SESSION 4. THEORETICAL SPECTROSCOPY

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DISTORTED WAVE CALCULATIONS: APPLICATION TO ASTROPHYSICS AND TOKAMAK PLASMA

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During the last few years, observations of solar phenomena have been carried out by rocket flights, manned satellites like Skylab, unmanned satellites like Orbiting Solar Observatories and more recently Solar Maximum Mission. The wavelengths, line intensities and line profiles in UV and X-ray regions of the solar spectra have been measured. The spectroscopic data obtained are of high spatial and spectral resolution. The goal is to understand the physical properties of the emitting plasma and determine the electron temperatures, densities and volume of the emitting plasma from UV and X-ray spectra.

Since emission lines are seen, this would imply plasma is hot and ionized. The lines are produced when the higher states of the positive ions excited by electron impact decay to the lower states. Therefore, it is necessary to understand the line forming processes and calculate the relevant atomic data for the interpretation of the spectroscopic data. Since the tokamak spectra are similar[1] to the flare spectra, the same atomic data can be used to interpret the tokamak spectra.

The intensity of the line due to the transition from j to i is given by

$$I_{ji} = N_j A_{ji} \frac{hc}{\lambda_{ij}} , \qquad (1)$$

where λ_{ij} is the wavelength of the line, A_{ji} is the transition rate and N_j is the population of the upper level. In the solar corona and in flares the electron densities are of the order of 10^9 to 10^{12} cm^{-3} which are not high enough to maintain a Saha-Boltzmann distribution of level populations. These must be obtained by solving the statistical equilibrium equations.

We assume that the collisional and radiative processes are much faster than the ionization and recombination processes so that the calculation of the level populations can be carried out separately by including only collisional and radiative processes. Therefore, we can deal with one ion at a time and assume that ionization equilibrium exists. This is a good approximation for the lower excited states but not for the higher excited states. We would also assume that the plasma is optically thin.

The level populations N_i are given by the rate equation

$$\frac{dN_i}{dt} = -N_e N_i \sum_{j>i} C^e_{ij} + \sum_{j>i} N_j A_{ji} - N_i \sum_{j<i} A_{ij} + N_e \sum_{j>i} N_j C^d_{ji} , \qquad (2)$$

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where C^e_{ij} is the collisional excitation rate coefficient from level i to j and is given by averaging over the Maxwellian distribution

$$C^e_{ij} = \frac{8.63 \times 10^{-6}}{\omega_i k T_e^{3/2}} \int_{\Delta E_{ij}} \Omega_{ij} \, e^{-E/kT_e} \, dE \qquad cm^{-3} \, s^{-1} . \tag{3}$$

T_e is the electron temperature. Collision strengths Ω_{ij}, dimensionless and symmetric in i and j, are related to the excitation cross section by

$$\Omega_{ij} = E \, \omega_i \, \sigma_{ij} \quad , \tag{4}$$

where E is the incident energy and ω_i is the statistical weight of the lower level i. The de-excitation rate coefficient C^d_{ji} is given by

$$C^d_{ji} = \frac{\omega_i}{\omega_j} \, C^e_{ij} \, e^{\Delta E_{ij}/kT_e} . \tag{5}$$

Other processes which can populate or depopulate the levels must be included in Eq. (2): photoexcitation by background radiation, as from the photosphere of the Sun, the rate for which is given by

$$F_{ij} = D(R) \, A_{ji} / \left(e^{\Delta E_{ij}/kT_R} - 1 \right) \quad , \tag{6}$$

where T_R is the temperature of the blackbody radiation and D(h) is the dilution factor. Stimulated emission, much smaller than spontaneous emission, and proton excitation rates[2] between the fine-structure levels should also be included.

A number of approximations have been made to calculate Ω_{ij}. The Coulomb Born approximation has been used extensively. This approximation overestimates collision strengths near the threshold for excitation. The Gaunt factor approximation based on the Bethe approximation, valid for allowed transitions, is not very reliable. The distorted wave approximation, which is valid when the coupling between the various channels is weak, has been widely used for the last few years. The total hamiltonian of the (N + 1) electron system is

$$H_{N+1} = - \sum_{i=1}^{N+1} \left(\nabla_i^2 + 2Z/r_i \right) + \sum_{i \neq j}^{N+1} 2/r_{ij} \quad , \tag{7}$$

where N is the number of target electrons and Z the nuclear charge. The total wave function is

$$\Psi_n = \mathcal{A} \, \Phi_n \, (1,2,\ldots, N) \, F_n \, (N+1) \quad , \tag{8}$$

where n is the initial or final state. F_n satisfies the equation

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$$\left(\frac{d^2}{dr^2} - \frac{\ell_n(\ell_n+1)}{r^2} + V_{nn}(r) + k_n^2\right) F_n(r) = 0 \quad . \tag{9}$$

In the distorted wave programs[3] developed at University College London (UCL) V_{nn} is chosen to be a central potential and is given by a scaled Thomas-Fermi potential such that

$$\lim_{r\to\infty} V_{nn}(r) = 2(Z-N)/r \quad . \tag{10}$$

The functions $F_n(r)$ which have the usual limit for $r > 0$ and ∞ are made orthogonal to the target orbitals having the same angular momentum. The reaction matrix is given by

$$\begin{aligned} K_{ij} &= -\langle \Psi_i | H_{N+1} - E_T | \Psi_j \rangle \\ &= -\langle F_i | V_{ij} + W_{ij} | F_j \rangle \quad , \end{aligned} \tag{11}$$

where V_{ij} and W_{ij} are the direct and exchange potentials. The short range correlations[3] can be improved by including quadratically integrable functions in the wave functions (8). The reaction matrix K_{ij} is modified then. The T matrix is given by

$$T = -\frac{2iK}{1+iK} \tag{12}$$

and the collision strength for a given parity and total angular and spin momenta L and S is given by

$$\Omega_{ij}^{\pi LS} = \frac{1}{2}(2L+1)(2S+1)\sum_{\ell_i,\ell_j} |T_{ij}|^2 \quad . \tag{13}$$

The total collision strength is given by

$$\Omega_{ij} = \sum_{\pi LS} \Omega_{ij}^{\pi LS} \quad . \tag{14}$$

In general, only the first few incident partial waves ℓ_i are used in the calculation. The contribution for $\ell > \ell_i$, for allowed transitions, is included in the Coulomb Bethe approximation[4].

A better approximation is a close coupling approximation[5]. Though the calculations tend to be difficult and expensive, they have the advantage of including resonances.

The target wave functions Φ_n are calculated using the 'Superstructure' program[6], also developed at UCL. The radial functions are again calculated in a scaled Thomas-Fermi Potential. As pointed out by Lazer[7] that to obtain accurate wave function of highly ionized systems, it is necessary to include all configurations in the same complex of a given principal quantum number and parity. The configuration interaction type wave functions can be used in this program to calculate the energy levels, oscillator strengths and radiative transition rates in LS and intermediate couplings. The term

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coupling coefficients are calculated in this program to transform LS coupling collision strengths to collisions strengths in intermediate coupling[8]. Since we require atomic data for high nuclear charge Z, the relativistic corrections are calculated using the Breit-Pauli Hamiltonian as a perturbation to the non-relativistic Hamiltonian. Atomic data have been calculated for a number of ions, and the level populations and intensity ratios have been calculated for diagnostic purposes by solving the statistical equilibrium equations (2) by assuming that the steady state $\frac{dN_i}{dt} = 0$ exists. We discuss some specific cases.

UV lines of Ca XVII have been observed by Doschek el al[9] in the August 9, 1973 solar flare by using NRL's slitless objective grating (171-630Å) aboard Skylab. Also X-ray lines have been identified by McKenzie and Landecker[10] in solar flares obtained from the Solex Bragg crystal spectrometer aboard the USAF P78-1 satellite. Bhatia and Mason[11] calculated the atomic data using three sets of configurations: Case A: $2s^2$, 2sp, $2p^2$; Case B: Case A + 2s3s, 2s3p, 2s3d; and Case C: Case B + 2p3s, 2p3p, 2p3d.

The energy values for Cases B and C are in good agreement with the observed values. The collision strengths are calculated using Case B configurations and scaled. The collision strengths are in good agreement with the close coupling calculations of Dufton el al[5].

The rates for electric dipole, electric quadrupole and magnetic dipole transitions are proportional to Z^4, Z^6 and Z^{10}, respectively. The rates for magnetic transitions at high Z become comparable to rates for the allowed transitions and therefore, the transitions become very important in the observations of tokamak plasma. The collision strengths for the dipole allowed, spin-forbidden and non-dipole allowed transitions behave like logE, $1/E^2$ and constant, respectively, as $E \to \infty$. Also $Z^2\Omega_{ij} \to$ constant for a fixed E/Z^2. These limits are useful for interpolation or extrapolation of A_{ji} and Ω_{ij}.

The level populations and intensity ratios have been calculated for UV and X-ray lines. The observed[9] intensity ratio for the lines 192.86 and 232.83 Å corresponding to the transitions $2s2p\ ^1P_1 \to 2s^2\ ^1So$ and $2p^2\ ^3P_2 \to 2s2p^3P_2$ is 60. The calculated ratios are 87.6, 62.9 and 59.1 for log Ne = 12, 13, and 14 cm^{-3}, respectively. A comparison with the observed value of 60 would imply an electron density of 5×10^{13} cm^{-3} which is much higher than 3×10^{11} cm^{-3} at 6.3×10^6 K obtained by Dere et al[12] from the measurements of Ca XV and XVI. This would imply an uncertainty in the calibration or the 233Å line is blended. In the X-ray region, the line at 20.456A° ($2s3d\ ^3D_3 \to 2s2p\ ^3P_2$) is density sensitive. But the electron density was not determined as the measured intensities are weak. A line observed at 22.025Å can be associated with the calculated line 22.152A° ($2s3s\ ^1So \to 2s2p\ ^1P_1$). A similar calculation has been carried out for Fe XXIII by Bhatia and Mason[13]. Since then the identification of the lines in the X-ray region given by them has been

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confirmed by McKenzie and Landecker[14]. The lines at 263.76 and 132.83Å due to the transitions $2s2p\ ^3P_1 \rightarrow 2s^2\ ^1S_0$ and $2s2p\ ^1P_1 \rightarrow 2s^2\ ^1S_0$ have been seen by Hinnov[15] in PLT tokamak. The line at 263.76Å obtained in NRL's spectroheliograph is an important line and has been used to study the energy release processes in solar flares. The most intense line of Fe XXIII in the UV region has been seen by Kastner et al[16] using the GSFC grating spectrometer on OSO-5.

The atomic data have been calculated for Mg VI, Si VIII, S X, Ar XII, etc by using the configurations $2s^22p^3$, $2s2p^4$ and $2p^5$ by Feldman el al[17]. The line ratios $(^2P_{3/2} \rightarrow {}^4S_{3/2})/(^2D_{3/2} \rightarrow {}^4S_{3/2})$ and $(^2D_{3/2} \rightarrow {}^4S_{3/2})/(^2D_{5/2} \rightarrow {}^4S_{3/2})$ are density sensitive but not temperature sensitive. These transitions are within the levels of the ground configuration $2s^2p^3$. S X lines have been observed in quiet and active regions of the Sun using NRL's spectrograph aboard Skylab. Using the observed ratios for the lines 1213.00 and 1196.26Å corresponding to the transitions $2s^22p^3\ (^2D_{3/2} \rightarrow {}^4S_{3/2})$ and $2s^22p^3\ (^2D_{5/2} \rightarrow {}^4S_{3/2})$ respectively, Feldman et al[17] inferred an electron density of 10^9 cm^{-3} at 1.3×10^6 K in quiet and active regions of the Sun. A similar calculation has been carried out for Fe XX. The line at 2665.1Å and 824.1Å corresponding to the transitions $2s^2p^3\ (^2D_{5/2} \rightarrow {}^2D_{3/2})$ and $2s^22p^3(^2D_{3/2} \rightarrow {}^4S_{3/2})$ have been seen by Suckewer and Hinnov[18] in PLT tokamak.

Doschek et al[19] inferred the densities in the quiet sun and in coronal holes by comparing the intensities of the intersystem and allowed lines emitted by the ions formed in the transition zone. They used the lines at 1402.77Å ($3p\ ^2P1/2 \rightarrow 3s\ ^2S_{1/2}$) in Si IV, 1908.73Å ($2s2p\ ^3P_1 \rightarrow 2s^2\ ^1So$) in C III, and 1666.15Å ($2s2p^3\ ^5S_2 \rightarrow 2s^2p^2\ ^3P_2$) in O III. But the intersystem and allowed lines were not close in wavelength. Therefore, when comparing the intensities of the various lines, it was necessary to take into account the change in temperature of the emitting plasma as well as the variation of the instrument reflectivity with wavelength. Those problems can be avoided by using the line ratios of the S IV 1406Å intersystem line and the 1403Å resonance line in Si IV. These lines have been observed from Skylab. Bhatia et al[20] calculated the atomic data for S IV using the $3s^23p$, $3s3p^2$ and $3s3d^2$ configurations. But the density they inferred for December 17, and 21, 1973 and January 21, 1974 flares was four times that inferred from O IV measurements. Bhadra and Henry[21], and Dufton and Kingston[22] by using a larger set of configurations calculated the collision strengths in close coupling approximation. The latter calculations include resonances as well. Dufton et al[23] calculated the densities in the quiet sun, coronal holes, active region B and active region C and these are closer to the densities deduced by using other ions.

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The intensity ratio of the allowed lines is temperature sensitive and it can be shown that

$$I_{ji}/I_{ki} \propto e^{-(\Delta E_{ij} - \Delta E_{ik})/kT_e} \quad . \tag{15}$$

This ratio is sensitive to changes to the electron temperature Te if $(\Delta E_{ij} - \Delta E_{ik})/kT_e \sim 1$. Feldman and Doschek[24] inferred the electron temperature ≈ ion temperature using Mg II allowed lines. The intensity ratio of the satellite line to the resonance line is a function of electron temperature and can be used for temperature diagnostics[25].

The Bowen fluorescence mechanism takes place when the wave length of a transition coincides with the wavelength emitted by another ion. This radiation when absorbed will populate the upper levels preferentially and therefore will change the level populations and intensities of the emitted radiation. He II Lyman α (304 Å) coincides with the O III $2p^2\ ^3P_2 > 2p3d\ ^3P_2$ wave length. Bhatia et al[26] calculated the atomic data for O III by using $2s^22p^2$, $2s2p^3$, $2p^4$, 2p3s, 2p3p and 2p3d configurations. The photoexcitation by He II was taken into account by increasing the electron excitation rate coefficient C by PC where C is the rate coefficient for exciting the $2p3d\ ^3P_2$ from $2p^2\ ^3P_2$. The total excitation rate is, therefore, KC, where K = 1+P The level populations e.g. of $2p3d\ ^3P_2$ and $2p3p\ ^3S_1$, were found to be K dependent. Choosing K = 1000 to obtain agreement of the calculated intensity of 304Å line with the intensity observed by Behring et al[27], they calculate the intensities of other lines and multiplets and compare with the observation.

The calculated intensities of the non-photosensitive multiplets 508, 526, 703 and 835Å are in good agreement with the observations of Varanazza and Reeves[28]. Also, the intensities of multiplet components 508.18, 703.85, and 702.90Å agree very well with the observations of Behring et al[27]. The intensity of the multiplet 374Å is higher when photoexcitation is included but is lower than the observed intensity given by Raymond[29]. Dere[30] has pointed out that this line is blended, and according to Raymond (private communication), the observed intensity should be lower than that given in Ref. 29. Finally, the line at 644Å will not be observed at all if photoexcitation is not present and the calculated intensity in the presence of photoexcitation agrees very well with the observation of Veranazza and Reeves[28] (see Fig. 4 of Ref. 26 for more details). Furthermore, the observed multiplet 644Å is due to O III and not N II or O II as suggested by Veranazza and Reeves[28].

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Though the bulk of the plasma is usually hydrogen or deuterium, other gases are added in controlled quantities for diagnostic purposes. Since the temperature in a tokamak is comparable to temperatures reached in solar flares, various stages of ionization of elements are present. Atomic data for various ions of interest have been calculated using UCL programs. The forbidden transitions, in particular magnetic dipole, are of special interest. These lines fall in the UV and EUV spectral regions and are due to transitions between the levels of the ground configurations $2s^2p^k$ of these ions. These lines are well separated in wave lengths and line blending is much less severe than in the case of allowed lines at shorter wave lengths. These transitions can be well observed to determine the line profiles. Ion temperatures can be inferred by measuring the full width at half maximum. Ion concentration and electron density can be determined from the intensities of these lines. Suckewer et al[31] observed lines from titanium ions and compared the observed intensities with the synthetic spectrum calculated by Bhatia et al[32] using the configurations $2s^2$, $2s2p^{k+1}$, $2p^{k+2}$. Suckewer el al[31] observed the Ti XIV 2115.3, Ti XV 2544.8, Ti XVII 3834.4 and 3371.5Å lines along with the allowed Ti XIX 169Å line and their intensity variation with time. The ion density can be calculated by noting that if the level population of the upper level does not vary with electron density, as for $2s^22p^4\ {}^3P_1$ of Ti XV, (see Fig. 3 of Ref. 32), then

$$I_{ji} = \frac{A_{ji}}{4\pi}\int N_j\, dV = \frac{n_j A_{ji}}{4\pi}\int N_T\, dV \quad , \tag{16}$$

where $n_j = N_j/N_t$ is the level of population of the level j. From the measured I_{ji} and the calculated n_jA_{ji} as indicated in Fig. 3 of Ref. 31, they obtained an ion density of 2.6×10^{10} cm^{-3}.

More recently Stratton et al[1] measured the intensity ratios of various lines in Fe XVIII to XXII and compared with intensity ratios inferred from the DW calculations. They conclude (See Table 1 of Ref. 1) that in general the agreement is within 30 percent, the expected accuracy of the distorted wave calculations.

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