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The RmaX Network: R-matrix calculations for X-ray atomic processes

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Abstract. The RmaX network ('R-matrix for X-rays') has been formed to calculate using ab-initio R-matrix techniques electron and photon collisional properties to higher precision than hitherto for transitions in the soft X-ray region, to improve understanding of the dynamics of X-ray transitions in astrophysical plasmas.

New opportunities are arising with the launch of the new generation X-ray observatories such as *Chandra* and *XMM*. A significant amount of theoretical work on atomic collisional processes is in train for these major space projects. Such work includes gathering and assessing existing data, and the generation of atomic data to higher accuracy and new data where appropriate.

The RmaX Network is an international partnership formed to manage the calculation of the new data, and follows previous successful projects, namely the Opacity Project (OP) for calculating radiative opacities (The Opacity Project Team 1995) and the Iron Project (IP) for collisional data for metal ions (Hummer et al. 1993). The name 'RmaX' refers to the use of ab-initio R-matrix methods (Burke and Berrington 1993) in the computation of atomic data for X-ray transitions.

What atomic data are required? X-ray emitting plasmas may be divided into two broad categories:

- Hot ($10^6 - 10^8$K), and maintained at a high degree of ionization by electron collisions (e.g. stellar coronae and shocked regions). In a 'coronal' plasma, line excitation is principally by electron collisions while the ionization state is determined by collisional ionization and dielectronic recombination. In this case K- and L-shell collisional processes predominate, although excitation to higher valence shells may be important also.

- Cool ($10^4 - 10^5$K) and ionized by some energetic photon source (e.g. AGN, XRB, CV). In these X-ray photoionized plasmas, line excitation is by a mixture of collisional excitation and recombination and cascading, while the ionization state depends upon photoionization by energetic photons and low temperature recombination. For this case, K- and L-shell photoionization predominates and excited state recombination coefficients may be derived from valence shell photoionization cross-sections. The ionization of metallic ions by energetic photons is also important in understanding the opacity of the ISM to X-rays, and in this case the absorption may be by inner-shell processes in near neutral species.

How are these data to be calculated?

One of the most widely used, and perhaps most fully developed, of the sophisticated models available to atomic physics today is the R-matrix approach. This is essentially a basis function approach, in which the wavefunction $\Psi(E)$ for an electron interacting with an N-electron target is expanded in a many-electron basis in a local region, while outside the system is reduced to a simple potential scattering

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problem. In each case the Shrödinger equation is used:

$$\Psi(E) = \sum_k A_k(E)\psi_k, \qquad H_{N+1}\Psi(E) = E\Psi(E)$$

$$H_{N+1} = \sum_{n=1}^{N+1} [\frac{1}{2}\nabla_n^2 - \frac{Z}{r_n} \qquad + \sum_{m>n}^{N+1} \frac{1}{|r_n - r_m|}] + H_{\text{Breit-Pauli}}.$$

The strength of the R-matrix method is that the ψ_k basis is energy independent, so that a single diagonalization of the internal-region Hamiltonian in this basis yields the expansion coefficients and wavefunctions at all energies – a vital advantage when physical properties are required over a large energy range. The R-matrix method is therefore an accurate general purpose method for the calculation of optical and electron-ion properties, including collisional excitation, photoionization and bound-state properties such as energy levels and transition probabilities. All of these properties can be obtained in intermediate coupling, incorporating relativistic effects through the use of the Breit-Pauli R-matrix method, as implemented in the R-matrix programs (Hummer etal 1993; Scott and Taylor 1982; Berrington etal 1995).

New directions in R-matrix models are concerned with 'discretising' the continuum, such that ionization can be described as an excitation process involving discrete states in the continuum (Berrington et al. 1997; Berrington and Nakazaki 1998). In the case of photoionization, these procedure allows for the investigation of soft X-ray ionization of atoms by ejection of the inner-shell electron(s).

Indeed, the optical properties of atoms and ions in X-ray fields are dominated by the inner-shell 'edge', where the cross section for photoionization for example can rise abruptly, often by at least an order of magnitude. The usefulness of the R-matrix method is that resonances, which modify the inner-shell 'edge' with quantum mechanical interference, are modelled ab initio, giving a highly accurate picture of the edge. In laboratory experiments on simple atoms R-matrix calculations are already modelling experiments to high accuracy (Berrington et al. 1997; Berrington and Nakazaki 1998). This confirmation by benchmarking of theory against experiment and observation is an essential part of the RmaX network, for scientific reliability.

We have identified four main tasks which define the goals of this proposal.

1. Electron impact excitation involving K- and L-shells of Fe ions. This includes inner-shell excitation as well as excitation to higher valence shells, neither of which was included in the Iron Project (which dealt with atomic data for IR, optical, UV and EUV transitions). These data will treat the problem of excitation in the "coronal" plasmas.

2. Photoionization of K- and L-shell electrons in light elements, C, N, O and Ne as well as in Fe ions. These data are required to treat the problems of ionization in the X-ray photoionized plasmas (e.g. AGN), as well as that of the X-ray opacity of the ISM.

3. Radiation damping and total dielectronic photorecombination rates. The aim here is two-fold: to include radiation damping in the excitation and photoionization cross sections obtained as above and to provide photorecombination data for Fe ions for use in calculating the ionization equilibrium of the 'coronal' plasmas.

4. Radiative transitions for fine-structure levels. We are extending our Opacity Project techniques to intermediate coupling, to obtain accurate and complete data sets of transition probabilities for fine-structure levels for the ions referred to above. These data are needed to carry out accurate level population calculations for heavy, or highly-ionized systems.

Finally, we aim to interface with the needs of the X-ray astrophysical community, in the provision of the new atomic data to the community via atomic databases and inclusion of the data in emission analysis codes.

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All data are available from TOPbase, access via web or telnet: european site at CDS Strasbourg, telnet 130.79.128.5; american site at the HEASARC GSFC, telnet 128.183.126.111; at either site, username=topbase, password=Seaton+

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