THE IRON PROJECT

Anil K. Pradhan
Department of Astronomy, The Ohio State University,
Columbus, Ohio, USA 43210

Abstract. Recent advances in theoretical atomic physics have enabled large-scale calculation of atomic parameters for a variety of atomic processes with high degree of precision. The development and application of these methods is the aim of the Iron Project. At present the primary focus is on collisional processes for all ions of iron, Fe I – FeXXVI, and other iron-peak elements; new work on radiative processes has also been initiated. Varied applications of the Iron Project work to X-ray astronomy are discussed, and more general applications to other spectral ranges are pointed out. The IP work forms the basis for more specialized projects such as the RMaX Project, and the work on photoionization/recombination, and aims to provide a comprehensive and self-consistent set of accurate collsional and radiative cross sections, and transition probabilities, within the framework of relativistic close coupling formulation using the Breit-Pauli R-Matrix method. An illustrative example is presented of how the IP data may be utilised in the formation of X-ray spectra of the Kα complex at 6.7 keV from He-like Fe XXV.

1 Introduction

The main purpose of the Iron Project (IP; Hummer *et al.* 1993) is the continuing development of relativistic methods for the calculations of atomic data for electron impact excitation and radiative transitions in iron and iron-peak elements. Its forerunner, the Opacity Project (OP; Seaton *et al.* 1994; The Opacity Project Team 1995), was concerned with the calculation of radiative parameters for astrophysically abundant elements, oscillator strengths and photoionization cross sections, leading to a re-calculation of new stellar opacities (Seaton *et al.* 1994). The OP work, based on the non-relativistic formulation of the close coupling approximation using the R-matrix method (Seaton 1987, Berrington *et al.* 1987), was carried out in LS coupling, neglecting relativistic fine structure that is not crucial in the calculation of mean plasma opacities. Also, collisional processes were not considered under the OP. The IP collaboration seeks to address both of these factors, and with particular reference to iron and iron-peak elements. The collaboration involves members from six countries: Canada, France, Germany, UK, US, and Venezuela.

The relativistic extension of the R-matrix method is based on the Breit-Pauli approximation (Berrington *et al.* 1995). Collisional and radiative processes may both be considered. However, the computational requirements for the Breit-Pauli R-matrix (hereafter BPRM) calculations can be orders of magnitude more intensive than non-relativistic calculations. Nonetheless, a large body of atomic data has been obtained and published in a continuing series under the title **Atomic Data from the Iron Project** in *Astronomy and Astrophysics Supplement Series*, with 43 publications at present. A list of the IP publications and related information may be obtained from the author's Website: www.astronomy.ohio-state.edu/ pradhan.

The earlier phases of the Iron Project dealt with (A) fine structure transitions among low-lying levels of the ground configuration of interest in Infrared (IR) astronomy, particularly the observations from the Infrared Space Observatory, and (B) excitation of the large number of levels in multiply ionized iron ions (with n = 2,3 open shell electrons, i.e. Fe VII – Fe XXIV) of interest in the UV and EUV, particularly for the Solar and Heliospheric Observatory (SOHO), the Extreme Ultraviolet Explorer (EUVE), and Far Ultraviolet Spectroscopic Explorer (FUSE). In addition, the IP data for the low ionization stages of iron (Fe I – Fe VI) is of particular interest in the analysis of optical and IR observations from ground based observatories. In the present review, we describe the IP work within the context of applications to X-ray spectroscopy, where ongoing calculations on collisional and radiative data for H-like Fe XXVI, He-like Fe XXV, and Ne-like Fe XVII are of special interest.

The sections of this review are organised as follows: 1. Theoretical, 2. collisional, 3. radiative, 4. collisional-radiative modeling of X-ray spectra, 5. atomic data, and 6. Discussion and conclusion.

2 The Close Coupling approximation and the Breit-Pauli R-matrix Method

In the close coupling (CC) approximation the total electron + ion wave function may be represented as

$$\Psi = A\sum_{i=1}^{NF}\psi_i\theta_i + \sum_{j=1} C_j\Phi_J, \tag{1}$$

where ψ_i is a target ion wave function in a specific state $S_i\ L_i$ and θ_i is the wave function for the free electron in a channel labeled as $S_iL_ik_i^2\ell_i(SL\pi)$, k_i^2 being its incident kinetic energy relative to $E(S_iL_i)$ and ℓ_i its orbital angular momentum. The total number of free channels is NF ("open" or "closed" according to whether $k_i^2 <$ or $> E(S_iL_i)$. A is the antisymmetrization operator for all $N+1$ electron bound states, with C_j as variational coefficients. The second sum in Eq. (1) represents short-range correlation effects and orthogonality constraints between the continuum electron and the one-electron orbitals in the target.

The target levels included in the first sum on the RHS of Eq. (1) are coupled; their number limits the scope of the CC calculations. Resonances arise naturally when the incident electron energies excite some levels, but not higher ones, resulting in a coupling between "closed" and "open" channels, i.e. between free and (quasi)bound wavefunctions. The R-matrix method is the most efficient means of solving the CC equations and resolution of resonance profiles (see reviews by K.A. Berrington and M.A. Bautista). The relativistic CC approximation may be implemented using the Breit-Pauli Hamiltonian.

Both the continumm wavefunctions at E $>$ 0 for the (e +ion) system, and bound state wavefunctions may be calculated. Collision strengths are obtained from the continuum (scattering) wavefunctions, and radiative transition matrix elements from the continuum and the bound wavefunctions that yield transition probabilities and photoionization and (e + ion) photo-recombination cross sections (see the review by S.N. Nahar).

Recent IP calculations for the n = 3 open shell ions include up to 100 or more coupled fine structure levels. Computational requirements are for such radiative and collisional calculations may be of the order of 1000 CPU hours even on the most powerful supercomputers.

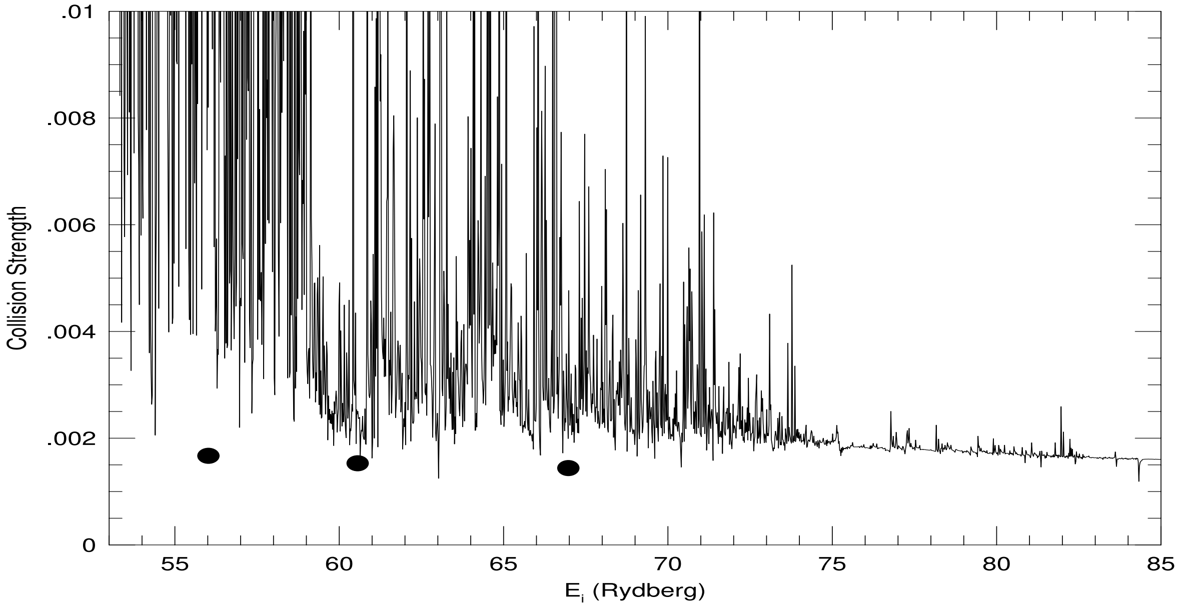

Figure 1: The BPRM collision strength $\Omega(2p^6\ {}^1S_0 \longrightarrow 2p^5\ 3s\ {}^3P_2)$ (Chen and Pradhan 2000); the relativistic distorted wave values are denoted as filled circles (H.L. Zhang, in Pradhan and Zhang 2000)

3 Electron Impact Excitation

Collision strengths and maxwellian averaged rate coefficients have been or are being calculated for all ions of iron. While some of the most difficult cases, with up to 100 coupled fine strcture levels from n = 3 open shell configurations in Fe VII – Fe XVII, are still in progress, most other ionization stages have been completed. In particular fine structure collision strengths and rates have been computes for thousands of transitions in Fe II – Fe VI. For a list of papers see "Iron Project" on www.astronomy.ohio-state.edu/ pradhan.

Work on K-shell and L-shell collisional excitations, begining with the H-like and the He-like ions will be continued under the new RMaX project, which is part of the IP and is focused on X-ray spectroscopy. Work is in progress on He-like Fe XXV (Mendoza *et al.*) and Ne-like Fe XVII. Fig. 1 presents the collision strength for a transition in Fe XVII from the new 89-level BPRM calculation including the n = 4 complex (Chen and Pradhan 2000). The extensive resonance structure is due to the large number of coupled thresholds following L-shell excitation.

4 Radiative transition probabilities

There are two sets of IP calculations: (i) with atomic structure codes CIV3 (Hibbert 1973) and SUPERSTRUCTURE (Eissner *et al.* 1974), and (ii) BPRM calculations. Of particular interest to X-ray work are the recent BPRM calcultions for 2,579 dipole (E1) oscillator strengths for

Fe XXV , and 802 transitions in Fe XXIV (Nahar and Pradhan 1999), extending the available datasets for these ions by more than an order of magnitude. Also, these data are shown to be highly accurate, 1 – 10%.

5 Collisional-Radiative model for He-like ions: X-ray emission from Fe XXV

Emission from He-like ions provides the most valuable X-ray spectral diagnostics for the temperature, density, ionization state, and other conditions in the source (Gabriel 1972, Mewe and Schrijver 1981, Pradhan 1982). The Kα complex of He-like ions consists of the principal lines from the allowed (w), intersystem (x,y), and the forbidden (z) transitions $1^1S \longleftarrow 2(^1P^o,\ ^3P^o_2,\ ^3P^o_1,\ ^3S_1$ respectively. (These are also referred as the R,I,F lines, where the I is the sum (x+y); we employ the former notation). Two main line ratios are particularly useful, i.e.

$$R = \frac{z}{x+y} \ , \tag{2}$$

and

$$G = \frac{x+y+z}{w} \ . \tag{3}$$

R is the ratio of forbidden to intersystem lines and is sensitive to electron density N_e since the forbidden line z may be collisionally quenched at high densities. G is the ratio of the triplet-multiplicity lines to the 'resonance' line, and is sensitive to (i) electron temperature, and (ii) ionization balance. Condition (ii) results because recombination-cascades from H-like ions preferentially populate the triplet levels, enhancing the z line intensity in particular (the level $2(^3S_1)$ is like the 'ground' level for the triplet levels). Inner-shell ionization of Li-like ions may also populate the $2(^3S_1)$ level $(1s^2\ 2s \longrightarrow 1s2s + e)$ enhancing the z line. The line ratio G is therefore a sensitive indicator of the ionization state and the temperature of the plasma during ionization, recombination, or in coronal equilibrium.

For Fe XXV the X-ray lines w,x,y,z are at $\lambda\lambda$ 1.8505, 1.8554, 1.8595, 1.8682 $\AA$, or 6.700, 6.682, 6.668, 6.637 keV, respectively. A collisional-radiative model (Oelgoetz and Pradhan, in progress) including electron impact ionization, recombination, excitation, and radiative cascades is used to compute these line intensties using rates given by Mewe and Schrijver (1978), Bely-Dubau *et al.* (1982), and Pradhan (1985a). New unified electron-ion recombination rates (total and level-specific) are being calculated by S.N. Nahar and collaborators, and electron excitation rates are being recalculated by C. Mendoza and collaborators; these will be employed in a more accurate model of X-ray emission from He-like ions.

Fig. 2 shows illustrative results for doppler broadened line profiles under different plasma conditions (normalized to I(w) = 1). All are at $N_e = 10^{10}\ cm^{-3} << N_c$, so that the R dependence is only on T_e. Figs. 2(a) and 2(b) are in coronal equilibrium, but differing widely in T_e, $10^7 - -10^8$K, as reflected in the broader profiles for the latter case. The ratios R and G show a significant (though not large) temperature dependence in this range. The ionization fractions Fe XXIV/FeXXV and Fe XXVI/FeXXV for the two cases are such that the Li-like iron dominates at 10^7K and the H-like at 10^8K. Figs. 2(a) and (b) illustrate a general property of the He-like line ratios: $G \approx 1$ *in cororal equilibrium* (for other He-like ions it may vary by 10-20%).

On the other hand, the situation is quite different when the plasma is out of equilibrium. In particular, it is known that the forbidden line z is extremely sensitive to the ionization state since it is predominantly populated via recombination-cascades (Pradhan 1985b). Fig. 2(c) illustrates a case where recombinations are suppressed, and the plasma is at $T_e = 10^8$ K. The total G value is now only a third of its coronal value, with the z/w ratio being considerably lower. Although the new recombination and excitation rates may change the number somewhat, it is seen that $G \approx 0.37$ *is a lower limit on an ionization dominated plasma.*

A reverse situation occurs in a recombination dominated plasma. It is known from tomakak studies (Kallne *et al.* 1984, Pradhan 1985b) that the z/w ratio, and hence G, increases practically without limit, as T_e decreases much below the coronal temperature of maximum abundance. $G >> 1$ *observed values imply a recombination dominated source.* However, the z/w ratio may also be enhanced by inner-shell ionization through the Li-like state. More detailed calculations are needed to distinguish precisely between the two cases, and to constrain the temperature and ionization fractions.

Di-electronic satellite intensities (Gabriel 1972) may also be computed using BPRM data for the autoionization and radiative rates of the satellite levels from recombination of e + FeXXV $\longrightarrow$ Fe XXIV (Pradhan and Zhang 1997). This work is in progress.

6 Atomic Data

The atomic data from the OP/IP is available from the Astronomy and Astrophysics library at CDS, France (Cunto *et al.* 1993). The data is also available from a Website at NASA GSFC linked to the author's Website (www.astronomy.ohio-state.edu/ pradhan).

A general review of the methods and data, ("Electron Collisions with Atomic Ions - Excitation", Pradhan and Zhang 2000) is available from the author's website. The review contains an evaluated compilation of theoretical data sources for the period 1992-1999, as a follow-up of a similar review of all data sources up to 1992 by Pradhan and Gallagher (1992) – a total of over 1,500 data sources with accuracy assessment. Also contained are data tables for many Fe ions, and a recommended data table of effective collision strengths and A-values for radiative-collisional models for ions of interest in nebular plasmas.

The collisional data from the IP is being archived in a new database called TIPBASE, complementary to the radiative database from the OP, TOPBASE (see the review by C. Mendoza).

7 Discussion and Conclusion

An overview of the work under the Iron Project collaboration was presented. Its special relevance to X-ray astronomy was pointed out since the IP, and related work, primarily aims to study the dominant atomic processes in plasmas, and to compute extensive and accurate set of atomic data for electron impact excitation, photoionization, recombination, and transition probabilities of iron and iron-peak elements. The importance of coupled-channel calculations was emphasized, in particular the role of autoionizing resonances in atomic phenomena. (A new project RMaX, a part of IP focused on X-ray spectroscopy, is described by K.A. Berrington in this review).

During the discussion, a question was raised regarding the resonances in Fe XVII collision strengths (e.g. Fig. 1), and it was mentioned that new experimental measurments appear

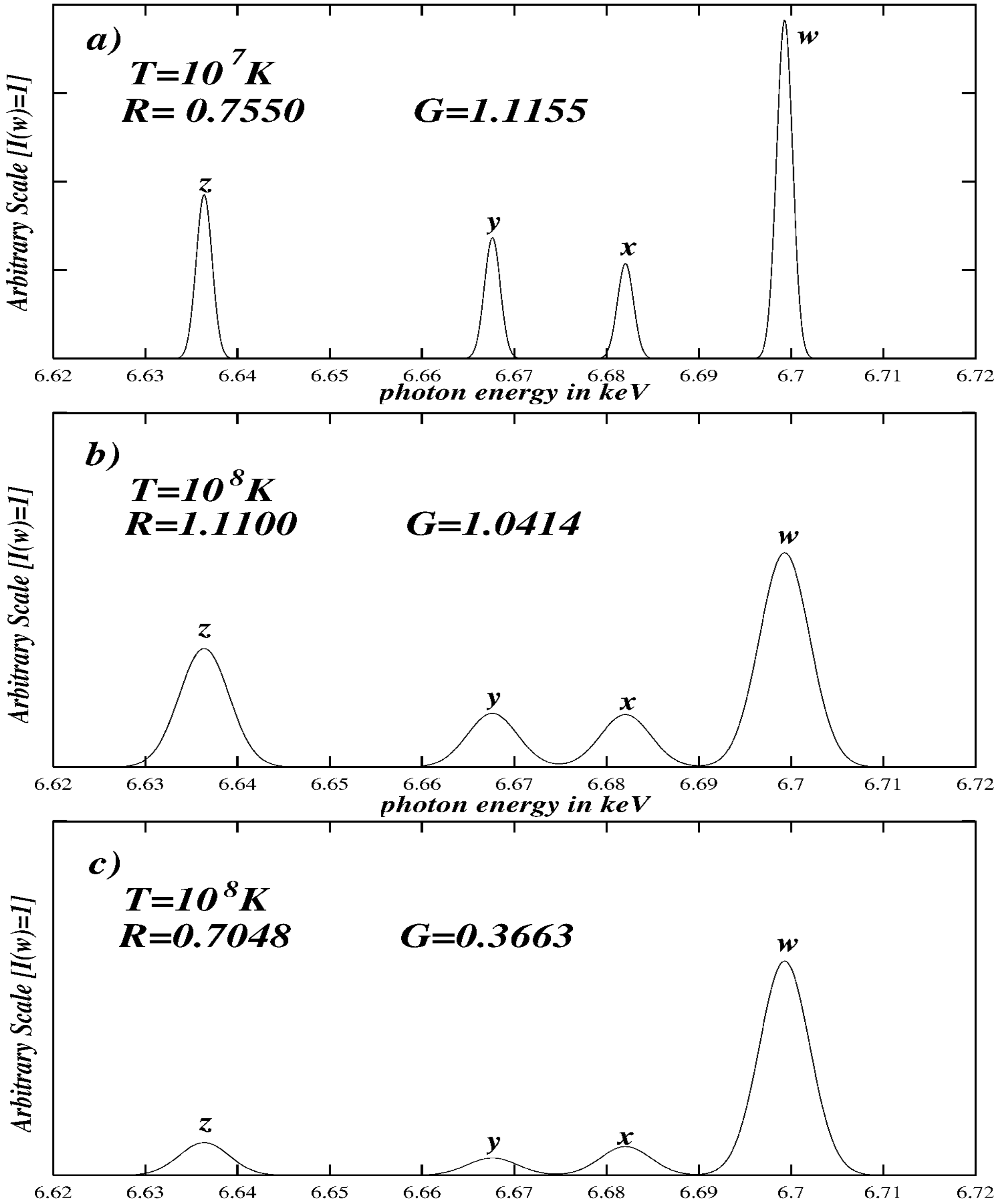

Figure 2: X-ray spectra of Fe XXV (Oelgoetz and Pradhan 2000). The principal lines w,x,y,z and the line ratios R and G are computed at plasma electron temperatues shown. The lines are Doppler broadened. I(w) is normalized to unity.

not to show the expected rapid variations in cross sections. A possible explanation may be that there are numerous narrow resonances in the entire near-threshold region, without a clearly discernible background or energy gap. The measured cross sections are averages over the resonances corresponding to the experimental beam-width. These averaged cross sections themselves may not exhibit sharp variations, unlike more highly charged He-like ions where the the non-resonant background and the resonance complexes are well separated in energy (e.g. He-like Ti XXI, Zhang and Pradhan 1993).

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