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ULTRAVIOLET EMISSION LINES OF Si II IN QUASARS—INVESTIGATING THE "Si II DISASTER"

Sibasish Laha[1], Francis P. Keenan[2], Gary J. Ferland[3], Catherine A. Ramsbottom[1], and Kanti M. Aggarwal[2]

[1] Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK; s.laha@qub.ac.uk

[2] Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

[3] Department of Physics and Astronomy, The University of Kentucky, Lexington, KY 40506, USA

ABSTRACT

The observed line intensity ratios of the Si II $\lambda1263$ and $\lambda1307$ multiplets to that of Si II $\lambda1814$ in the broad-line region (BLR) of quasars are both an order of magnitude larger than the theoretical values. This was first pointed out by Baldwin et al., who termed it the "Si II disaster," and it has remained unresolved. We investigate the problem in the light of newly published atomic data for Si II. Specifically, we perform BLR calculations using several different atomic data sets within the CLOUDY modeling code under optically thick quasar cloud conditions. In addition, we test for selective pumping by the source photons or intrinsic galactic reddening as possible causes for the discrepancy, and we also consider blending with other species. However, we find that none of the options investigated resolve the Si II disaster, with the potential exception of microturbulent velocity broadening and line blending. We find that a larger microturbulent velocity (~500 km s^{-1}) may solve the Si II disaster through continuum pumping and other effects. The CLOUDY models indicate strong blending of the Si II $\lambda1307$ multiplet with emission lines of O I, although the predicted degree of blending is incompatible with the observed $\lambda1263/\lambda1307$ intensity ratios. Clearly, more work is required on the quasar modeling of not just the Si II lines but also nearby transitions (in particular those of O I) to fully investigate whether blending may be responsible for the Si II disaster.

Key words: atomic processes – quasars: emission lines

1. INTRODUCTION

Emission and absorption lines of Si II provide important diagnostics of the plasma conditions in the low-temperature clouds of quasars and other active galactic nuclei (AGNs; Laor et al. 1997; Vestergaard & Wilkes 2001; de Kool et al. 2002; Leighly et al. 2007; Moe et al. 2009; Shull et al. 2011; Borguet et al. 2012, and references therein). The relevant transitions are from the lower-lying energy levels to the ground state and lie in the UV wavelength range from ∼1000 to 2500 Å. Baldwin et al. (1996) studied Si II emission lines arising from the quasar broad-line region (BLR) using data from the 4 m Cerro Tololo Inter-American Observatory telescope and found that the observed ratios of the Si II line fluxes at 1263 Å ($3s^23p\,^2P$–$3s^23d\,^2D$) and 1307 Å ($3s^23p\,^2P$–$3s3p^2\,^2S$) to that of the $\lambda1814$ multiplet of Si II ($3s^23p\,^2P$–$3s3p^2\,^2D$) are both more than an order of magnitude larger than the theoretical values. They termed this the "Si II disaster," which forms the main focus of our paper. Since the Baldwin et al. work, there have been several observations of the BLR clouds in narrow-line quasars using high-resolution *Hubble Space Telescope* (*HST*) data, which show similar discrepancies between theory and observation for the Si II emission lines (Laor et al. 1997; Vestergaard & Wilkes 2001; Leighly et al. 2007).

In this paper we address this discrepancy in three ways. First, using recently published Si II atomic data by Aggarwal & Keenan (2014), we check whether the discrepancy could be due to inaccurate atomic data being adopted by Baldwin et al. (1996) in their plasma modeling. Second, we investigate whether continuum pumping by the quasar/AGNs may have a selective effect on the excitation of the $\lambda1263$ and $\lambda1307$ multiplet emission lines compared to that at 1814 Å. Finally, we assess the impact of blending of the Si II transitions with other emission features as a possible source of the discrepancy.

Our paper is arranged as follows. In Section 2 we discuss observations of narrow-line quasars and the discrepancies with theory known as the Si II disaster, while in Section 3 we describe the new theoretical models. Finally, in Section 4 we provide a discussion of our results.

2. OBSERVATIONS

Baldwin et al. (1996), in their study of the optical and UV spectrum of the quasar Q0207–398, detected several emission lines from ions such as O I, N V, O VI, Fe II, Si II, and Si III in the (rest-frame) wavelength range 970–2400 Å. These emission lines are from the BLR of the quasar, where the plasma is typically photoionized by the incident AGN radiation. Using the measured line intensities and their ratios, Baldwin et al. constrained the ionizing photon flux and the density of the BLR cloud through a comparison with theoretical simulations. From the ionization state of the cloud defined by $U = \Phi_H/(n_H c)$, where Φ_H is the incident photon flux, n_H is the hydrogen density, and c is the speed of light, one can determine the location R of the cloud by knowing Φ_H and the total photon flux Q_H of the source, where $\Phi_H = Q_H/4\pi R^2$. Baldwin et al. extensively spanned the parameter space of Φ_H and n_H and found that the regions that best describe the various line ratios from several ions are unable to reproduce the observed Si II emission line intensities, even though their similar Doppler widths (~1000 km s^{-1}) point to a common region of origin. In particular, the ratios of the observed Si II $\lambda1263$ and $\lambda1307$ multiplet line intensities to that of Si II $\lambda1814$ were both more than an order of magnitude larger than the theoretical values. This problem was referred to as the "Si II disaster" by Baldwin et al., who discussed several possibilities for this anomaly, such as the effects of dielectronic recombination, charge transfer, collisional excitation, and selective excitation, but could not

Table 1
Observed and Theoretical Si II Emission Line Intensity Ratios

Ratio	Q0207–398[a]	I Zw 1[b]	I Zw 1[c]	PHL 1811[d]	CLOUDY1[e]	CLOUDY2	CLOUDY3[f]	CLOUDY3[g]
1263/1814	6.6	5.2	2.1	$\geqslant 8.5$	0.15	0.20	0.63	4.80
1307/1814	5.7	2.8	4.1	$\geqslant 2.4$	0.17	0.12	0.40	2.62

Notes.
[a] From Baldwin et al. (1996).
[b] From Vestergaard & Wilkes (2001).
[c] From Laor et al. (1997).
[d] From Leighly et al. (2007).
[e] See Section 3 for details of the different CLOUDY models.
[f] Calculations for microturbulent velocity = 0 km s^{-1}.
[g] Calculations for microturbulent velocity = 500 km s^{-1}.

resolve the issue. In Table 1 we list the Si II line intensity ratios measured by Baldwin et al. for QSO Q0207–398, and below we discuss a few more instances of quasars that exhibited such Si II emission line discrepancies.

The narrow-line quasar I Zw 1 has been studied several times over the past 20 yr in the optical and UV wavelength bands (Laor et al. 1997; Vestergaard & Wilkes 2001; Véron-Cetty et al. 2004). It has been paid such attention because its narrow-line profiles show minimal blending, thus allowing emission lines to be individually identified and measured. Laor et al. (1997) observed this source using the Faint Object Spectrograph (FOS) on board *HST* and detected the Si II emission line multiplets at 1263, 1307 and 1814 Å. However, the authors pointed out a possible blend of O I with the Si II multiplet at 1307 Å. Table 1 lists the Si II emission line ratios measured by Laor et al. (1997).

Vestergaard & Wilkes (2001) similarly studied I Zw 1 with *HST*/FOS, with the aim of providing an empirical UV template for Fe emission in quasars. Their Si II line intensity ratios are also reported in Table 1.

Optical and UV spectra of the quasar PHL 1811 were obtained by Leighly et al. (2007) using the Space Telescope Imaging Spectrograph on board *HST*, plus the 2.1 m telescope at the Kitt Peak National Observatory. This is a narrow-line quasar whose UV spectrum is dominated by Fe II and Fe III lines and unusual low-ionization species such as Na I and Ca II. The higher ionization stage emission lines are very weak, which Leighly et al. attribute to an unusually soft spectral energy distribution. They detected the Si II emission lines in the UV spectrum, and their intensity ratios are summarized in Table 1.

In all the above cases we find that the observed fluxes for the Si II multiplets at 1263 and 1307 Å are 5–10 times larger than that of Si II $\lambda 1814$. By contrast, the simulations predict larger fluxes for the multiplet at 1814 Å, as discussed in Section 3.

3. CLOUDY MODELS

We have used the photoionization code CLOUDY (Ferland et al. 1998, 2013) for our modeling work, which was also adopted by Baldwin et al. (1996). The CLOUDY models generated by Baldwin et al. employed Si II transition probabilities (TPs) from the compilation of Morton et al. (1988) and the results of Dufton & Kingston (1991) for electron impact excitation effective collision strengths (ECS). Over the past 20 yr, the available data for these atomic processes have been improved, and the most recent release of CLOUDY (Ferland et al. 2013) employs Si II TP and ECS values from Nahar (1998) and Tayal

(2008), respectively. However, very recently Aggarwal & Keenan (2014) have produced new calculations of TP and ECS for Si II, considering all 1540 transitions among the lowest 56 energy levels. These are estimated to be accurate to ±20% for most transitions, and in some instances they are very different from previous work. For example, for the $3s^2 3p\ ^2P_{1/2}$–$3s3p^2$ $^2D_{3/2}$ (1808.01 Å) transition at an electron temperature of $T_e = 10,000$ K, the Tayal (2008) value of ECS = 2.74, about 40% larger than that of Aggarwal & Keenan (ECS = 1.91). Similarly, the Nahar (1998) TP for $3s^2 3p\ ^2P_{3/2}$–$3s^2 3$ d $^2D_{5/2}$ (1264.73 Å) is $3.04 \times 10^9\,\mathrm{s}^{-1}$, over 30% larger than the Aggarwal & Keenan calculation of $2.31 \times 10^9\,\mathrm{s}^{-1}$. For some transitions, the differences in TP are even larger, such as $3s^2 3p$ $^2P_{1/2}$–$3s3p^2$ $^2D_{3/2}$, where the Nahar calculated value is more than a factor of 10 greater than that of Aggarwal & Keenan ($2.54 \times 10^6\,\mathrm{s}^{-1}$ compared to $1.0 \times 10^5\,\mathrm{s}^{-1}$). See Table 1 of Laha et al. (2016) for a comparison of the TP and ECS values between the various atomic data sets of Si II.

In view of the above, we investigate whether the "Si II disaster" anomaly may be due to the adoption of inaccurate atomic data. Specifically, we have created three CLOUDY models with differing atomic data sets. The first (termed CLOUDY1) employs the same Si II TP and ECS as Baldwin et al. (1996), i.e., those from Morton et al. (1988) and Dufton & Kingston (1991), while the second (CLOUDY2) is the Ferland et al. (2013) CLOUDY model with the atomic data of Nahar (1998) and Tayal (2008). In the third (CLOUDY3) we adopt the TP and ECS of Aggarwal & Keenan (2014). All three models consist of the energetically lowest 148 fine-structure levels of Si II with energies from the NIST database.[4] However, the calculations of Aggarwal & Keenan only consider the lowest 56 fine-structure levels. Hence, CLOUDY3 is a merger of the data sets of Aggarwal & Keenan and CLOUDY2, where we use the results of the former for the first 56 levels and data from the latter for the remainder. The TP values from Aggarwal & Keenan were wavelength-corrected to the NIST observed wavelengths.

For each CLOUDY model we have calculated the Si II emission line strengths in a BLR cloud. Baldwin et al. (1996) generated grids of CLOUDY models covering a large range of hydrogen density ($10^7 \leqslant n_H \leqslant 10^{14}\,\mathrm{cm}^{-3}$) and ionizing photon flux ($10^{17} \leqslant \Phi_H \leqslant 10^{24}$ photons cm^{-2} s^{-1}). They used contour plots of these parameters to determine values that could produce the observed spectrum, and for component A in Q0207–398 they found that the Si II lines are emitted in a BLR cloud with $n_H = 10^{12.7}\,\mathrm{cm}^{-3}$ and $\Phi_H = 10^{20.7}\,\mathrm{cm}^{-2}\mathrm{s}^{-1}$. These

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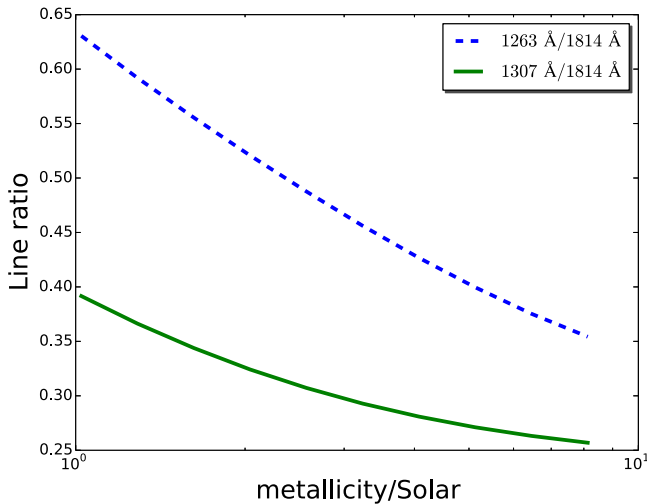[4] http://www.nist.gov/pml/data/asd.cfm

Figure 1. Si II line ratios plotted as a function of cloud metallicity (in units of the solar value).

parameters are hence used as representative values to model the BLR clouds in our CLOUDY simulations, and in Table 1 we list the resultant theoretical Si II line intensity ratios. We note that the "stopping" criterion for the CLOUDY calculations is when the total hydrogen column density N_H of the cloud reaches 10^{23} cm^{-2}, which yields the optically thick case. The equivalent width of the Si II $\lambda1814$ multiplet ($W_\lambda \sim 1.81$ Å) observed in the quasar Q0207–398 by Baldwin et al. (1996) compares well with that calculated using CLOUDY ($W_\lambda \sim 2.11$ Å), using the BLR parameters mentioned above, and a unit cloud covering fraction. We note that we have assumed a solar metallicity in the above calculations, but consider nonsolar values in Section 4.

4. RESULTS AND DISCUSSION

As noted in Section 3, the recent TPs for the Si II $\lambda1814$ (3s^{2}3p ^{2}P–3s3p^2 ^{2}D) multiplet lines calculated by Aggarwal & Keenan (2014) are more than a factor of 10 smaller than the earlier values of Nahar (1998). This would hence appear to potentially provide an explanation for the Si II disaster, as reducing the TP for the Si II $\lambda1814$ multiplet might be expected to similarly reduce the theoretical line intensity, hence increasing the predicted values of the $\lambda1263/\lambda1814$ and $\lambda1307/\lambda1814$ ratios, hopefully to match the observations and hence solve the Si II disaster problem. However, from Table 1 we see that the observed values of the $\lambda1263/\lambda1814$ and $\lambda1307/\lambda1814$ ratios range from 2.1 to 6.6 and from 2.8 to 5.7, respectively, while the CLOUDY3 calculations (which use the Aggarwal & Keenan TP data) are 0.63 and 0.40, respectively. These theoretical values are significantly larger than those from CLOUDY1 and CLOUDY2, but still not by a sufficient amount to resolve the Si II emitted spectrum discrepancy. Hence, we conclude that the latest atomic data do not solve the Si II disaster.

Ferland et al. (1996) found that the BLR clouds may have supersolar metallicities ($\sim 5\,Z_\odot$), which can change the ionic column densities and hence the optical depths of different emission lines, in turn affecting the line ratios. Figure 1 shows the Si II emission line ratios calculated as a function of cloud metallicity, which is varied from 1 to 10 times solar. We find that the resultant theoretical line ratios decrease with increasing

metallicity of the cloud and are in worse agreement with observation. Hence, enhancing the metallicity of the cloud does not solve the Si II disaster.

However, another possible explanation is continuum pumping. In AGNs, the continuum photoionizes the BLR gas clouds and can selectively pump specific levels and hence lines. The optimal way to test whether the Si II $\lambda1263$ and $\lambda1307$ lines are selectively pumped by the continuum would be to switch off and on the continuum and compare the intensities. However, the emission-line strength is dependent on the ionization and thermal equilibrium of the BLR cloud, and upon changing the spectral energy distribution or switching it off, the equilibrium will be disturbed and the line ratios will change not only because of photoionization but also because of other effects. Therefore, we have adopted an alternative method to test this effect, by first reducing the number of available levels of Si II in the CLOUDY3 model to 11 (the minimum number required to produce the Si II emission lines) and then allowing all 148 levels to be in use. By comparing the predicted line intensities in the two instances, we can estimate the effect of indirect photoexcitation, whereby the Si II electrons are pumped to higher levels by the continuum and then cascade to strengthen the lines of interest. However, we note that in all cases the Si II line fluxes changed by $\leqslant 5\%$, and thus continuum pumping by indirect photoionization cannot be a possible solution to the Si II problem.

The microturbulent velocity of a cloud is also a potential source of continuum pumping. Turbulence broadens the local line width, which can then absorb a larger fraction of the continuum, leading to increased line intensity. Also, the presence of turbulence in a cloud reduces the optical depth and hence increases the line intensities, as the emitted photons can escape more easily. The effect of microturbulent velocity on BLR clouds has been studied extensively by Bottorff et al. (2000) using CLOUDY. These authors found that the Si II line multiplets at 1263 and 1307 Å are selectively pumped by the continuum to a far greater extent than the $\lambda1814$ multiplet, for turbulent velocities ranging from 100 to 10^4 km s^{-1}. By default, CLOUDY adopts a microturbulent velocity of 0 km s^{-1}, and hence we have undertaken calculations with CLOUDY3 data for a turbulent velocity of 500 km s^{-1} and derived $\lambda1263/\lambda1814$ and $\lambda1307/\lambda1814$ ratios of 4.80 and 2.62, respectively. These values are much larger than the results for a turbulent velocity of 0 km s^{-1} and closer to the observed ratios (see Table 1). Therefore, the microturbulent velocity broadening of the BLR clouds could be a possible solution to the Si II disaster. However, there is an important caveat to this exercise. The introduction of turbulent velocity into a cloud changes its entire properties, including temperature and ionization structure. Hence, it is hard to isolate the effect of continuum pumping on the emission lines, as several other factors also affect the line emissivity.

A potential source of the Si II discrepancy could be intrinsic reddening by Galactic-like dust that produces a pronounced broad absorption feature in the range 1800–2500 Å, which reduces the intensity of the Si II $\lambda1814$ feature and hence leads to enhancements in the $\lambda1263/\lambda1814$ and $\lambda1307/\lambda1814$ ratios over their true values and the Si II disaster. Laor et al. (1997) discuss this effect in detail for I Zw 1, but note that there was little evidence for the presence of such intrinsic reddening. This therefore appears to be an unlikely cause for the Si II problem.

In a typical BLR plasma, the clouds are in a Keplerian orbit about the supermassive black hole at velocities of ~ 1000 km s^{-1},

Table 2
Theoretical Intensity Ratios for Possible Blending Lines

Line Ratio	CLOUDY1	CLOUDY2	CLOUDY3
S II $\lambda1259.52$/Si II $\lambda1263$	0.120	0.107	0.104
Si I/Si II $\lambda1263$	0.049	0.044	0.043
P II $\lambda1301.87$/$\lambda1307$	0.065	0.073	0.073
O I $\lambda1302.17$/Si II $\lambda1307$	2.3	2.6	2.6
Si III $\lambda1303.32$/Si II $\lambda1307$	0.50	0.57	0.57
P II $\lambda1304.49$ /Si II $\lambda1307$	0.066	0.075	0.075
P II $\lambda1304.68$/Si II $\lambda1307$	0.061	0.069	0.069
O I $\lambda1304.86$/Si II $\lambda1307$	2.1	2.4	2.3
P II $\lambda1305.50$/Si II $\lambda1307$	0.065	0.073	0.073
O I $\lambda1306.03$/Si II $\lambda1307$	1.7	2.0	1.9
P II $\lambda1309.87$/Si II $\lambda1307$	0.072	0.082	0.082
$\lambda1263$/$\lambda1814$[a]	0.18	0.23	0.72
$\lambda1307$/$\lambda1814$[a]	1.4	1.1	3.6

Note.
[a] Revised theoretical values of line ratios with the addition of the predicted blending lines.

which would lead to line broadening of approximately 4 and 6 Å at 1300 and 1800 Å, respectively. Hence, the Si II disaster may simply be due to blends, as found for other such long-standing problems. For example, Dufton et al. (1990) found discrepancies between theory and observation for emission lines of Fe XV in solar flares, which they attributed to either errors in the adopted atomic data or the effects of atomic processes that were not considered in their flare models. However, subsequently Keenan et al. (2006) showed that line blending was responsible. To investigate this for Si II, we have used CLOUDY to calculate the intensities of possible blending lines in the wavelength ranges 1258.4–1267.0 Å (i.e., spanning the components of the $\lambda1263$ multiplet, plus ±2 Å), 1302.4–1311.3 Å (the same for the $\lambda1307$ multiplet), and 1805.0–1820.5 Å (spanning the components of the $\lambda1814$ multiplet, plus ±3 Å in this instance). We list the calculated intensities of the blending lines in Table 2 relative to that of the relevant Si II multiplet. Only lines that are predicted to be ∼5% of the intensity of the Si II feature or greater are included in the table, and we note that no blending lines were found for the $\lambda1814$ multiplet in any of the CLOUDY models. Also shown in Table 2 are the revised theoretical Si II line ratios taking into account the effect of the blends. An inspection of the table reveals that the revised values of $\lambda1307$/$\lambda1814$ are now closer to the observational results, with the CLOUDY3 theoretical ratio (3.6) being in reasonable agreement with the observations (which range from 2.8 to 5.7). However, the revised estimates for $\lambda1263$/$\lambda1814$ remain significantly lower than the measured values. In addition, the predicted ratios for the line blend flux ratios of $\lambda1263$/$\lambda1307$ are 0.13 (CLOUDY1), 0.21 (CLOUDY2), and 0.20 (CLOUDY3), much smaller than the observed values of 0.51–1.9. This discrepancy arises due to the prediction of very strong O I emission in the CLOUDY models, with in fact this species dominating the $\lambda1307$ feature. The O I lines are excited by the H I Lyβ Bowen fluorescence process, which we treat as in Elitzur & Netzer (1985). This process is complex and depends on the detailed velocity and density structure of the plasma. Given the

complexity in dealing with O I, it is possible (and indeed perhaps likely) that the predicted O I intensities are not reliable, so that our estimates of line blending are in turn not highly accurate. There is also no a priori reason to believe that our calculations of blends for the $\lambda1263$ and $\lambda1814$ multiplets are reliable. We therefore conclude that blending cannot be ruled out as a source of the Si II discrepancy, but clearly more work is required on the calculation of the intensities, and hence impact, of blending species.

In summary, we have ruled out several possible explanations for the Si II disaster observed in quasar spectra, including errors in atomic data, continuum pumping, and the presence of intrinsic reddening in the source. We find that an enhanced microturbulent velocity in the BLR plasma can solve the Si II disaster. However, the caveat is that changing the turbulent velocity also changes the ionic structure and several other properties of the cloud, and hence the effect of continuum pumping on the line ratios may not be isolated. Another possible explanation for Si II disaster, line blending, cannot, we believe, be completely ruled out at this stage, and more detailed calculations of the intensities of possible blending species are required.

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