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Atomic Data Needs for Modeling Photoionized Plasmas

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Abstract.

Many of the fundamental questions in astrophysics can be addressed using spectroscopic observations of photoionized cosmic plasmas. However, the reliability of the inferred astrophysics depends on the accuracy of the underlying atomic data used to interpret the collected spectra. In this paper, we review some of the most glaring atomic data needs for better understanding photoionized plasmas.

1. Introduction

Spectroscopic observations of photoionized plasmas can be used to address many of the fundamental questions in astrophysics. Planetary nebulae (PNe) and H II regions provide information about the primordial He abundance which is an important constraint for theories of cosmological nucleosynthesis (Pagel 1997). In addition, PNe can be used to study the processing and dredging that goes on during the lifetime of a star (Clegg et al. 1987; Boroson et al. 1997; Hyung, Aller, & Feibelman 1997). H II regions can also be used to determine galactic abundance gradients (Pagel 1997). Stellar winds from hot stars input energy, momentum, and nuclear processed material into the interstellar medium and are vital for the evolution of galaxies (Kudritzki & Puls 2000). Active galactic nuclei (AGN) and quasars can be used to study General Relativity (Nandra et al. 1997), the physics of matter-radiation interaction in extreme environments (Kahn & Liedahl 1995), and through measurements of the chemical abundances in the emitting gas, the chemical evolution of massive galaxies (Hamann & Ferland 1993, 1999). Low-redshift Lyα clouds can be used to study the origin and chemical evolution of gas at large distances from galaxies and also to provide constraints on the ionizing spectrum between 1 and 4 Ryd in order to discriminate between an extragalactic radiation field due to AGN or due to O stars from starburst galaxies (Shull et al. 1998). Studies of the IGM yields information on the chemical evolution of the universe and the shape of the metagalactic radiation field as a function of redshift (Songaila & Cowie 1996; Giroux & Shull 1997; Savin 2000).

The physical conditions in photoionized plasmas are governed by a host of microphysical atomic processes. Ionization of the plasma is due to photoionization (PI), Auger ionization, collisional ionization, and charge transfer (CT). Electron-ion recombination occurs through radiative recombination (RR), dielectronic recombination (DR), three-body recombination, and CT. Line emission is due to RR, DR, CT, and electron impact excitation (EIE). Bound-bound transitions due to photoabsorption can be important. Free electrons are assumed to have a predominately Maxwellian velocity distribution with a kinetic temperature T_e determined by the balance between the processes of heating (photoelectric, mechanical, cosmic ray, etc.) and cooling (predominantly inelastic collisions between electrons and other particles). Together these various processes determine the ionization structure, the electron temperature, the level populations of excited states, and all emission and absorption features. The observed spectrum results from transport of radiation through the depth-dependent physical conditions. No analytical solutions are possible because of the intricacies, and large-scale numerical simulations must be performed instead.

Interpreting the spectra of photoionized cosmic sources is carried out using spectral simulation codes such as CLOUDY (Ferland et al. 1998), ION (Netzer 1996; Kaspi et al. 2001), NEBU (Péquignot et al. 2001) and XSTAR (Kallman & Bautista 2001). Codes which have the capabilities of modeling stars with extended outflowing atmospheres (i.e., stellar winds) have been written by Hamann & Koesterke (2000), Haser et al. (1998), Hillier & Miller (1998), Short et al. (2001), and others. Fundamental to the reliability of these simulations and any inferred astrophysical conclusions is an accurate understanding of the underlying atomic physics which produces the observed spectra. In this overview we will briefly outline some of the most glaring atomic data needs which were presented at this conference.

2. Atomic Data Needs

Reliable atomic data are needed for nearly every atomic process involving the first 30 elements of the periodic table. The vast quantity of needed data is overwhelming. Given the limited resources currently devoted worldwide to this task, it will likely take decades to produce all the needed data. Here we attempt to identify high priority atomic data needs. In specific, our aim is to help researchers identify and address those uncertainties in our understanding of atomic physics which have the largest impact on our ability to address the fundamental questions in astrophysics.

The easiest selection criterion which can be used to prioritize the needed atomic data is for researchers to focus on the twelve most abundant elements, namely H, He, C, N, O, Ne, Mg, Si, S, Ar, Ca, and Fe. But even within this set of twelve, the amount of needed atomic data is still vast. To provide further guidance, we discuss below some of the specific atomic physics which needs to be better understood for astrophysics. Our discussion focuses on those issues which were raised during the conference as being important for the understanding of photoionized plasmas. The review here is complementary to the recent article by Ferland et al. (1998) which also discusses the atomic data needs for modeling photoionized plasmas.

2.1. Charge Transfer (CT)

The importance in photoionized plasmas of CT on H and other atoms, as well as on H_2, has long been recognized (e.g., Péquignot et al. 1978; Péquignot & Aldrovandi 1986). At the relevant temperatures ($k_B T_e \sim 1$ eV), CT on H is the dominant recombination mechanism, for many one- to four-times charged ions in photoionized plasmas (Kingdon & Ferland 1996). Surprisingly, modeling has also shown that CT on H of iron ions five-times charged and higher can significantly affect photoionized plasmas (Ferland et al. 1997). This may also hold for ions of other elements.

Total CT rates are needed for ionization balance calculations. State specific partial rates are needed for line emission predictions. Most of the rates currently being used for plasma modeling have been calculated using a Landau-Zener (LZ) approximation and are not expected to be reliable to better than a factor of ~ 3, but the error may be even larger. Recent laboratory measurements have shown LZ calculations can be off by an order of magnitude (Thompson et al. 2000). Much theoretical and experimental work is needed to provide reliable CT rates for modeling cosmic plasmas.

2.2. Dielectronic Recombination (DR)

DR rates at the low temperatures appropriate for photoionized plasmas are theoretically and computationally challenging. It is particularly difficult to calculate accurate resonance energies for DR resonances at electron-ion relative energies close to zero eV. Laboratory measurements have consistantly found errors even in state-of-the-art theory for resonance energies and strengths below ~ 3 eV (DeWitt et al. 1996; Schippers et al. 1998; Schippers et al. 2001; Savin et al. 2001). These near zero eV resonances often dominate the DR rate in photoionized plasmas.

Care also needs to be given to states which are forbidden to autoionize in LS coupling. Recent measurements of DR onto C IV have shown the importance at low temperatures of DR via these LS forbidden autoionizing states (Mannervik et al. 1998; Schippers et al. 2001).

Currently, the majority of DR rates for modeling photoionized plasmas come from older calculations. These rates, given the computational power available at the time and the theoretical approximations used to make the calculations tractable, are expected to be somewhat unreliable, particularly at low temperatures. This lack of reliable low temperature DR rates is one of the dominants uncertainties in the ionization balance in photoionized plasmas (Ferland et al. 1998).

Modern calculational techniques can be used to produce the needed DR rates. However, given the discrepancies found between theory and experiment at low energies, it is clear that improvements to the theoretical techniques are called for. Until these needed theoretical advances are achieved, the only way to produce reliable low temperature DR rates will involve a co-ordinated effort between laboratory measurements and theoretical calculations.

2.3. Electron Impact Excitation (EIE)

Many plasma diagnostics used for interpreting spectra of AGN, H II regions, and PNe use EIE-generated line emission from transitions between low-lying energy levels of various atomic ions (Osterbrock 1989). The upper state in the observed transitions can be populated by direct EIE (a one-step processes) or by resonant EIE (a two-step processes). Particularly challenging to calculate is the contribution to the total EIE rate due to resonant EIE. This channel involves dielectronic capture to an excited (autoionizing) state of the recombined system which then autoionizes to the upper level of interest in the initial ion. This indirect excitation process is the dominant population mechanism for many important transitions. For example, for $^3P_1 - {}^3P_2$ and $^2P_{1/2} - {}^2P_{3/2}$ transition within the valence shell, calculations carried out including resonance effects can yield EIE rates over an order of magnitude larger than calculations which do not account for resonances (Oliva, Pasquali, & Reconditi 1996). For situations where resonance EIE is important, reliable EIE rates requires knowing the position of those autoionizing levels lying within $\sim$ 4 eV of the ground state (Oliva et al. 1996). Accurately determining these resonance energies is extremely challenging theoretically and experimentally.

2.4. Energy Levels

Reliable energy levels are important for modeling and interpreting spectra from stellar winds of hot stars. Bound-bound photoabsorption transitions between 800 and 1300 Å can dramatically affect stellar spectrum (Hillier 2001) and type Ia supernovae spectra (Pauldrach et al. 1996). A significant number of these transitions are due to states involving electrons in $n \geq 4$ levels, up to $n = 15$ in some situations (Kurucz 2001). For many ions, no accurate measured wavelengths exist for the corresponding transitions. Theoretical energy levels must be used and the resulting wavelengths can be shifted by $\sim$ 1 Å or sometimes more (Haser et al. 1998). Once the energy levels are reliably known, then improved (photoabsorption) oscillator strengths can be calculated.

Of all the cosmically-abundant heavy metals in stellar atmospheres, iron has the richest spectrum. Of particular importance for understanding stellar atmospheres and wind are states involving $n \geq 4$ levels in Fe IV, V, and VI. The article by Hillier (2001) in this conference proceedings briefly discusses and demonstrates the importance of these high-lying levels in models of stellar winds from O stars.

2.5. Photoionization (PI)

The majority of PI cross sections currently used by astrophysicists for valence shell electrons come from OPACITY Project (OP) calculations (Opacity Project Team 1995). The OP energy levels are uncertain by 1-2% (Verner, Barthel, & Tytler 1994). This translated directly into uncertainties in the resonance structure of the PI cross section and can introduce significant uncertainties when calculating PI rates due to spectral lines (Verner et al. 1996). Accurate knowledge of this resonance structure is particularly important in the wavelength regions around H I Lyα, He I Kα, and He II Lyα, as well as near other astrophysically important lines. To reduce the effects of accidental coincidences between resonances and spectral lines, OP results are often averaged over resonances (Verner et al. 1996, Kallman & Bautista 2001). It is also worth noting that the OP assumption of LS-coupling is not satisfactory for closed shell systems (Verner et al. 1994).

Recent laboratory advances have finally allowed PI measurements of valence shell for a few astrophysically important singly- and doubly-charged ions (e.g. Kjeldsen et al. 1999, 2000, 2001). Reasonable agreement has been found between theory and experiment for most of these systems. But for Fe II, which is one of the astrophysically most important ions (Viotti, Vittone, & Friedjung 1988), significant discrepancies remain (Kjeldsen 2000).

Innershell PI of ions plays an important role in determining the ionization and thermal structures and line emission of X-ray photoionized plasmas. The innershell PI cross sections currently used for modeling these plasmas have been calculated using a Hartree-Slater central field approximation (Reilman & Manson 1979; Verner et al. 1996). The calculations do not account for any of the structure in the PI cross section near the innershell ionization thresholds. To date, these calculations have been benchmarked only with measurements on atoms.

Multielectron ionization can occur as a result of innershell PI. This is due to Auger processes which occur as the electronic structure of the ion relaxes to fill the innershell hole. Auger yields are currently estimated using theoretical and experimental results for atoms from the early 1970's (Kaastra & Mewe 1993 and references therein). These estimates have never been tested for ions and their reliability is highly questionable.

3. Conclusions

Shortcomings in our current theoretical and experimental capabilities in atomic physics as well as a lack of available atomic data hinder our ability to infer reliably the properties of many cosmic plasmas. This in turn limits our ability to address many of the fundamental issues in astrophysics. In order to help improve the situation, we have attempted to list here some of the most glaring atomic data needs for a better understanding of photoionized cosmic plasmas. It is our hope that this review will help to guide the future research of theoretical and experimental atomic physicists. Given the current resources being devoted to removing the above described uncertainties in our understanding of atomic physics, it seems likely that it will require decades to remove these uncertainties and provide data needed by the astrophysicists.

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