^+	1^+-1^+	-1^+0^+	
0		1^-0^+	1^--1^+	-1^-0^+	
-1		1^-0^-	1^--1^-	-1^-0^-	
0			0^+0^-		

Ch. 2. Atomic Structure

1. Pauli Exclusion Principle and Spectral States:

In §2.5 we discuss the formation of spectral states — LS terms — from a given configuration of electrons. As described, when the electrons in a configuration are non-equivalent, that is when they have different principal quantum numbers (viz. 2p3p), the Pauli exclusion principle does not exclude any combination of quantum numbers. In general the two-electron configuration $npn'p$ gives rise to six LS terms or states: $^3D, ^1D, ^3P, ^1P, ^3S, ^1S$. But when the electrons in a configuration are equivalent, with the same n, then one needs to work out in some detail as to how the exclusion principle applies. That is exemplified in Table 2.1 for three p-electrons in configuration np^3.

A simpler example is that of the configuration np^2 discussed in this note. The distribution of the two $2p$ electrons can be expressed as (1^+0^+), (1^+1^-) etc. Since electrons are indistinguishable they may be permuted without affecting the distribution; thus (1^+0^+), (0^+1^+) are the same. These electrons are grouped according to their respective values of M_L and M_S. Since

$$M_L = \sum_i m_l; \;\; M_S = \sum_i m_s \tag{11}$$

a distribution of (1^+0^+) is associated with values M_L = 1 and M_S = 1. For the np^2 configuration, Table 2 in this note shows all 15 possible distributions of (m_l, m_s) following the exclusion principle, ordered according to M_L and M_S. The highest value of $M_L= \pm 2$ allows only $M_S = 0$ since the spin quantum numbers must have opposite sign and cancel; hence they correspond to a single LS term ^1D. But $\mathbf{M}_L$ components for a given term range from $+\mathbf{M}_L$ to $-\mathbf{M}_L$. For ^1D the remaining components are $M_L = 0, \pm 1$, and therefore 5 intries in the table correspond to it, and can be excluded. The next highest value of $M_L= \pm 1$ associates with $M_S = 0, \pm 1$. These entries belong to the ^3P state, which takes out a total of nine entries ($M_L = 0, \pm 1$ and $M_S = 0, \pm 1$). The single remaining entry with M_L=0 and $M_S = 0$ must then correspond to the LS term ^1S. Thus six possible states resulting from two non-equivalent p-electrons are reduced to three LS states $^3P, ^1D, ^1S$ in the case of two equivalent electrons; the other three terms are excluded by the Pauli exclusion principle. We have listed the terms in order in which they are observed, with the term of highest spin-multiplicity, ^3P, lying the lowest in energy, i.e. the ground state of all atoms with two equivalent p-electrons (see Hund's rules).

2. Hydrogenic radial functions and charge densities

In §2.1.4 the mathematical expressions for the radial part of the wavefunctions of hydrogen are given. For the first few nl orbitals the spatial distributions are graphically illustrated in Fig. 2. On the top we have the radial wavefunctions and on the bottom the probability distribution of each electron in respective orbitals. In general the nodes in the radial wavefunctions are of crucial importance in the calculation of transition amplitudes from one initial state to another, such as oscillator strengths (Ch. 4) and photoionization cross sections (Ch. 6). The transition matrix elements contain an interaction operator and the overlap of the
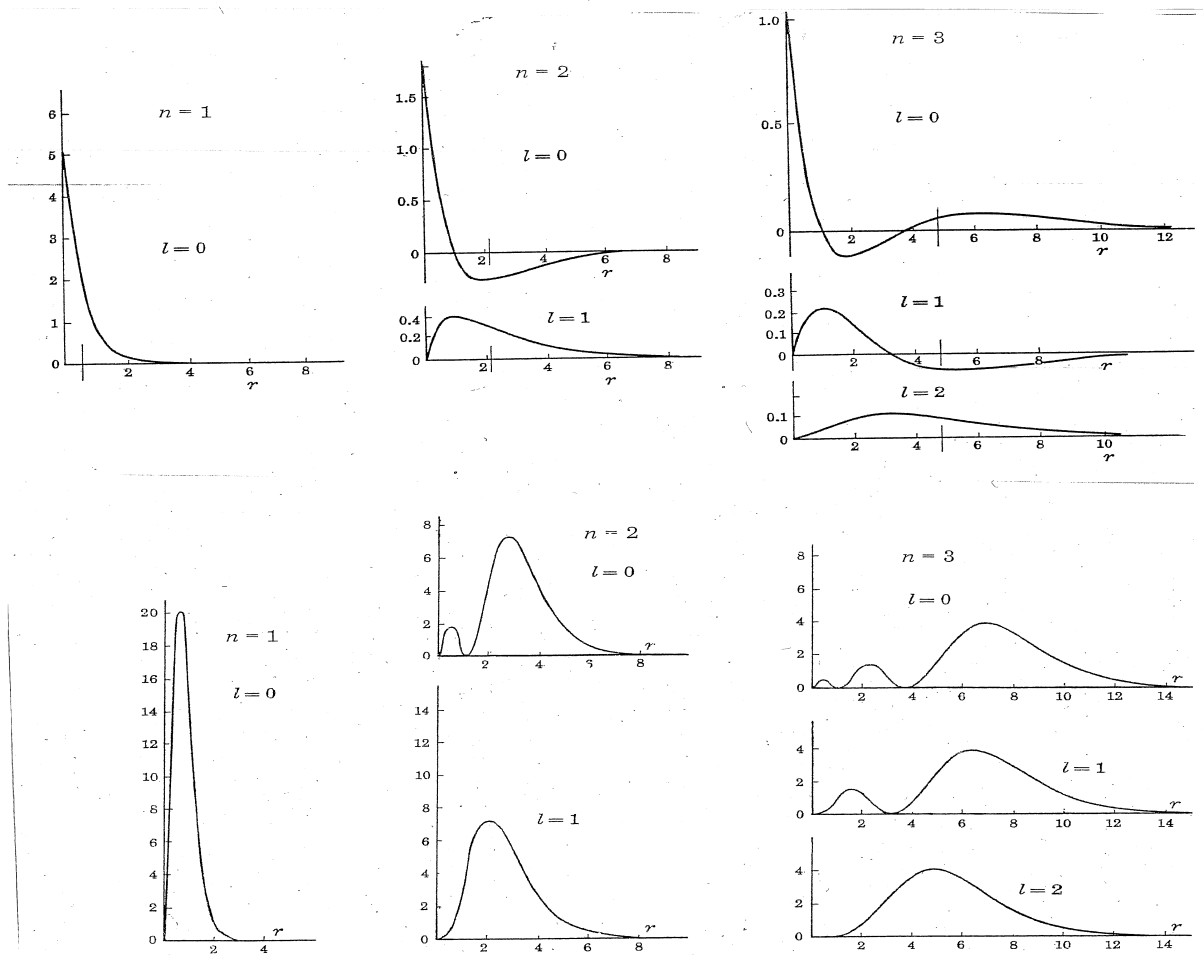
Figure 2: Top: Radial functions $R_{nl}(r)$ for 1s, 2s, 2p, 3s, 3p, 3d orbitals. Bottom: Radial charge densities $[P_{nl}(r)]^2$, with radial distance r in bohr radii.

initial and final wavefunctions, discussed in Ch. 4. The nodes determine the extent of overlap, and may lead to destructive interference due to cancellation and small transition amplitudes, or constructive interference and large transition amplitudes. An exmaple of the former is the minimum in photoionization cross sections of alkali atoms shown in Fig. 6.2.

Table 4.3 - Detailed explanation

It is necessary to specify several variables for full spectroscopic information involving many radiative transitions. Table 4.3 is a small sample from a large-scale calculation for radiative transition probabilities for boron-like ion Fe XXII. The iniital and final electronic configurations $C_i - C_k$ are listed in Column 1. The ground configuration is $2s^2 2p$ and the next excited configuration is $2s2p^2$ (the superscript '1' in Col. 1 is usually omitted if there is only one electron in the orbital). The ground LS term and fine structure J-components are $^2P^o_{1/2,3/2}$ (the second column should be read with '2', '4' etc. as superscripts for (2S+1), the spin-multiplicity). The third column labeled '$g_i : I - g_j : K$' denotes the statistical weight (e.g. $g_i = 2$ for J = 1/2), and an index I or K which refers to the order in which the bound levels occur in the computed energy spectrum. For example, in row 6, $2s2p^2 - 2p^3$, and column 3, we have $g_i = 2$, I = 1 and $g_k = 2$, K = 2. That means that the initial level $4P$ (column 2) belonging to $2s2p^2$ is the *lowest* energy level with SLJ symmetry J = 1/2, i.e. $4P_{1/2}$. Likewise, the final level is $2p^3$ $^2P^o_{1/2}$, but with K =2, i.e. the *second level* with J = $(1/2)^o$ (odd parity 'o' is denoted with a superscript, but even parity superscript 'e' is usually omitted). Note that the lowest J = $(1/2)^o$ levels is of course the ground level $2s^2 2p$ $^2P^o_{1/2}$, with corresponding index I = 1 (rows 1-5).

Ch. 12. Gaseous Nebulae and H II Regions

Emission Measure

In spatially diffuse nebulae, generally H II regions, the total intensity emitted in a line depends on the product of the number density of electrons n_e and the number density of ions n_i, integrated over the volume of the emitting region. Since the abundance of ions is related to electron density, it is useful to define a quantity called the *Emission Measure* (EM)

$$EM \equiv \int_V n_e^2 dV. \tag{12}$$

In H II regions the proton density tracks the hydrogen density N(H) and is close to n_e. The element abundnace N(X) and ion density N(X^{z+}) are relative to N(H), and hence EM $\sim n_e^2$. The EM is often used to obtain the flux in an optically thin line. We ended Ch. 8 on multi-wavelength emission line analysis by writing down Eq. (8.45) for a single [C II] line at 158 μm due to the forbidden transition $2s^2 2p$ ($^2P_{3/2}^o \longrightarrow ^2 P_{1/2}^o$). More generally, for a transition $j \to i$ from an excited level j in an ion X^{z+} to a lower level i, we can write the number density as

$$N_j(X^{z+}) = \frac{N_j(X^{z+})}{N(X^{z+})} \times \frac{N(X^{z+})}{N(X)} \times \frac{N(X)}{N(H)} \times \frac{N(H)}{n_e} \times n_e. \tag{13}$$

The flux in the line is then

$$F_{ij} = \left(\frac{1}{4\pi r^2}\right) \int N_j(X^{z+}) A_{ji} dV, \tag{14}$$

where r is the distance of the source from the Earth, A_{ji} the radiative decay rate, and the integrand is the emissivity per unit volume. Also recall that the flux is different from intensity in that it also considers geometrical dilution with distance.

Kα lines

The physics of Kα lines is rather more involved than appears at first sight. Although they correspond to the simplest possible transition array, 1s-2p, the corresponding spectroscopic designations require some study. Whereas Kα lines are ubiquitous in X-ray spectroscopy, we begin with their discussion in the context of AGN spectra.

Table 13.3 lists the transitions for Fe Kα lines. Starting at the bottom, the two Kα_1, Kα_2 transitions for H-like Fe XXVI are straightforward. However, note that for He-like Fe XXV there are also only two dipole allowed transitions, $1s^2\ (^1S_0) \rightarrow 1s2p\ (^3P_1^o,^1\ P_1^o)$ (recall the $\Delta J = \pm 1$ selection rule from Table 4.4), in spite of the fact that the 1s2p configuration gives rise to 4 levels; transitions from all other levels to the ground state are forbidden (Fig. 4.3).

But it is the other ions, Li-like Fe XXIV to F-like Fe VIII, that are more complex. They correspond to resonances, where the final state is an autoionizing state, unlike Fe XXVI and Fe XXV where the final level is a bound state. Let us consider the six Fe XXIV Kα transitions corresponding to the transition array $1s^22s \rightarrow 1s2s2p$. These transitions are explicitly listed in Table 7.1, where they give rise to the dielectronic satellite lines q, r, s, t, u, v, discussed in in §7.6. Note that there are only two final $J\pi$ symmetries for the 1s2p2s configuration with J-values 1/2 and 3/2. But the six final levels are non-degenerate in energy because the *parent levels* are different. The 4 levels of the parent configuration $1s2p\ (^1P_1^o,^3\ P_{0,1,2}^o)$ yield 6 distinct levels when coupled with another 2s-electron in the final 1s2p2s (or the equivalent 1s2s2p) configuration. Hence there are 6 Kα transitions for dipole allowed transitions in Fe XXIV, as listed in Table 13.3. Note that the J = 5/2 - 1/2 transitions $1s2p2s\ (^4P_{5/2}^o) \rightarrow 1s^22s(^2S_{1/2})$ is forbidden. The six transitions refer to the other 1s2s2p levels with J = 1/2 and 3/2.

Proceeding in this way for the other ions with an L-shell vacancy, we find that there are no less than 112 Kα transitions, not only for iron but for *all* elements and ions with more than 10 electrons, all the way up to uranium. This fact is also of great importance in other fields, as diverse as biomedicine and nanotechnology, where X-ray interaction with high-Z atoms entails Kα transitions. This is one of the reasons we discuss the atomic structure of gold (Z = 79) in §5.9 on the **Auger effect** in Ch. 5. The ionization structure of gold atoms (see Table 5.3) may potentially lead to their use as nanoparticles in cancer research (Ref. Pradhan *et al.* , J. Phys. Chem. A 113, 12356, 2009 and Montenegro *et al.* , J. Phys. Chem. A 113, 12364, 2009).

N.B. There is a typo in listing the parent level of six lines $q, .., v$ in Table 7.1. For example, $1s2p\ ^1(P^o)$ should be $1s2p\ (^1P^o)$, i.e. the superscript for spin multiplicity should be inside the parenthesis (..).