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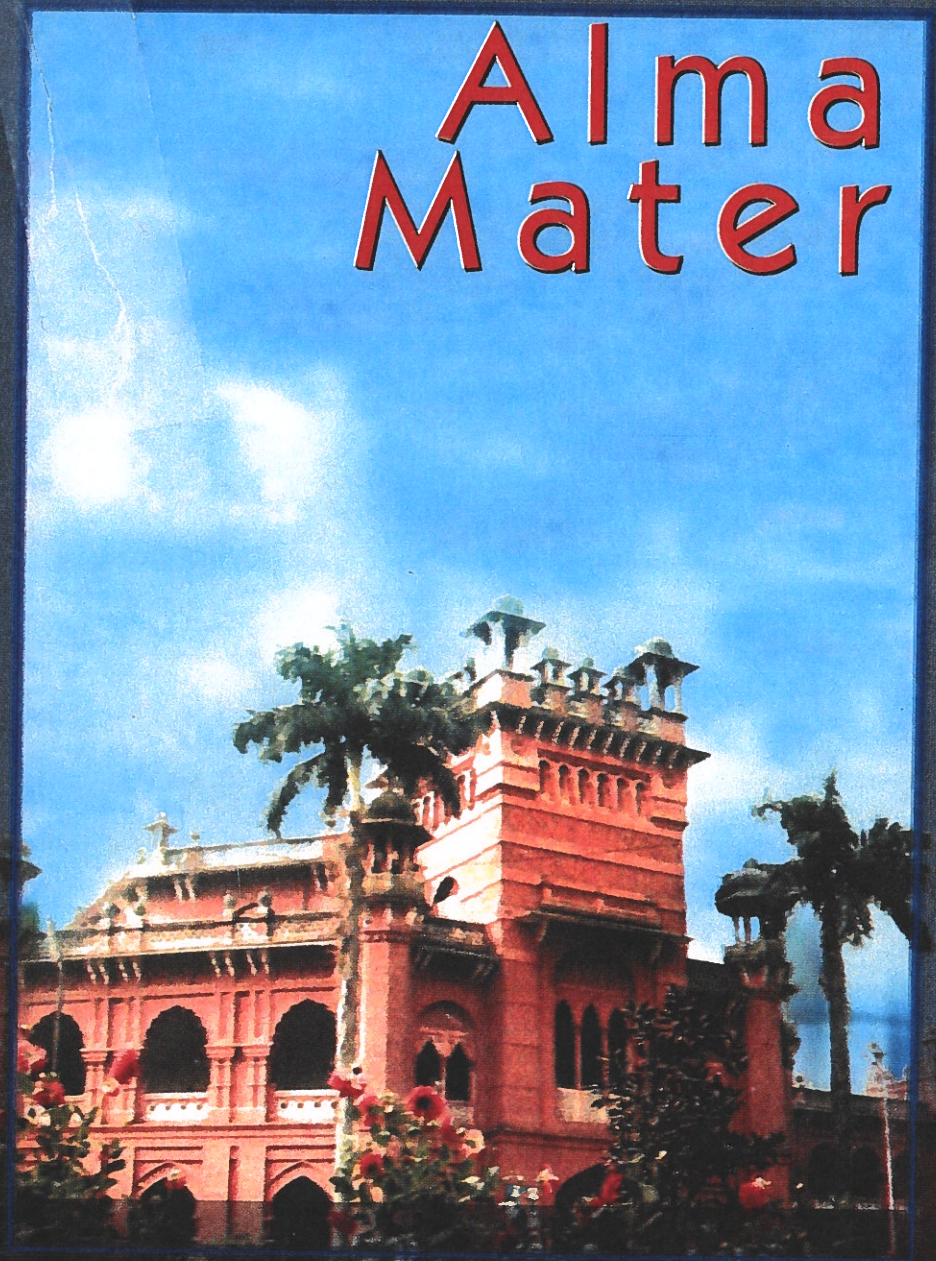

Dhaka Physics Group

With Warmest
Compliments
to
Prof. Sultana Nahar

H. abdullah
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The Dhaka Physics Group is a nebulous collection of some kindred spirits, all coming out of Curzon Hall at various times after getting training in physics from some of the most dedicated and inspiring teachers of the subject. This group is distinguished by its love of physics, and of the Department of Physics , many of them were not actually teachers here but they always share in the joys and sorrows of Curzon Hall. For example, we can never forget that one of us Mr. Ataur Rahmam Khan Khadim was brutally murdered by the Pakistan Army in a dormitory behind the Curzon Hall on the fateful night of 25th March, 1971 when this nation was born in glory and in pain. Another of our very dear friends was A.K. Rafiqullah who in a barely audible voice narrated to some of us about that time :" The first bullet hit my nephew and then his mother and both were instantly killed. Then I heard my eldest son scream and I knew that this was the end. But it was not the end. It was only a beginning of a long journey out of the Waste Land.

What are the roots that clutch,
What branches grow
Out of this stony rubbish ?
Son of man
You can not say or guess.
For you know only
A heap of broken images.

Many people have lent their willing and helping hands in the arduous task of bringing out this volume of broken images and we especially remember with gratitude the co-operation we have received from Mr.A.M. Mozharul Haque, the authorities of the Bank Asia, the Standard Bank and the Editor of the Daily Star. We are also grateful for the unstinted co- operation and help we have received from C.M. Tufail Sami, Jamilur Reza Chowdhury, Abdul Qurder, Mrs, Shawar Sadeque, Md. Tauhid Hossain, Baman Das Basu , Subhas Ch. Biswas, Anwar Motin Chaudhury, Prasad Ranjan Das, Amitav Manzoor, Tanvir Habib, Monoranjan Acharyaa, and Subal Chandra Dey. A special word of thanks goes to Md. Mosharof Hossain Titas for his cheerful handling of our endless demands in the actual process of composition and printing of this labour of love.

Board of Editors

Dhaka
1st May, 2006

Some Recent Publications From Curzon Hall Alumni : Cosmic Strings, Collapsing Matter, Wavelets and All that

Some Popular Writings of Curzon Hall Alumni : "I want to know how God created this world."

Atomic Processes in Astrophysical Plasmas

Sultana N. Nahar

1 Introduction

The basic atomic processes that dominant the astrophysical plasmas are:

i) Radiative bound-bound transition for excitation and de-excitation:

$$X^{+z} + h\nu \Leftrightarrow X^{+z*},$$

where the ion, X, is of charge, Z. The atomic parameters of interest are the oscillator strengths (f) for excitation and the radiative decay rate or Einstein's coefficient for radiative transition probability (A-value) for de-excitation.

ii) Photoionization (PI) and radiative recombination (RR):In a single step process, an electron goes to continuum by absorption of a photon:

$$X^{|z} + h\nu \Leftrightarrow X^{|z|1} + \varepsilon$$

The inverse process is the radiative recombination (RR): These are non-resonant processes.

iii) Autoionization (AI) and dielectronic recombination (DR):

$$e + X^{+z} \leftrightarrow (X^{+z-1})^{**} \leftrightarrow \begin{cases} e+X^{+z} & AI \\ X^{|z-1}+h\nu & DR \end{cases}$$

In this two step process, the electron is colliding with an ion, excites the target as well as attaches itself to a highly excited level forming a doubly excited state, known as the autoionizing state. This state either leads to autoionization (AI), a radiationless process where

the electron goes free and the target goes to ground state, or to dielectronic recombination (DR) when the electron is captured by emission of a photon. The inverse of DR is phtoionization. Autoionizing states introduce resonances in atomic processes.

The atomic parameters of interest for phoptoionization and recombination process are the photoionization cross sections (σ_{PI}), recombination cross sections (σ_{RC}) and recombination rate coefficients (α_{RC}).

iv) The collisional process of electron-impact excitation (EIE) is

$$e + X^{+z} \rightarrow e' + X^{+z*}$$

This is one of the primary processes for spectral formation in astrophysical plasmas since the excited ion decays by emission of a photon. Collisional excitation may also go through an intermediate doubly excited autoionizing states introducing resonances in the cross sections. The relevant atomic parameters of interest are collisional cross sections (σ_{EIE}) and the collision strengths (Γ).

v) The collisional process of electron-impact ionization is

$$e + X^{|z} \rightarrow e' + e + X^{|(z|1)}$$

The atomic parameters of interest, ionization cross sections (σ) and collision strengths (S), for this process can be obtained experimentally more accurately than theoretical calculations and measured values are in general available. We are not concerned with this process at this time.

Each of the above processes needs to be treated separately to obtain the relevant parameters. Astrophysical model applications, such as determination of radiation transfer in plasmas for the

opacities, need a large amount of atomic data as these deal with many atomic levels and over a wide energy ranges. The Close Coupling (CC) R-matrix method employed by the Opacity Projcct (1995, 1996) and the Iron Projcct (Hummer et al. 1993) enable computation of such large scale atomic data.Work under these two projects have produced the detailed features of autoinizing resonances in the radiative and collisional processes for most of atoms and ions for the first time.The method enables self-consistent sets of atomic parameters if the atom or the ion is described by the same wavefunction expansion for each process. This reduces the uncertainty introduced in applications involving different processes and approximations.

The large amount of atomic data and plasma opacities obtained under the OP and the IP are available electronically from databases, such as TOP base and TIPTOPBASE at CDS (Astronomy and Astrophysics Journal, France), Goddard-NASA, and the Ohio State University.

2 Theory

The R-matrix method in the close-coupling (CC) approximation (Burke & Robb 1975) is the most powerful method for ab initio atomic calculations. The entire region is divided in to two, the inner and the outer regions of the R-matrix sphere with the atom or ion at the center. The inner region wavefunction is represented by a basis set known as the R-matrix basis. The size of the sphere is chosen such that the effects of the electron-electron correlation and other short-range Potentials is zero at the boundary. The method has been extended extensively under the OP for radiative processes (Seaton 1987, Berrington et al 1987, Nahar and Pradhan 1994a, 1995) and the IP for electron Collisional as well radiative processes (Hummeretal).

1993, Berrington et al. 1995). Futher extension was made by developing the new unified treatment for total electron-ion recombination (Nahar and Pradhan 1992, 1994a). The computational packages of codes span a number of stages before obtaining the atomic parameters.

A brief summary of the theories to treat the atomic processes is given below.

a) The Hamiltonian

In non-relativistic atomic structure calculations, the energies and wavefunctions of an N-electron ion are obtained through optimum solution of the Schrodinger equation,

$$\left[\sum_{i=1}^{N}\left\{-\nabla_i^2-\frac{2Z}{r_i}+\sum_{j>i}^{N}\frac{2}{r_{ij}}\right\}\right]\psi=E\psi, \qquad (1)$$

where $\psi=\psi(\gamma SLM_S M_L|r_{1,\ldots,r_N})$ are the bound solutions consisting of a linear combination of configuration state functions.

We include the relativistic effects through Breit-Pauli approximation. The approximation is more suitable for multi-electron systems than one-particle Dirac equations. The relativistic N-electron Hamiltonian in the Breit-Pauli (BP) approximation is (e.g. Eissner 1991)

$$H_{BP}=H_{NR}+H_{mass}+H_{Dar}+H_{so}+ \frac{1}{2}\sum_{i\neq j}^{N}\left[g_{ij}(so+so')+g_{ij}(ss')+g_{ij}(css')+g_{ij}(d)+g_{ij}(oo')\right] \qquad (2)$$

where H_{NR} is the non-relativistic Hamiltonian, and

$$H_{mass} = -\frac{\alpha^2}{4}\sum_i p_i^4, \quad H_{Dar} = -\frac{\alpha^2}{4}\sum_i \nabla^2(\frac{Z}{r_i}), \qquad H_{so} = \alpha^2 \sum_{i=1} \frac{Z}{r_i^3} l(i).S(i) \quad (3)$$

are the relativistic one-body mass correction, Darwin, and spin-orbit interaction terms. The rest are two-body interaction terms with notation c for contraction , d for darwin, o for orbit, s for spin and a prime indicates 'other'. The last three two-body terms very weak and may be igorned. The fine structure terms, that is spin-other-orbit (os') and spin-other-spin (ss') terms,

$$g_{ij}(so + so') = -\alpha^2(\frac{r_{ij}}{r_{ij}^3} \times P_i)(s_i + 2s_j) + \frac{r_{ij}}{r_{ij}^3} \times p_j).(s_j + 2s_i),$$

$$g_{ij}(ss') = 2\alpha^2 \frac{s_i.s_j}{r_{ij}^3} - 3\frac{(s_i.r_{ij})(s_j.r_{ij})}{r_{ij}^5} \quad (4)$$

together form the full Breit interaction term,

$$H^B = \sum_{i>j} \left[g_{ij}(so + so') + g_{ij}(ss')\right].$$

Spin-orbit interaction splits the LS terms into fine-structure levels labeled by $J\pi$ where J is the total angular momentum π is the parity. Rest of the relativistic terms improve the energy values and the wavefunctions.The electron-electron correlations contribute dominantly through $1/Z$ dependence compared to the relativistic effects. Hence, in the Breit-Pauli R-matrix (BPRM) approximation, where correlation effects are treated more accurately, only the one-body relativistic terms are included.

However, for weak bound-bound radiative transitions of type intercombination and forbidden the relativistic corrections play an important role in general to fine structure components.The one-body terms very as α^2Z^4 and contribute in general more than the two-body terms with one less power of Z. We include the contribution of the one-body terms and the full Breit interaction term for such transitions through atomic structure calculations.

b) Coupled Channel Wavefunction

The atomic system is representcd by a coupled eigenfunction expansion in the close-coupling approximation. The ion or atom trcated as a (N+1) electron system where the core, called the" target" in CC approximation, has N number of electrons and the (N+1)th electron is the interacting electron which can be bound or in continuum. The total wavefunction of the (N+1) electron system is described as :

$$\Psi_E(c+ion) = A\sum_i^N X_i(ion)\theta_i + \sum_j c_j\Phi_j(e+ion), \qquad (5)$$

where X_i is the target ion or core wavefunction in a specific state $S_iL_i\pi_i$ or level $J_i\pi_i$, θ_i is the wavefunction of the interacting (N+1)th electron in a channel labeled as $S_iL_i(J_i)\pi_i k_i^2\ell_i(SL\pi\ or\ J\pi); k_i^2$ is the incident kinetic energy. Φ_j is the correlation functions of (e+ion) system that compensates the orthogonality condition and short range correlation interations.

The complex resonant structures in photoionization, recombination, and in electron impact excitation are included through couplings of channels in Ψ_E. To each excited target state, there corresponds to a series of doubly excited states, $S_iL_i(J_i)\pi_i vl$, know as the Rydberg series, most of which are autoionizing states as they lie above the ionizing potential and cause resonances. v is the effective quantum number.

The wavefunction X_i of the core or "target" is obtained through a configuration interaction atomic structure calculations before starting the R-matrix calculations. Most commonly used code for the purpose is SUPERSTRUCTURE (Eissner et al 1974. Eissner and Zeippen 1981, Eissner 1991, Nahar et al. 2003). The nuclear and electron-electron potential is represented by the statistical Thomas-Fermi-Dirac-Amaldi model potential $V^{sm}(r) = \frac{z_{eff}(\lambda_{nl,r})}{r}$ where $Z_{eff}(\lambda_{nl,r}) = Z\left[e^{-zr/2} + \lambda_{nl}(1-e^{-zr/2})\right]$ and λ_{nl} are the Thomas-Fermi scaling parameters for each orbital. The calculations include relativistic effects in Breit-Pauli approximation. The target wavefunctions are used as the input for the R-matrix suite of codes.

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