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Cross Sections for Electron Impact Excitation of Astrophysically Abundant Atoms and Ions

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ABSTRACT

Electron collisional excitation rates and transition probabilities are important for computing electron temperatures and densities, ionization equilibria, and for deriving elemental abundances from emission lines formed in the collisional and photoionized astrophysical plasmas. Accurate representation of target wave functions that properly account for the important correlation and relaxation effects and inclusion of coupling effects including coupling to the continuum are essential components of a reliable collision calculation. Non-orthogonal orbitals technique in multiconfiguration Hartree-Fock approach is used to calculate oscillator strengths and transition probabilities. The effect of coupling to the continuum spectrum is included through the use of pseudostates which are chosen to account for most of the dipole polarizabilities of target states. The B-spline basis is used in the R-matrix approach to calculate electron excitation collision strengths and rates. Results for oscillator strengths and electron excitation collision strengths for transitions in N I, O I, O II, O IV, S X and Fe XIV have been produced.

1. INTRODUCTION

Collisions of electrons with atoms and ions are major excitation mechanism in a wide range of astrophysical objects such as planetary nebulae, H II regions, stellar and planetary atmospheres, active galactic nuclei, novae and supernovae. The astrophysical plasma diagnostic techniques based on spectroscopic line intensities, profiles and wavelengths have been used to determine temperatures, densities, emission measures, mass motions and elemental abundances. The high quality of spectroscopic data made available by the recent flight instruments has highlighted the need for improvements in the number and accuracy of atomic data. In many cases the accuracy of the astrophysical analysis is limited by the inadequacy of atomic data. Spectral synthesis codes have been developed to generate synthetic spectrum by converting a database of atomic quantities into a model spectrum that can be compared with the observed spectrum. The relative ion abundances can be determined by generating isothermal models for each ion.

Electron collisional excitation rates and transition probabilities are important for computing plasma electron temperatures and densities, ionization equilibria and to derive abundances from emission lines formed in the collisional and photoionized plasmas. The photoionization cross sections are needed for the radiative transfer calculations. Oscillator strengths of abundant and trace elements are needed to study absorption by gases in the interstellar medium. Hot plasmas can be diagnosed using both emission and absorption lines. The computation of true opacity of stellar matter requires both continuum and line opacities.

2. THEORETICAL DETAILS

Recently our research program has been focused to produce accurate and extensive data for transition probabilities and oscillator strengths, photoionization cross sections and electron excitation rates for a large number of lines of O I, N I, O II, O IV, S II, S X and Fe XIV. Being open-shell systems, these atoms and ions pose a serious theoretical challenge because of the difficulty in the determinations of accurate target wave functions and slow convergence of the close-coupling expansion. An accurate description of target wave functions is essential for a reliable scattering calculation. The short-range correlation and long-range polarization effects are expected to be very important for an open-shell system. Consequently, accurate representations of the target wave functions require extensive configuration expansions, with additional complications arising from a strong term dependence of the valence orbitals. The effect of coupling to the continuum is included through the use of pseudostates which are chosen to account for most of the dipole polarizabilities of target states. The non-orthogonal orbitals technique in the multiconfiguration Hartree-Fock approach has been successfully used to describe term dependence of target wave functions and to represent correlation corrections and interactions between the Rydberg states and the perturber states.

The wave function describing the (N+1)-electron system in an internal region surrounding the atom with radius r is expanded in terms of energy-independent functions (Zatsarinny & Tayal 2001; Zatsarinny 2006)

$$\Psi_k \ = \ A \sum_{ij} a_{ijk} \overline{\Phi_i} u_j(r), \tag{1}$$

where $\overline{\Phi_i}$ are channel functions formed from the multi-configurational functions of the target states and the operator A antisymmetrizes the wave function. The radial functions u_j are expanded in the B-spline basis. Use of the B-spline basis leads to a generalized eigenvalue problem of the form

$$\mathbf{H}c = E\mathbf{S}c \tag{2}$$

where **S** is the overlap matrix, which in the case of the usual orthogonal conditions on scattering orbitals reduces to the banded matrix, consisting of overlaps between individual B-splines, but in the more general case of non-orthogonal orbitals has more complicated structure.

3. A BRIEF SUMMARY OF NEW RESULTS

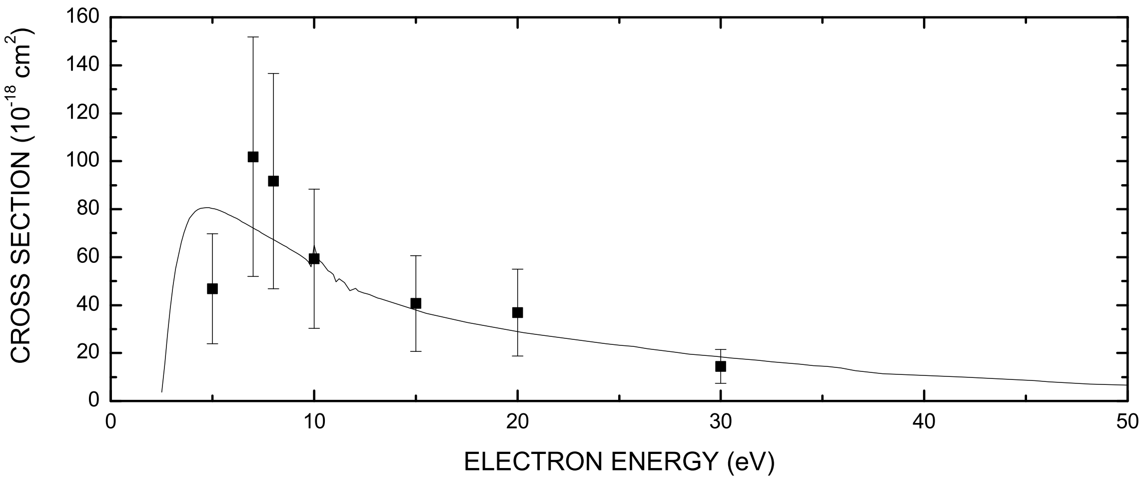

Fig. 1.— Excitation cross section for the N I 5200 Å line as a function of electron energy. Solid curve: 39-state theory; soild rectangles: measured cross sections (Yang & Doering 1996).

The O I ultraviolet features at 1304 and 1356 Å due to excitation of the 3s $^3S^o$ and $^5S^o$ levels are among the dominant features in the spectra of atmospheres of Io, Mars and Venus. In recent years we have carried a collaborative effort with experimental group at the Jet Propulsion Laboratory and our 52-state R-matrix with pseudostates calculation shows excellent agreement with experiment for the 1304 Å resonance line (Johnson et al. 2005). The cross sections for this prominent transition are now considered very well established. We also reviewed O I data and made recommendations regarding the existing theoretical and experimental data sets (Johnson et al. 2005). Collisions of electrons with N I are responsible for many of the strong emission lines observed in the atmospheres of Titan, Sun and in a variety of other astrophysical objects. The 39-state B-spline R-matrix with pseudostates approach has been used to calculate excitation rates (Tayal & Zatsarinny 2005; Tayal 2006). The measured cross sections are available only at a limited number of energies for lines at 5200, 1200 and 1135 Å. A good agreement with measured cross sections can be seen in Fig. 1 except at 5 eV for the forbidden line at 5200 Å. We also recently completed a 47-state

B-spline Breit-Pauli R-matrix calculation for electron impact excitation of O II. Several O II lines are temperature and density sensitive and can provide useful astrophysical plasma diagnostics.

Electron collisional excitation rates for ultraviolet and X-ray lines arising from transitions in S X have been calculated using the Breit-Pauli R-matrix method (Tayal 2005). The 25-state R-matrix theory was used for O IV and the rich resonance structure for the $2s^22p\ ^2P^o$ - $2s2p^4\ ^4P$ transition showed excellent agreement with experiment (Smith et al. 2003). The electron impact excitation calculation for O IV is now extended to 54-state Breit-Pauli R-matrix calculation to cover a large number of transitions in a wide range of temperature. We have investigated electron impact excitation of Fe XIV in collaboration with the experimental group at the Jet Propulsion Laboratory where cross sections have been measured for the $3s^23p\ ^2P^o$ - $3s3p^2\ ^4P$ transition in the low-energy region close to threshold using merged-beams electron-energy-loss method. There is excellent agreement between theory and experiment.

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