X-RAY PHOTOABSORPTION IN KLL RESONANCES OF O VI AND ABUNDANCE ANALYSIS

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ABSTRACT

It is shown that photoabsorption via autoionizing resonances may be appreciable and used for abundance analysis. Analogous to spectral lines, the “resonance oscillator strength” $f$ may be defined and evaluated in terms of the differential oscillator strength $df/d\epsilon$ that relates bound and continuum absorption. X-ray photoabsorption in KLL ($1s^22s2p$) resonances of O vi is investigated using highly resolved relativistic photoionization cross sections with fine structure. It is found that $f$ is comparable to that for UV dipole transition in O vi ($2s-2p$) and the X-ray ($1s^21s^22p^5P^0$) transition in O vii. The dominant O vi (KLL) components lie at 22.05 and 21.87 Å. These predicted absorption features should be detectable by the Chandra X-Ray Observatory and the X-Ray Multimirror Mission. The combined UV/X-ray spectra of O vii/O vii should yield valuable information on the ionization structure and abundances in sources such as the “warm absorber” region of active galactic nuclei and the hot intergalactic medium. Some general implications of resonant photoabsorption are addressed.

Subject headings: atomic processes — line: formation — line: identification — radiation mechanisms: thermal — ultraviolet: general — X-rays: general

1. INTRODUCTION

Whereas line absorption has been well studied and used for diagnostics and abundance analysis (Spitzer 1978), resonant absorption does not appear to have been similarly considered. This is probably due to the general complexity of resonances that require rather elaborate atomic physics calculations. On the other hand, resonances are ubiquitous and may considerably affect the effective cross sections. In this Letter the theoretical treatment of resonant absorption is generalized using the quantity of the differential oscillator strength that describes both bound-bound and bound-free absorption on either side of the ionization threshold. The method is applied to K shell X-ray absorption in lithium-like oxygen.

The O vi UV absorption in the $2s^-2p$ $^2P^2_{3/2, 1/2}$ transition at 1031.91 and 1037.61 Å is widely observed in sources such as quasars and active galactic nuclei (AGNs; Mathur et al. 1994; Tripp, Savage, & Jenkins 2000) and Far-Ultraviolet Spectroscopic Explorer sources (e.g., Savage et al. 2000). Hellsten et al. (1998) have predicted an “X-ray forest” of O vii and O viii absorption lines from the low-$\zeta$ hot intergalactic medium as a probe of baryonic matter. Recently, X-ray absorption and emission-line spectra have been reported from the Chandra X-Ray Observatory (CXO) from H- and He-like ions such as O vii and O viii (Kaspi et al. 2000; Kaastra et al. 2000). In their work, Mathur et al. (1994) reported on UV/X-ray absorption from the same element but in different ionization states, O vi and O vii, from the “warm absorber” region of AGNs. The possibility of the same ionic species (O vii) as both the UV and X-ray absorber is therefore of further interest for ionization structure and abundance studies. It is shown in this Letter that resonant K shell X-ray absorption by O vii should lie among, but distinct from, the prominent emission lines of O vii due to $2s^-2p^5P^0 \rightarrow 1s^2S^0$ transitions.

KLL resonances are normally seen as emission lines (Gabriel 1972). Dielectronic recombination of highly ionized ions—for example, $e + Fe \rightarrow Fe^{24+}$—leads to dielectronic satellite (DES) lines that are useful diagnostics of high-temperature sources such as tokamaks and solar flares (e.g., Bely-Dubau et al. 1982; Beiersdorfer et al. 1992). The radiative decay rates of many DES lines of Fe xxv approach or exceed autoionization rates (e.g., Pradhan & Zhang 1997). For lighter elements, such as oxygen, radiative decays are much smaller, and these resonances should manifest themselves primarily in absorption, as demonstrated in this work.

2. THEORY AND COMPUTATIONS

The differential oscillator strength may be used to relate bound-bound and bound-free absorption as follows (e.g., Seaton 1983; Fano & Rau 1986; Pradhan & Saraph 1977):

$$\frac{df}{d\epsilon} = \frac{(\nu/2\zeta^2)f_{\text{line}}, \epsilon < I,}{(1/4\pi^2\alpha a_0^2)\sigma_{\text{pi}}, \epsilon > I,} (1)$$

where $f_{\text{line}}$ is the line absorption oscillator strength, $\sigma_{\text{pi}}$ is the photoionization cross section, $I$ is the ionization potential, $\zeta$ is the ion charge, $\nu$ is the effective quantum number at $\epsilon = -z^2/\nu^2$ in rydbergs, and $\alpha$ and $a_0$ are the fine-structure constant and the Bohr radius, respectively. The quantity $df/d\epsilon$ describes the strength of photoabsorption per unit energy, in the discrete bound-bound region as well as the continuum bound-free region, continuously across the ionization threshold. We may write

$$\lim_{\epsilon \to 0} \left(\frac{\nu^2}{2\zeta^2}\right)f(I_j - I_a) = \lim_{\epsilon \to 0} \left(\frac{1}{4\pi^2\alpha a_0^2}\right)\sigma_{\text{pi}}[I_j - \epsilon(I_j)] (2)$$

where $I_j, I_a$ represent the symmetries of the initial and final bound levels and $J$ represents the continuum symmetry, governed by the usual dipole selection rules $\Delta J = 0, \pm 1$; $\pi \to -\pi$. The photoionization cross sections contain Rydberg series of autoionizing resonances converging on the excited levels of the residual (photoionized) ion. The effective photoabsorption is generally enhanced in the vicinity of resonances.

The $df/d\epsilon$ reflects the same resonance structure as the $\sigma_{\text{pi}}$ in the bound-free continuum. Combining the two forms of $df/d\epsilon$, we therefore define, in the vicinity of a resonance, the
integrated “resonance absorption oscillator strength” as

$$\tilde{f}_{res}(J_i \rightarrow J_f) = \int \frac{df(J_i \rightarrow J_f)}{de} \, de,$$

where $J_i, J_f$ represent the initial bound and the final continuum symmetries. Equation (3) may be evaluated from the detailed $\sigma_{\text{res}}$ for the symmetries concerned provided the resonance profile is sufficiently well delineated. In practice this is often difficult, and elaborate methods need to be employed to obtain accurate positions and profiles (the background and the peaks) of resonances. Relativistic effects need to be included to differentiate the fine-structure components. Using the coupled channel formulation based on the $R$-matrix and the relativistic Breit-Pauli $R$-matrix (BPRM) method (Burke, Hibbert, & Robb 1971; Berrington, Eissner, & Norrington 1995), a large number of photoionization cross sections have been calculated for all astrophysically abundant elements, including resonance structures, particularly in the Opacity Project and the Iron Project works (Seaton et al. 1994; Hummer et al. 1993). The BPRM formulation has been extended to theoretically self-consistent calculations of photoionization/recombination of atomic systems (e.g., Nahar, Pradhan, & Zhang 2000a, 2000b; Zhang, Nahar, & Pradhan 1999), including a unified treatment of total non-resonant and resonant recombination (radiative and dielectronic recombination).

Photoionization of, and electron recombination to, an atom is described in terms of the same eigenfunction expansion over coupled levels of the residual (“core” or “target”) ion. Recently, BPRM photoionization/recombination calculations have been carried out for Li-/He-/H-like carbon and iron: C iv/C v/C vi (Nahar et al. 2000a) and Fe xxiv/Fe xxv/Fe xxvi (Nahar et al. 2000b) for applications to X-ray photoionization and non-LTE modeling. We similarly consider the photoionization of the ground state of O vi, 1s$^2$2s (2$^2$D$_{3/2}$), into all $n = 1, 2, 3$ fine-structure levels of O vii—1s$^2$2s$^2$(2$^2$S), 1s$^2$2s$^2$(2$^2$P), 1s$^2$2p$^2$(3$^2$P, 3$^2$S), and 1s$^2$2p$^2$(3$^2$D). The autoionization and radiative decay rates and cross sections with and without radiative decay of resonances are calculated by analyzing the poles in the complex dipole matrix elements using the method described in (Pradhan & Zhang 1997). The cross sections are resolved on a very fine mesh of up to $10^{-6}$ eV.

3. RESULTS

Figure 1a shows the photoionization cross section of O vi from the L shell (2s) ionization threshold at O vii (1s$^2$2s$^2$) up to the K shell ionization thresholds at 1s$^2$2s, 1s$^2$2p levels of O vii. Converging on to the K shell edges are the KLL n ≥ 2 complexes of resonances. We resolve the lowest resonance “doublet” feature at $E \approx 41.5$ ryd into four fine-structure com-

**Fig. 1.**—(a) Photoionization cross section of O vi. The KLL resonance complexes at 22.05 and 21.87 Å are resolved in (b) and (c) including the fine-structure $J$-components. Note the different energy and cross section scales: the break at 40 ryd in (a) and log $\sigma$ in (b) and (c). The resonance peaks in (b) and (c) are up to 4 orders of magnitude higher than in (a).
TABLE 1
CALCULATED PARAMETERS FOR THE PHOTOOBSORPTION RESONANCES IN O VI

| Identification | \(\lambda_{ex}\) (Å) | \(E_r\) (KeV) | \(j_r\) | \(\Gamma_r\) (ryd, s\(^{-1}\)) | \(\Gamma_r\) (ryd, s\(^{-1}\)) |
|---------------|----------------|--------|------|----------------|----------------|
| 1s2p(^3P)2s \(^1P_{1/2}\) (t) ........ | 22.05 | 0.56227 | 0.1410 (0.1924) | 3.11 (−4), 6.42 (12) | 1.26 (−4), 2.60 (12) |
| 1s2p(^3P)2s \(^3P_{1/2}\) (u) ........ | 22.05 | 0.56231 | 0.2670 (0.3837) | 2.76 (−4), 5.70 (12) | 1.28 (−4), 2.65 (12) |
| (\(j_r\)(\(\lambda_{22.05}\)) = 0.408 (0.5761) |
| 1s2p(^3P)2s \(^3P_{3/2}\) (t) ........ | 21.87 | 0.56696 | 0.0216 (0.0217) | 3.41 (−3), 7.11 (13) | 1.46 (−5), 3.01 (11) |
| 1s2p(^3P)2s \(^3P_{3/2}\) (s) ........ | 21.87 | 0.56700 | 0.0390 (0.0391) | 3.43 (−3), 7.09 (13) | 1.32 (−5), 2.72 (11) |
| (\(j_r\)(\(\lambda_{21.87}\)) = 0.0606 (0.0608) |

Components of the 1s2s2p complex in detail in Figures 1b and 1c. The peak values in Figures 1b and 1c are up to 4 orders of magnitude higher than the “edges” in Figure 1a and are indicative of the corresponding photoabsorption resonance (PAR) strengths. We label these as PAR in absorption to distinguish them from the same resonances seen as DES lines in emission for other Li-like ions such as Fe xxiv, mentioned above. The computed wavelengths of the two features in Figure 1a are at 22.05 and 21.87 Å, each with twin \(J = 0.5, 1.5\) components shown in Figures 1b and 1c. (The energy scale is also given in units of KeV on the top of Fig. 1a.)

It is clearly important to resolve the resonances completely in order to evaluate the PAR strength \(j_r\), according to equation (3). The probability of resonances decaying radiatively back to the bound state(s) of O vi, versus the autoionization probability, is included using the radiation damping procedure described in Pradhan & Zhang (1997). Although not obvious on the log scale, the radiatively damped cross sections (solid lines) are up to 40% lower than undamped ones (dashed lines) at peak values. The resonances in Figure 1c have no significant damping (dashed and solid lines merge). The computed resonance positions \(E_r\), the autoionization and radiative decay rates \(\Gamma_i\) and \(\Gamma_r\), and the PAR strengths \(f\) using radiatively damped and undamped cross sections (the latter in parenthesis) are given in Table 1.

Figure 2 shows the computed differential oscillator strength \(df/d\varepsilon\) for O vi photoabsorption over a wide energy range, from the 2s−2p transition in UV to the X-ray absorption in KLL. The fine-structure \(J = 0.5, 1.5\) has been summed over in oscillator strengths and photoionization cross sections. The BPRM line oscillator strengths for the discrete (2s \(^1S_{1/2}\)−np \(^3P_{1/2, 3/2}\)) transitions were also computed. In accordance with equation (2), there is smooth continuation of \(df/d\varepsilon\) across the 2s ionization threshold. Equation (2) provides a stringent check on both the line oscillator strengths and photoionization cross sections for each symmetry.

The relative line and resonance strengths in O vi are quali-

FIG. 2.—Differential oscillator strength \(df/d\varepsilon\) (summed over fine structure) for bound-bound and bound-free photoabsorption in O vi from the lowest energy UV transition 2s−2p at 1034 Å to the predicted X-ray PAR transitions at 22.05 and 21.87 Å.
tatively apparent from Figure 2. Quantitatively, the computed PAR strengths are given Table 1. Identification of the PAR “satellites” is in accordance with the standard DES notation (Gabriel 1972), where the KLL resonances are labeled by letters a–v. The four dominant components of the 1s22s2p complex according to the calculated $\Gamma_o, \Gamma_i, \Gamma_r, \Gamma_u$ are the ones labeled $i, u, r, v$. Two weaker components, $g$ and $s$, are not resolved since their autoionization rates are about $2$ orders of magnitude smaller, and therefore their contribution to photoabsorption should be negligible (see, for example, the corresponding $\Gamma_o$ for Fe xxv in Bely-Dubau et al. 1982 and Pradhan & Zhang 1997). The calculated $\Gamma_o$ for resonances at 21.87 Å are roughly $2$ orders of magnitude smaller than the $\Gamma_u$, whereas for the resonances at 22.05 Å, $\Gamma_o$ and $\Gamma_i$ are comparable. That accounts for the significant radiation damping in the latter case (Fig. 1b). The computed $f_i$ (eq. [3]) for the PAR satellites are found to be comparable to typical line oscillator strengths $f_i$ for dipole transitions. The combined $f_i(\lambda 22.05) = 0.408 \, (0.576)$ and $f_i(\lambda 21.87) = 0.0606 \, (0.061)$. By comparison, the $O \, vi$ $f_i(2s-2p)$ for the UV fine-structure doublet $\lambda \lambda 1031.91, 1037.61$ are 0.199 and 0.066, respectively, and the $O \, vii$ $f_i(1s^2-2p^*)$ is 0.6944 (Wiese, Fuhr, & Deters 1996); the latter is equal to the sum of the (undamped) $f_i$.

4. DISCUSSION

Significant X-ray absorption by $O \, vi$ at 22.05 Å, and a weaker one at 21.87 Å, is expected based on the theoretically computed resonance strengths. These wavelengths lie in the range spanned by the emission lines of $O \, vii$ due to electron impact excitation and recombination cascades (e.g., Pradhan 1982) in transitions $2(^3S, ^1P, ^3P) \rightarrow 1(^1S, 0)$ at 22.101, 21.804, and 21.602 Å, usually labeled as $i, u, r$ for forbidden, intercombination, and resonance transitions. Although the $O \, vi$ absorption and $O \, vii$ emission features lie close together, they should be distinguishable with the CXO resolution (e.g., C. R. Canizares et al. 2000). An inspection of the X-ray spectra of the Seyfert galaxy NGC 5548, reproduced in Figure 3 from Kaasra et al. (2000), appears to show absorption dips at 22.05 and 21.87 Å (dashed lines), both lying in between the $i$ and $f$ emission lines of $O \, vii$. Furthermore, the $\lambda 22.05$ dip is much stronger, as inferred by the $f_i$ given in Table 1. Kaasra et al. (2000) do not comment on these features; however, the combined $O \, vi$ absorption might be comparable to the net absorption in the resonance line of $O \, vii$ (albeit reduced by $r$ emission). Since the $O \, vii$ and $f$ lines at 21.804 and 22.101 Å are forbidden, with $Einstein\, A$ values $0.14 \times 10^3$ and $3.31 \times 10^3\, s^{-1}$, respectively (Wiese et al. 1996), they should not exhibit significant absorption, unlike the $r$ line, with an $A$-value of $3.309 \times 10^3\, s^{-1}$, which does have an absorption component (Kaasra et al. 2000). It might be noticed from Figure 3 that fits to all features are slightly shifted in $\lambda$ due to velocity fields.

In addition to the KLL PARs described herein, the closely spaced KLn ($2 < n \leq \infty$) absorption may be discernible as a pseudospectrum below the 1s2K shell ionization edges; for $O \, vi$ (Fig. 1a) these higher energy features might be between 17.6 and 19.4 Å ($0.64-0.71\, \text{keV}$). The KLn are not fully resolved in Figure 1a. Being much narrower than the KLL, since $\Gamma_i \sim n^{-3}$, they are also more likely to be radiatively

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1 In Atomic Data Needs in X-Ray Astronomy, ed. M. A. Bautista, T. R. Kallman, & A. K. Pradhan; see http://heasarc.gsfc.nasa.gov/docs/heasarc/atomic/proceed.html.
and X-ray provides an additional tool for ionization and abundance studies. An examination of X-ray spectra is suggested for both the O vii emission and the O vi absorption features.

3. Radiative decay rates for autoionizing resonances may be obtained from the integrated $dI/dE$ since the Einstein $A$-values are related to $f$-values (Wiese et al. 1996). As confirmation of accuracy of the method presented, the computed $f$ in Table 1 are nearly equal (to two decimal figures) to those obtained from $f$. However, the quantity $dI/dE$ is more general and represents photoabsorption in lines, resonances, and the nonresonant background at all energies. As such, it may be useful in complex cases with many overlapping resonances or lines.

4. The PAR features in absorption should manifest themselves as DES lines along an isoelectronic sequence as $\Gamma_r \sim Z^4$. Contrary to heavier elements like iron, where the DES lines are strong, for lighter elements like oxygen DES emission is very weak (possibly undetectable), and the PAR satellites could be important absorption-line diagnostics.

5. Radiative transfer in resonances may be significant and should be considered in non-LTE and photoionization models.

These and other points will be discussed in subsequent works.

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