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Approximating the X-ray Spectrum Emitted from Astrophysical Charge Exchange

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Charge Exchange (CX), both onto ions in the solar wind and potentially in other astrophysical contexts, can create X-ray emission lines largely indistinguishable from those created in collisional or photoionized plasmas. The prime distinguishing characteristic is in the distinctly different line ratios generated by the CX process. A complete astrophysical model of the process would require a vast number of atomic calculations; we describe here an approximate approach that will allow astronomers to evaluate the likely contribution of CX to an observed spectrum. The method relies upon an approximate calculation of the CX cross section paired with detailed atomic structure calculations used to determine the emission lines. Simulated spectra based on observed solar wind CX data are shown for both current (Suzaku) and near-term (Astro-H) missions.

1 Introduction

X-ray astrophysicists were alerted to the importance of Charge Exchange (CX) when Cravens (1997) showed that electrons from neutral hydrogen and helium transferring into highly-excited states of solar wind ions could explain why comet C/Hyakutake 1996 B2 appeared to emit X-rays (Lisse et al. 1996). The Solar Wind CX (SWCX) process creates an entirely line-dominated spectrum, primarily in the 0.05-1.0 keV bandpass. Cox (1998) pointed out that although CX is not intrinsically bright, its bandpass and location could mean that it a significant contributor to the soft X-ray background, and thus that it is a major contamination source in many diffuse sources (*e.g.* Smith et al. 2005; Miller et al. 2008). CX has also been suggested as a possible source of some distant astrophysical emission (Lallement 2009, Liu, Mao & Chen 2011). In all likelihood, X-ray satellites such as *Chandra, XMM–Newton,* and *Suzaku* regularly observe CX spectra, but the lack of parameterized models hinders both the identification and analysis of such sources. We describe here a simplified method to calculate model spectra from an astrophysical plasma undergoing CX. While not exact, this method will allow astrophysicists to determine if an observation is likely to contain CX emission lines and estimate the plasma parameters necessary to generate such lines.

2 Method

The charge exchange process involves an electron transferring from one atom or ion to another. Typically, the type of charge exchange relevant to X-ray astrophysics involves a donor hydrogen atom and a highly ionized metal recipient such as O^{+7} or Si^{+10}, although in some cases such as comets (*e.g.* Cravens 2002) or planets in the Solar system (*e.g.* Bhardwaj et al. 2007) the donors can be metals or molecules. The electron maintains roughly the same binding energy in the process, leaving the recipient ion in an excited state that then radiatively decays. Evaluating the impact of this process on the emitted X-ray spectra involves some fundamental difficulties, both in atomic physics and astrophysics. From an atomic physics perspective, the exact cross section for charge exchange into a particular quantum state at low impact energies is difficult to calculate theoretically, although a number of results are now available for selected ions (*e.g.* Kharchenko & Dalgarno 2001, Kharchenko et al. 2003). It is clear that the CX cross section dominates other possible processes that lead to X-ray emission, such as collisional excitation or recombination. A related uncertainty also exists in the astrophysical modeling, as it is not possible to determine with any accuracy the density of donor atoms and recipient ions in a given region of space. Individual situations do exist where these can be estimated, such as charge exchange in the solar wind where ions in the solar wind are directly measured by satellites like ACE and WIND and models exist for the geocoronal or heliospheric neutral atoms (Koutroumpa et al. 2006, 2009). Thus, while there remain many ions without explicit cross section calculations, this omission is matched by our lack of knowledge of the mixing in hot plasma / dense cloud interaction regions that could lead to CX spectra. Although not ideal, these difficulties mean that we may assume that CX, if possible, will occur and any approximations in the model should not undermine the final result.

We will therefore use an enhanced version of the basic method described by Wegmann et al. (1998), which uses a hydrogenic model for the CX cross section into the highly-excited state:

$$\sigma = 8.8 \times 10^{-17}\mathrm{cm}^2 \, \frac{q-1}{\frac{q^2}{2n^2} - |I_p|} \tag{1}$$

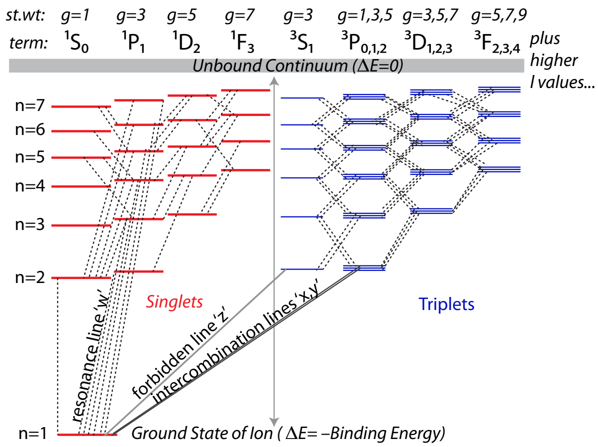

Fig. 1 *Schematic Grotrian diagram for a Helium-like ion with selected radiative (downward) transitions marked as dashed lines. Charge exchange transitions between a hydrogenic ion and a neutral hydrogen atom with binding energy -13.6 eV will result in an ionized hydrogen ion and a highly excited Helium-like state whose binding energy is again -13.6 eV; as an example, for O VII this is* $n \approx 7$.

where q is the charge of the ion, n the principal quantum number, and I_p is the ionization potential in atomic units (*i.e.*, 1 au = 27.2 eV). Once the charge has been 'exchanged' onto a highly-excited level of the ion, our model tracks the emission resulting from radiative decays of the ion using detailed calculations of the ionic structure (see Figure 1 for the He-like case). Effectively, the electron decays towards the ground state like a pachinko ball, radiating photons at each step. As implied by Figure 1, this means for example that CX into a He-like triplet state will lead to enhanced forbidden and intercombination lines (as almost any exchange into a triplet state results in such lines). Meanwhile, CX into the He-like singlet state will lead to enhanced (relative to a purely collisional model in the ground state) high-n resonance transitions from np^1P_1 to the ground state.

Predicting the actual line emission requires first determining the exact atomic level (or distribution of levels) of the charge-exchanged ion. We follow the approximation described by Janev & Winter (1985), which found that the peak of the principle quantum number n distribution is at

$$n' = q\sqrt{\frac{I_H}{I_p}}\left(1 + \frac{q-1}{\sqrt{2q}}\right)^{-1/2} \quad (2)$$

where again q is the charge of the ion, I_H is the ionization energy of the neutral ion (assumed here to be hydrogen), and I_p is the ionization potential in atomic units. Although this is only the peak of the distribution, for this initial work we assumed all the ions ended up in this level; we will relax this assumption in future work, although we do not expect it to change our results qualitatively.

The final line strengths are determined using the atomic structure and radiative transition data available in the AtomDB v2.0.1 (`http://www.atomdb.org`), to follow the various paths available as the ion stabilizes by radiative decay. In some cases, however, we found that the initial electron transfer would put the ion in a higher state than is available in the AtomDB (which typically extends to $n = 5$ at a minimum for ions that can emit X-rays in a collisional plasma and to $n = 10$ for the hydrogenic and helium-like isosequences). Following these ions required that we perform a large atomic structure calculation to determine the energies and radiative transition rates of all levels up to at least n', the predicted state of the post-CX system. We calculated all ions of astrophysical interest up to $n \leq 13$ (in Ni^{+27}) using the AUTOSTRUCTURE (Badnell 1986) code. The largest number of levels needed (for the ion Ni^{+20}) was 2,374. Until fairly recently, these calculations were simply not feasible given computational limitations, but now the primary limitation is the time required to set up the calculations and to check the results.

The primary uncertainty in the process, given that the Wegmann et al. (1998) cross section is summed over all LS states for a given n, is the total final angular momentum (L) of the exchanged electron. The correct result will be velocity-dependent, which is problematic since in most cases the input ion velocity (or position) will not be known. Following the approximate nature of this model, we address this uncertainty by simply providing a range of options for the model. The four different distributions considered were:

1. "Even:" weighted evenly by total angular momentum L
2. "Statistical:" weighted by the relative statistical weight of each level
3. "Landau-Zener:", weighted by the function
$$W(l) = \frac{l(l+1)(2l+1) \times (n-1)! \times (n-2)!}{(n+l)! \times (n-l-1)!} \quad (3)$$
4. "Separable:" weighted by the function
$$W(l) = \frac{(2l+1)}{Z} \times \exp\left[\frac{-l \times (l+1)}{z}\right] \quad (4)$$

The latter two methods are from Janev & Winter (1985). We will use method (1) as the default, but by providing the alternative models we will allow users to test the sensitivity of their data to the model approximation. Despite the simple nature of these models, we expect they will be useful to check if charge exchange could or could not be responsible for some or all of an observed spectrum.

3 Results

Solar wind charge exchange (SWCX) primarily affects the 0.1-1 keV X-ray band, due to the relatively low ionization temperature of the solar wind. The exact distribution of ion states depends upon the wind type (fast or slow), and a flare or coronal mass ejection will have an entirely different set of ionization states. Von Steiger et al. (2000) used data from the *Ulysses* satellite to measure a range of solar wind ion parameters and found that the ionization states of most ions of C, O, Si, and Fe can be described as being from a plasma in collisional ionization equilibrium at temperatures between $0.9 - 1.6 \times 10^6$ K, with the exception of a secondary peak

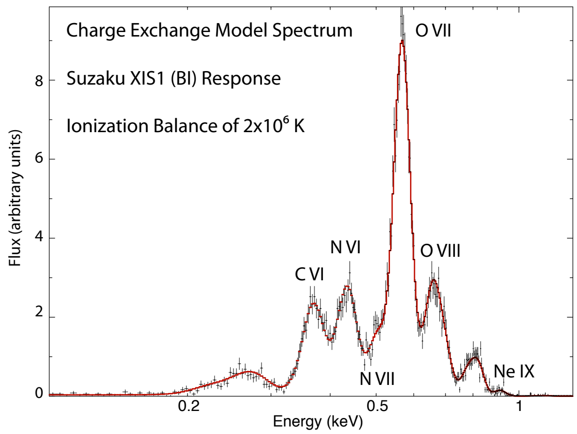

Fig. 2 Predicted SWCX as observed by the Suzaku BI CCD from a plasma with photospheric abundances and the ionization distribution of a plasma in collisional equilibrium at 2×10^6 K.

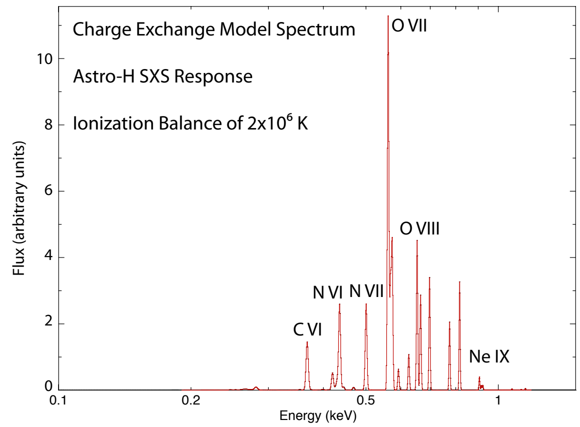

Fig. 3 Same model as Figure 2 simulated using the Astro-H SXS X-ray microcalorimeter. Only a fraction of the visible lines are labelled; many of the higher energy lines are higher n transitions from the same ions.

in iron ions at a temperature around $2 - 3 \times 10^6$ K. While von Steiger et al. (2000) found there was variation in the ionization temperature and abundances as a function of the origin of the wind (*i.e.* the 'fast' wind from the polar coronal holes, or the 'slow' wind from the solar equator), the overall picture is one of relatively low ionization states. While a coronal mass ejection could easily have much higher ionization states, these are rare and should not affect the average observation of SWCX emission.

Figure 2 shows the shape of pure SWCX emission in the Suzaku BI CCD assuming solar photospheric abundances and an ionization balance from a 2×10^6 K plasma in collisional ionization equilibrium (Bryans et al. 2006, 2009). At this temperature, 7% of Oxygen ions are fully stripped (O^{+8}), while 44% have one electron (O^{+7}). Nitrogen is 50% fully-stripped (N^{+7}) and 40% hydrogen-like (N^{+6}), and Carbon is 90% fully stripped (C^{+6}). Neon, for comparison, is only 2% hydrogen-like (Ne^{+10}) and 97% helium-like (Ne^{+9}). As a result, the Ne IX lines are quite weak, while the O VII lines are strong due to the abundance of oxygen in general and the large number of O^{+7} ions available to recombine. Observationally, Suzaku has detected strong evidence of O VII and O VIII SWCX lines (Smith et al. 2007), but calibration uncertainties at lower energies and other processes at higher energies makes other detections hard. Astro-H should be able to detect these lines and determine their origin based on their unique line ratios; Figure 3 shows this same model as observed by the Astro-H X-ray microcalorimeter SXS.

While the model in Figure 2 shows that SWCX can create a spectrum where O VII dominates, the ionization temperature modestly exceeds the *Ulysses* measurements. Figure 4 shows a more realistic simulation of the three strongest elements in a SWCX spectrum as would be observed in the full field of view (2.8x2.8 arcmin^2) of the Astro-H SXS. These results have been scaled such that the overall O VII flux is in rough agreement with observations, which show that that the O VII surface brightness varies between 1-6 ph cm^{-2}s^{-1}sr^{-1} (Koutroumpa et al. 2011). The ionization

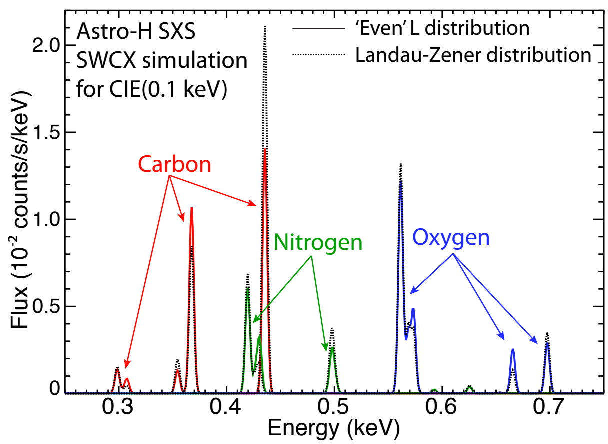

Fig. 4 Predicted SWCX from carbon, nitrogen, and oxygen as observed by the Astro-H SXS X-ray microcalorimeter from a plasma with solar abundances and the ionization distribution of a plasma in collisional equilibrium at 1.2×10^6 K. Both an 'even' distribution of angular momenta and a Landau-Zener distribution is shown.

temperature is 0.1 keV, or $\sim 1.2 \times 10^6$ K, in line with the predicted results. The elemental abundances were still assumed to be photospheric, but the von Steiger et al. (2000) results imply this is a reasonable assumption for C, N, and O, although elements with low first ionization potentials (*e.g.* Mg, Si, S, and Fe) are typically overabundant.

Figure 4 not only shows the predicted spectrum, it also shows the variation expected between two different models of the exchanged ion's total angular momentum. Although the two models ("Even" and "Landau–Zener") predict quite different distributions, the variations in the final spectrum remain similar, with only modest differences. Examinations of the other two models show that this is a characteristic result in the X-ray band emission. Transitions between high-n states do vary quite a bit, but these primarily lead to optical or UV lines which will be difficult to detect. The X-ray lines, however, do not show differences larger than a factor of 50% or so – comparable to the estimated accuracy of the entire approach.

4 Conclusions

Calculating an accurate and complete model for the charge exchange spectrum from the solar wind spectrum has been long considered a completely intractable problem, due to the difficulty of complete cross section calculations, the vast number of ions and energy levels, and our uncertainty about the location of the solar wind ions and heliospheric neutral elements.

This project achieves an approximate but useful answer by avoiding the difficult cross section and ion position questions, assuming these will be simply fit to the available data. Meanwhile, the problem of large structure calculations has been largely solved by the growth of computing power and the easy availability of large disks (each CX model calculation take nearly 0.3 GB to store, or 1.2 GB for the complete set). Our results show that different assumptions for the angular momentum distribution of the exchanged electron do affect the final spectrum, but generally the differences are quantitative rather than qualitative. Foster et al. (2012, in prep.) will describe these results in more detail, including a new model for use in XSPEC.

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References

Badnell, N. R. 1986, JPhysB, 19, 3827
Bhardwaj, A., et al. 2007, P&SS, 55, 1135
Bryans, P. et al. 2006, ApJS, 167, 343
Bryans, P., Landi, E. & Savin, D. W. 2009, ApJ, 691, 1540
Cox, D. P. 1998, LNP, 506, 121
Cravens, T. E. 1997, Geophys. Res. Lett. 24, 105
Cravens, T. E. 2002, Science, 296, 1042
Foster, A. et al. 2010, BAAS, 41, 524
Janev, R. K., & Winter, H. 1985, Phys. Rep., 117, 265
Kharchenko, V. & Dalgarno, A. 2001, ApJ, 554, L99
Kharchenko, V. et al. 2003, ApJL, 585, L73
Koutroumpa, D. et al. 2006, A&A, 460, 289
Koutroumpa, D. et al. 2009, ApJ, 697, 1214
Koutroumpa, D. et al. 2011, ApJ, 726, 91
Lallement, R. 2009, SSR, 143, 427
Lisse et al. 1996, Science, 274, 205
Liu, J., Mao, S. & Wang, Q. D. 2011, MNRAS, 415, L64
Miller, E. et al. 2008, PASJ, 60S, 95
Smith, R. K. et al. 2005, ApJ, 623, 225
Smith, R. K. et al. 2007, PASJ, 59S, 141
von Steiger, R. et al. 2000, JGR, 105, 27217
Wegmann, R. et al. 1998, P & SS, 46, 603

