PHYSICAL CONDITIONS IN THE X-RAY EMISSION-LINE GAS IN NGC 1068

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ABSTRACT

We present a detailed, photoionization modeling analysis of XMM-Newton/Reflection Grating Spectrometer observations of the Seyfert 2 galaxy NGC 1068. The spectrum, previously analyzed by Kinkhabwala et al., reveals a myriad of soft X-ray emission lines, including those from H- and He-like carbon, nitrogen, oxygen, and neon, and M- and L-shell iron. As noted in the earlier analysis, based on the narrowness of the radiative recombination continua, the electron temperatures in the emission-line gas are consistent with photoionization, rather than collisional ionization. The strengths of the carbon and nitrogen emission lines, relative to those of oxygen, suggest unusual elemental abundances, which we attribute to the star formation history of the host galaxy. Overall, the emission lines are blueshifted with respect to systemic, with radial velocities \( \sim 160 \text{ km s}^{-1} \), similar to that of \([\text{O} \text{III}] \lambda 5007\), and thus consistent with the kinematics and orientation of the optical emission-line gas and, hence, likely part of an active galactic nucleus driven outflow. We were able to achieve an acceptable fit to most of the strong emission lines with a two-component photoionization model, generated with CLOUDY. The two components have ionization parameters and column densities of \( \log U = -0.05 \) and 1.22 and \( \log N_{\text{H}} = 20.85 \) and 21.2 and covering factors of 0.35 and 0.84, respectively. The total mass of the X-ray gas is roughly an order of magnitude greater than the mass of ionized gas determined from optical and near-IR spectroscopy, which indicates that it may be the dominant component of the narrow-line region. Furthermore, we suggest that the medium that produces the scattered/polarized optical emission in NGC 1068 possesses similar physical characteristics to those of the more highly ionized of the X-ray model components.

Key words: galaxies: active – galaxies: individual (NGC 1068) – galaxies: Seyfert – X-rays: galaxies

1. INTRODUCTION

Active galactic nuclei (AGNs), of which Seyfert galaxies are relatively low luminosity \( (L_{\text{bol}} \lesssim 10^{45} \text{ erg s}^{-1}) \) examples in the local universe (\( z \lesssim 0.1 \)), are thought to be powered by accretion of matter onto supermassive black holes, which reside at the gravitational centers of the host galaxies. The properties of Seyfert galaxies and how these are understood within the context of the unified model (Antonucci 1993) have been discussed in several of our previous papers (e.g., Kraemer et al. 2009). However, it is useful in the context of this paper to mention the scales of the various regions that contribute to the spectra of Seyferts. The continuum source, which is approximately light-hours in extent (e.g., Edelson et al. 1996), and the surrounding broad emission-line region, which ranges in size from several to tens of light-days (e.g., Peterson et al. 2004), are only directly observable in Seyfert 1 galaxies. In contrast, the narrow-line region (NLR), which is composed of lower-density gas in which the forbidden lines and narrower components of the permitted lines form, can extend out to \( \sim 1 \text{ kpc} \) (e.g., Pope 1988).

Owing to its proximity, the Seyfert 2 nucleus of the barred spiral galaxy NGC 1068 (Bland-Hawthorn et al. 1997) is the most extensively studied such object to date. Redshift-independent distance estimates place the host galaxy between 10 and 16 Mpc away (e.g., Tully et al. 2009; Sofue & Wakamatsu 1991). To be consistent with the bulk of the current literature, here we adopt the mean value of 12.65 Mpc from NED,\(^4\) such that 1" is roughly equivalent to 60 pc.

\(^4\) The NASA/IPAC Extragalactic Database (NED) is operated by the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration.
the observer, which is consistent with the morphology of the H\textsubscript{i} 21 cm emission (Gallimore et al. 1994). The maximum deprojected outflow velocity is $\sim$2000 km s\textsuperscript{-1}, with a peak $\sim$140 pc from the central nucleus, after which there is rapid deceleration to systemic. Although outflowing, photoionized gas is suggestive of radiative acceleration, the velocity profiles are not fully consistent with any simple form of AGN-driven flow (Das et al. 2007; Everett & Murray 2007). The main issue is that the flow appears to accelerate much more gradually than predicted. One possibility is mass loading, perhaps in the form of AGNs by photoionized gas (now generally referred to as “warm absorbers”). In fact, Netzer (1993, 1996) had predicted that there would be strong soft X-ray emission lines associated with warm absorbers.

The unprecedented X-ray spectral resolution afforded by the XMM-Newton (hereafter XMM) Reflection Grating Spectrometer (RGS) and the Chandra High Energy Transmission Grating (HETG) and Low Energy Transmission Grating (LETG) has revealed the myriad of emission lines predicted by Netzer (1993). Furthermore, based on Chandra/HETG observations, Ogle et al. (2000) found extended soft X-ray emission in the Seyfert 1 galaxy, NGC 4151. As it is roughly spatially coincident with the optical [O \textsc{iii}] emission and radio continuum, it likely arises in the NLR. Similarly, the NLR is the source of the soft X-ray emission in Seyfert 2 galaxies. For example, X-ray observations of NGC 1068 show an extended region of soft X-ray emitting gas, broadly coincident with the [O \textsc{iii}] bicone (Young et al. 2001; Ogle et al. 2003). The extended emission component likely has contributions from both line emission and a small electron-scattered component of the X-ray continuum.

Previous analyses, based on RGS (Kinkhabwala et al. 2002) and Chandra/LETG (Brinkman et al. 2002) and HETG (Ogle et al. 2003) observations, have revealed a multitude of emission lines in NGC 1068. Particularly prominent are strong H- and He-like lines of C, N, and O. These are accompanied by weaker highly ionized lines from Ne, Mg, Si, S, and Fe. Via its superior spatial resolution, the Chandra observations revealed two peaks of X-ray emission, one centered on the nucleus and the other $3''$–$4''$ to the northeast. The overall emission-line spectra were found to be similar in both regions (Brinkman et al. 2002; Ogle et al. 2003). Ogle et al. (2003) suggested that the X-ray emission line was the source of the scattered optical continuum, detected via spectropolarimetry (Miller et al. 1991). Consideration of the ensemble of line measurements has suggested that both photoionization and photoexcitation are important ionization processes for the X-ray emitter (Kinkhabwala et al. 2002; Ogle et al. 2003), with no clear evidence of a collisionally ionized component. However, none of these authors generated detailed photoionization models to analyze the physical properties of the emission-line gas.

More recently, Kallman et al. (2014) analyzed a 450 ks Chandra/HETG spectrum of NGC 1068, using photoionization models generated with the code xstar (Kallman et al. 2004). Overall, their results support the claims in Kinkhabwala et al. (2002) and Ogle et al. (2003), specifically that the emission-line gas is photoionized, with some evidence for photoexcitation, and the emission lines are blueshifted, indicative of outflows. They found that multiple zones, characterized by a range of ionization parameters and column densities, were required to match the measured emission-line fluxes. Furthermore, in order to fit the spectra, they allowed the oxygen and iron abundances to vary among the components. However, Chandra/Medium Energy Grating has a low effective area at wavelengths >25 Å. As a result, Kallman et al. (2014) were unable to compare the oxygen lines with many of the strong lines of nitrogen and none of carbon, and therefore they were unable to determine how their assumed abundances might result within the constraints of nucleosynthesis models. We will revisit these points in Section 3.

In this paper, we reinvestigate the soft X-ray spectra obtained using the RGS in the context of photoionization models generated with cloudy (Ferland et al. 1998). The goals of our study include a reassessment of the physical processes responsible for ionizing the X-ray gas and a better understanding of the relationship between the X-ray emitter and other key components of the nuclear outflow. Progress on these questions will, in turn, lead to a better understanding of the energy and material transport between the active nucleus and the host galaxy.

2. OBSERVATIONS AND DATA ANALYSIS

The observation of NGC 1068 reported here was made by XMM on 2000 July 29–30 (OBSIDs 011100101, 011120201). The standard RGS and PN data products were extracted from the archive, having been produced by the XMM Science Analysis Software (SAS) v6.6.0. The RGS offers a useful bandpass $\sim$0.4–2.0 keV ($\sim$6–31 Å). As a result of the failure of RGS1 CCD7 and RGS2 CCD4 (soon after launch), there are no useful data over the wavelength range 11–14 Å (0.9–1.2 keV) and 20–24 Å (0.51–0.62 keV) for RGS1 and RGS2, respectively. Subsequent reprocessing and analysis were performed using a more recent version of SAS\(^5\) (v10.0.0) and various tasks from the heasoft\(^6\) (v6.9) software suite.

In order to determine the RGS wavelength scale, the position of the zeroth order must be determined. This is not possible using the RGS instrument alone. Thus, we used the HEASoft “xrtcentroid” task (within ximage v0.2.9) to determine the centroid of the image from the co-aligned PN instrument in the RGS wavelength band. The centroid position was found to be at R.A. = $02^h42^m40^s70$, decl. = $-0^\circ00'46''24''$ (J2000). We estimated the uncertainty of our centroid position to be $1''$ based on repeated trials of the task, i.e., less than one image pixel ($1''$ on a side). Our X-ray centroid position is consistent with that derived from Chandra observations of the source (Young et al. 2001) but is $\sim$6/3 away from the position assumed in the (SAS v6.6.0) processing of the RGS data that created the archived data products. (The processing software uses the position supplied by the principal investigator) We also note that our centroid position is $\sim$5'' away from the X-ray centroid position determined by Kinkhabwala et al. (2002) for this XMM observation, attributable to improvements in attitude determination software between the original processing of the data and the current archived version.

As the RGS energy scale is determined by the angle a photon makes with the optical axis, it is important to compare the energy scale of the RGS with the energy scale of the PN camera.

\(^5\) http://xmm.esac.esa.int/sas/
\(^6\) http://heasarc.gsfc.nasa.gov/docs/software/lheasoft
difference in attitude solution does not affect the line energy determination relative to that performed by Kinkhabwala et al. (2002). In addition to the uncertainty on photon energy related to the statistical uncertainty in determination of the centroid and therefore the dispersion angle, there is another uncertainty in the absolute energy scale that corresponds to a 1σ uncertainty in velocity of 105 km s\(^{-1}\) at 20 Å.

Given the above, we reprocessed the RGS data from both ObsIDs using SAS v10.0.0 to produce co-added source and background spectra for each RGS, based on our X-ray centroid position. The total exposure times were 84.7 ks and 82.5 ks for RGS 1 and RGS 2, respectively. The mean source count rates (in the 0.4–2 keV band) were 0.568 ± 0.003 counts s\(^{-1}\) and 0.516 ± 0.003 counts s\(^{-1}\) for RGS 1 and RGS 2, respectively. The background constituted ∼20% of the total count rate.

2.1. Spectral Analysis

2.1.1. Initial Line Fitting

The source spectral (without background subtraction), background, and response files obtained after reprocessing the data (as discussed above) were loaded into xspec (Arnaud 2010) to create the background-subtracted source spectra from RGS 1 and RGS 2, as shown in Figure 1 (orange color). This methodology allows xspec to perform the background subtraction and preserve the full statistical information from the data. The RGS spectra contained >10 counts in most of the channel range used, allowing us to utilize the \(\chi^2\) statistic for fitting.

Inspection of the spectra revealed several prominent lines (Figure 1), including those from H-like and He-like transitions of O, C, N, Ne, Mg, and Si. Of particular interest are the very prominent triplets that arise from He-like species, such as N\(\text{vi}\), O\(\text{vii}\), and Ne\(\text{ix}\), which can yield constraints on the gas density and excitation mechanism (Porquet & Dubau 2002).

To extract the parameters for these lines, narrow sections of the data were fit using xspec. As far as was possible, the lines were isolated (by ignoring data around the selected range) and fit individually such that each line could be fit accurately. Each line profile was modeled using a Gaussian component whose flux, width, and energy were allowed to vary (Table 1). The Galactic column density was accounted for in the spectral analysis by using the neutral absorption model \(\text{tbabs}\) (Wilms et al. 2000). The column density for the \(\text{tbabs}\) component was allowed to vary between 2.92 \(\times\) 10\(^{20}\) cm\(^{-2}\) (Dickey & Lockman 1990) and 3.53 \(\times\) 10\(^{20}\) cm\(^{-2}\) (Kalberla et al. 2005), to account for the uncertainty in this quantity. The best-fit value of the Galactic column, pegged at the high end of this range in the fit, was therefore initially fixed at 3.53 \(\times\) 10\(^{20}\) cm\(^{-2}\) (but see Section 3.2.1). The continuum close to each line was fit with a power-law component that was allowed to vary. The best-fit line parameters are detailed in Table 1 for lines above the threshold of observed flux >10\(^{-6}\) photons cm\(^{-2}\) s\(^{-1}\). We tabulated 1σ errors on each parameter (i.e., calculated at 68% confidence).

As expected, our measured emission-line fluxes are in good agreement with those of Kinkhabwala et al. (2002). However, the RGS fluxes are ∼2 greater than those measured in Chandra/HETG spectra (Ogle et al. 2003; Kallman et al. 2014). The difference is due to the much larger extraction region for the RGS. To illustrate this, in Figure 2, we show the RGS and Chandra/HETG extraction windows, overlaid on a Chandra/ACIS image. Clearly, much of the X-ray emission-line region is outside the Chandra window.
Fe M- and L-shell transitions (Fe xiv to Fe xxiv) are heavily blended with H- and He-like lines of Ne (Figure 1); therefore, the strengths of these lines could not be usefully constrained. The higher-order transition lines of Mg, Si, and S are barely resolved owing to the low sensitivity of the RGS in the wavelength regime (6–10 Å).

2.1.2. Kinematics

We have identified the observed lines using the expected laboratory energies from the National Institute of Standards and Technology (NIST), supplemented by the Kentucky atomic database (Table 2). Most of the emission lines show a significant blueshift relative to the host galaxy (cζ = 1137 ± 3 km s⁻¹; Huchra et al. 1999), indicating an origin in outflowing gas, as previously found by other authors (e.g., Kinkhabwala et al. 2002). Based on the strongest, most isolated lines from He-like N and O and H-like C, N, and O, there is evidence for two kinematic components, with the N vi and O viii f lines having more negative radial velocities than the N vii and O viii Lyα lines (see Figure 3). However, the velocities of the latter are consistent with those of the N vi and O vii r lines, within the uncertainties. Unfortunately, the Ne ix and Ne x lines are weaker and heavily blended with Fe lines; hence, it is impossible to see whether the same trend is present. Overall, the radial velocities are on the same order as that measured for [O iii] λ5007, v rad ∼ 160 km s⁻¹ (Crenshaw et al. 2010b), which suggests that the X-ray and optical emission-line gas have similar kinematics. Note that these velocities are not deprojected and the actual outflows may be much faster (e.g., Das et al. 2006). As we also note in Section 3.2.1, while the kinematics are consistent with distinct low- and high-ionization zones, their radial velocities cannot be well constrained with these data.

Velocity widths (FWHM) were determinable for a few strong lines (Table 2). The strongest lines, e.g., N vi f and O viii f, are resolved using RGS, with velocity widths FWHM ∼ 800–1000 km s⁻¹ (Whittle 1992), again indicative of similar kinematics for the X-ray and optical emission-line gas. The values are in excess of the radial velocities and most likely result from the superposition of different kinematic components along our line of sight.

### Table 1 Comparison of the Observed and Predicted Emission-line Fluxes

| Line ID | Observed | Absorption-corrected | Total Model | Low T | High T |
|---------|----------|----------------------|-------------|-------|--------|
| C iv Hef | 1.16 ± 0.31 | 3.24 ± 0.86 | 1.09 | 1.09 |
| C iv Heδ | 2.45 ± 1.30 | 4.62 ± 2.08 | 0.59 | 0.59 |
| C vi Lyα | 9.48 ± 0.41 | 23.35 ± 1.01 | 16.57 | 9.55 | 7.02 |
| C vi Lyβ | 1.76 ± 0.21 | 3.18 ± 0.38 | 2.58 | 0.87 | 1.71 |
| C vi Lyγ | 0.60 ± 0.14 | 0.95 ± 0.22 | 1.41 | 0.53 | 0.88 |
| C vi Lyδ | 1.07 ± 0.16 | 1.94 ± 0.29 | 0.87 | 0.41 | 0.46 |
| N vi Heγ | 0.47 ± 0.14 | 0.67 ± 0.20 | 0.42 | 0.42 |
| N vi r | 3.32 ± 0.48 | 6.08 ± 0.87 | 4.13 | 3.62 | 0.51 |
| N vi i | 0.93 ± 0.37 | 1.72 ± 0.68 | 1.80 | 1.80 |
| N vi f | 7.37 ± 0.12 | 13.20 ± 0.60 | 9.77 | 9.77 |
| N vi Lyα | 6.01 ± 0.26 | 8.92 ± 0.39 | 6.45 | 1.99 | 4.46 |
| N vi Lyβ | 0.95 ± 0.09 | 1.45 ± 0.16 | 1.62 | 0.43 | 1.19 |
| N vii Lyγ | 0.40 ± 0.16 | 0.53 ± 0.16 | 0.88 | 0.27 | 0.61 |
| N vii Lyδ | 0.35 ± 0.10 | 0.40 ± 0.10 | 0.51 | 0.19 | 0.32 |
| O vii r | 4.96 ± 0.28 | 7.85 ± 0.68 | 5.30 | 3.97 | 1.33 |
| O vii i | 1.00 ± 0.44 | 1.94 ± 0.70 | 3.13 | 3.13 |
| O vii f | 9.25 ± 0.18 | 14.99 ± 0.29 | 12.57 | 12.07 | 0.50 |
| O vii Heβ | 0.73 ± 0.15 | 0.99 ± 0.22 | 0.88 | 0.54 | 0.34 |
| O vii Heγ | 0.67 ± 0.09 | 0.88 ± 0.14 | 0.36 | 0.30 |
| O viii Heδ | 0.38 ± 0.08 | 0.49 ± 0.12 | 0.30 | 0.30 |
| O viii Lyα | 5.37 ± 0.30 | 7.44 ± 0.64 | 8.94 | 1.25 | 7.69 |
| O viii Lyβ | 0.96 ± 0.44 | 1.22 ± 0.28 | 1.59 | 0.32 | 1.27 |
| Ne ix r | 1.74 ± 0.13 | 2.08 ± 0.15 | 1.46 | 0.45 | 1.01 |
| Ne ix f | 1.11 ± 0.15 | 1.32 ± 0.18 | 0.79 | 0.38 | 0.41 |
| Ne ix Heβ | 0.21 ± 0.09 | 0.24 ± 0.09 | 0.45 | 0.16 | 0.29 |
| Ne x Lyα | 1.34 ± 0.11 | 1.52 ± 0.12 | 2.07 | 2.07 |
| Mg xi r | 0.90 ± 0.17 | 0.96 ± 0.19 | 1.46 | 1.46 |
| Mg xi Lyα | 0.27 ± 0.11 | 0.29 ± 0.12 | 0.95 | 0.95 |

Notes.

a Fluxes obtained by fitting a Gaussian to each line as identified in the combined spectra of RGS 1 and RGS 2; all fluxes × 10⁻⁶ photons cm⁻² s⁻¹.

b Absorption-corrected line fluxes predicted by cloudy in the total model.

c Fluxes predicted by cloudy for LOWION, after scaling to that of O vii f.

d Fluxes predicted by cloudy for HIGHION, after scaling to that of O vii Lyα.

3. PHOTOIONIZATION MODELING

3.1. Inputs to the Models

Previous analyses for the soft X-ray emitting gas in NGC 1068 have used selected line measurements to explore the conditions

7 The RGS FWHMs at these wavelengths, linearly extrapolating between the values at 35.4 Å and 15.5 Å, are 775 km s⁻¹ and 1000 km s⁻¹.
in the emitting gas (Kinkhabwala et al. 2002). Here we aim to construct a self-consistent photoionization model for the X-ray emitter. To this end, we have made use of the photoionization code, cloudy version C10.00, last described by Ferland et al. (2013). As usual, our model results depend on the choice of input parameters, specifically the spectral shape of the incident radiation or spectral energy distribution (SED), the radial distances of the emission-line gas with respect to the central source, the number density of atomic hydrogen (\(n_H\)) and column density (\(N_H\)) of the gas, and its chemical composition. Given the large radial distances (>tens of parsecs) of the emission-line gas, we have assumed open, or slab-like, geometry. The models are parameterized in terms of the dimensionless ionization parameter \(U\), the ratio of ionizing photons per nucleon at the illuminated face of the slab, or

\[
U = \frac{Q}{4\pi R^2 cn_H},
\]

where \(R\) is the distance to the continuum source, \(c\) is the speed of light, and the total number of Lyman continuum photons s\(^{-1}\)

\[
Q = \int_{13.6\text{eV}}^\infty (L_v/\hbar v)dv,
\]

emitted by a source of luminosity \(L_v\).

### 3.1.1. The Ionizing Continuum

We assumed an SED in the form of a broken power law \(F_v = K v^{-\alpha}\), with \(\alpha = 1.0\) below 13.6 eV, \(\alpha = 1.7\) from 13.6 eV to 0.5 keV, and \(\alpha = 0.8\) from 0.5 keV to 30 keV (Kraemer & Crenshaw 2000b), where \(\alpha\) is the energy index. We also included a low-energy cutoff at 1 eV and a high-energy cutoff at 100 keV.

Since our view of the central source is blocked in NGC 1068, we estimated the ionizing luminosity using an “isotropic” quantity, specifically the [O\(\text{iv}\)] 25.89 \(\mu\)m emission line (see Meléndez et al. 2008). The [O\(\text{iv}\)] flux, detected with the Infrared Space Observatory–Short Wave Spectrometer, is approximately \(1.9 \times 10^{-11}\) erg cm\(^{-2}\) s\(^{-1}\) (Lutz et al. 2000), which corresponds to a line luminosity \(L_{\text{O iv}} \approx 10^{31.53}\) erg s\(^{-1}\). Using the linear regression fit to \(L_{\text{O iv}}\) and the 2–10 keV \((L_{2-10\text{keV}})\) luminosity for Seyfert 1 galaxies calculated by Meléndez et al. (2008), we estimate \(L_{2-10\text{keV}} \sim 10^{43.8}\) erg s\(^{-1}\), which, for a bolometric correction of \(\sim 30\) (Awaki et al. 2001), yields \(L_{\text{bol}} \sim 10^{45.3}\) erg s\(^{-1}\). The corresponding mass accretion rate is \(\dot{M} = L_{\text{bol}}/\eta c^2\), or \(0.35 M_\odot\) yr\(^{-1}\), for \(\eta = 0.1\). Interestingly, given a black hole mass of \(1.5 \times 10^7\) \(M_\odot\) (Greenhill & Gwinn 1997), the central source is radiating at approximately its Eddington limit. Based on these values and our assumed SED, we find the ionizing luminosity \(L_{\text{ion}} \sim 10^{44.2}\) erg s\(^{-1}\) and \(Q \sim 10^{54.4}\) photons s\(^{-1}\).

### 3.1.2. Elemental Abundances

Our initial approach was to find an approximate solution for the gas by comparing the ratio of intensities of selected strong emission lines in the data with those predicted by the cloudy model. The line ratios selected were for the strengths of H-like and He-like ions relative to O\(\text{vii}\) \(\lambda\)22.10 (the latter was selected by virtue of being the strongest line detected in the RGS data), similar to the approach used in the analysis of the RGS spectrum of the Seyfert 1 galaxy NGC 4151 by Armentrout et al. (2007). We first generated cloudy

![Figure 2. XMM/RGS and Chandra extraction cells, overlaid on the Chandra/ACIS image. Declination is along the y axis, right ascension is along the x axis, and the colors in the image correspond to the following: red, 0.2–1.5 keV; green, 1.5–2.5 keV; and blue, 2.5–8.0 keV. The extraction cells are square with size of ∼100″ and ∼9″ for XMM/RGS and Chandra/HETG, respectively, oriented with respect to the roll angles for these observations (Kinkhabwala et al. 2002; Kallman et al. 2014).](image-url)
photoionization models assuming solar abundances (Grevesse & Sauval 1998). This initial comparison revealed no single-zone gas solution that could adequately describe the observed line ratios. Specifically, models with solar abundances overpredicted the strongest oxygen lines, $\text{O v}^7f, \lambda 22.10$ and $\text{O v}^8 \text{Ly} \alpha$, relative to the lines from other abundant elements/ions, in particular, and He-like carbon and nitrogen. Interestingly, in photoionized gas, the X-ray emission lines from second-row elements are primarily produced by recombination or, for permitted transitions if the lines are optically thin, by photoexcitation. The other strong features in the RGS spectrum include radiative recombination continua (RRCs), which are obviously formed via recombination. Hence, the strengths of these features are quite sensitive to relative elemental abundances. Notably, it has been argued that optical and UV recombination lines are more reliable indicators of elemental abundances than collisionally excited forbidden lines, which are typically used to estimate elemental abundances in optical spectra, owing to the sensitivity of the latter on temperature and density fluctuations (Peimbert 1967).

In the analysis of RGS spectra of the Seyfert 1 NGC 3516, Turner et al. (2003) found that the model fit was improved by assuming both supersolar N/O and subsolar C/O abundance ratios. They argued that this was consistent with conversion of carbon to nitrogen via the CNO cycle in intermediate-mass stars ($M \lesssim 7 M_\odot$; e.g., Maeder & Meynet 1989), and that fairly large N/O ratios, e.g., a few times solar, could occur in stars with initially roughly solar abundances. However, the NGC 1068 spectra also show strong carbon lines (see Figure 1), which are not consistent with the loss of carbon, at least if the overall abundances were approximately solar. In studies of H II regions in the Milky Way, evidence has been found for a C/O gradient, with a C/O ratio $\sim$unity, while O/H ratio was roughly solar, at radial distances $\lesssim 7$ kpc (e.g., Esteban et al. 2005). The enhancement of carbon in the Milky Way interstellar medium could be due to either stellar winds from massive stars, $8 \lesssim M/ M_\odot \lesssim 80$ (Henry et al. 2000), or a combination of high-metallicity, massive stars and low-metallicity, low- to intermediate-mass stars, $0.8 \lesssim M/ M_\odot \lesssim 8$ (Carigi et al. 2005). In either case, if the carbon were significantly enhanced in a star with otherwise solar abundances, the conversion of carbon to nitrogen described above could lead to both high C/O and N/O ratios while O/H evolved as $Z/Z_\odot$. Based on this, we assumed that metallicities of progenitor stars were solar (Asplund et al. 2005), although with C/O approximately $3 \times$ solar, compared to the roughly twice solar values found by Esteban et al. (2005). We further assumed that nucleosynthesis brings the overall metallicity to $1.5 \times$ solar, but with all the added carbon going into the production of nitrogen. The resulting abundances, with the log values, relative to H by number, are as follows: He, $-0.83$; C, $-3.06$; N, $-3.36$; O, $-3.13$; Ne, $-3.90$; Na, $-5.59$; Mg, $-4.23$; Al, $-5.39$; Si, $-4.32$; P, $-6.42$; S, $-4.71$; Ar, $-5.43$; Ca, $-5.49$; Fe, $-4.33$; and Ni, $-5.61$. Here the N/H and C/H ratios are $6$ and $3.2 \times$ solar, respectively, while the other heavy-element abundance ratios are $1.5 \times$ solar. It should be noted that Brinkman et al. (2002) suggested supersolar nitrogen abundance and Kallman et al. (2014) required nonsolar heavy-element abundances for their photoionization models. Based on the strong C and Fe emission in the RGS spectra, there is
no evidence for depletion of these elements onto dust grains. Therefore, we did not include cosmic dust in the models.

3.2. Spectral Fitting Results

The range in ionization states detected in these spectra suggests the presence of the two distinct components of emission-line gas; therefore, our approach was to generate two model grids with CLOUDY. Consideration of the ratio N v f/O v f and Ne x/O viii suggested that these lines lie in the ranges logU ~ −1 to 0, logN_H ~ 20–22 and logU ~ 0–2, logN_H ~ 20–23.

3.2.1. The Final Model

To refine our solution, the RGS spectra were compared to a model comprising two “candidate” model zones. Based on the initial results from the line ratio analysis, we ran CLOUDY with model step intervals of 0.1 in the log of U and N_H, across the ranges −2 < logU < 2 and 20 < logN_H < 24, using the elemental abundances noted above. Initially, the resonance lines of the He-like triplets (only) were underpredicted compared to the forbidden lines. Thus, to boost the strength of these resonance lines, we included microturbulence of 35 km s−1. This corresponds to an FWHM = 82 km s−1, which is significantly less than that of the resolved lines discussed in Section 2.1.2, which likely result from the superposition of kinematic components along our line of sight. Following Porter et al. (2006), we then created a FITS format ATABLE from the CLOUDY output. To facilitate a comparison of the model tables with the ensemble of line results, we performed spectral fitting of the RGS data using our ATABLE.

| Line ID | λ_m (Å) | E_m (eV) | ΔE* (eV) | Velocity Shift (km s−1) |
|---------|---------|----------|----------|-------------------------|
| C v He β | 34.9728 | 354.516 | 0.444 ± 0.085 | −490 ± 80 |
| C v He δ | 32.7542 | 378.529 | 0.969 ± 0.205 | −680 ± 120 |
| C v Lyα | 33.7342 | 367.533 | 0.333 ± 0.019 | −270 ± 50 |
| C v Lyβ | 28.4663 | 435.547 | 0.582 ± 0.065 | −400 ± 70 |
| C v Lyγ | 26.9900 | 459.369 | 0.618 ± 0.040 | −400 ± 80 |
| C v Lyδ | 26.3572 | 470.399 | 0.459 ± 0.135 | −290 ± 10 |
| N v Heγ | 23.7710 | 521.578 | 0.685 ± 0.161 | −400 ± 110 |
| N v r | 28.7870 | 430.695 | 0.376 ± 0.042 | −260 ± 70 |
| N v i | 29.0815 | 426.333 | 0.342 ± 0.069 | −240 ± 70 |
| N v f | 29.5343 | 419.797 | 0.495 ± 0.018 | −350 ± 60 |
| N v r Lyα | 24.7792 | 500.356 | 0.318 ± 0.045 | −190 ± 70 |
| N v Lyβ | 20.9095 | 592.957 | 0.498 ± 0.141 | −251 ± 102 |
| N v Lyγ | 19.8261 | 625.358 | 0.513 ± 0.161 | −250 ± 110 |
| N v Lyδ | 19.3614 | 640.368 | 0.841 ± 0.235 | −390 ± 130 |
| O vi r | 21.6020 | 573.947 | 0.483 ± 0.046 | −250 ± 80 |
| O vi i | 21.8014 | 568.620 | 0.539 ± 0.111 | −260 ± 90 |
| O vi f | 22.1012 | 560.983 | 0.708 ± 0.221 | −660 ± 130 |
| O vi Heβ | 18.6270 | 665.615 | 1.516 ± 0.174 | −680 ± 120 |
| O vi Heγ | 17.7682 | 697.787 | 1.414 ± 0.221 | −610 ± 130 |
| O vi Heδ | 17.3958 | 712.722 | 1.145 ± 0.310 | −480 ± 150 |
| O vi Lyα | 18.9725 | 653.493 | 0.337 ± 0.036 | −150 ± 80 |
| O vi Lyγ | 16.0867 | 774.577 | −0.111 ± 0.194 | +40 ± 120 |

Notes.

a Theoretical wavelengths from NIST/Kentucky atomic database.

b Theoretical line energies.

ΔE = E_a − E_b, with uncertainties of 1σ (68% confidence level).

d The quoted errors are statistical (1σ) and systematic (derived from the centroid position uncertainty), combined in quadrature.
LOWION, respectively. One additional check on whether the models are physically plausible is the requirement that the depth of the model, $\Delta R/R = N_{\text{H}}/n_{\text{H}}$, is less than the component’s radial distance, $R$ (e.g., Blustin et al. 2005; Crenshaw & Kraemer 2012). For these model parameters, $\Delta R/R = 0.02$ and 0.68 for LOWION and HIGHTION, respectively.

Based on the fitting, LOWION and HIGHTION contribute 0.96 and 0.04 of O$_{\text{vii}}$ $f$ and 0.14 and 0.86 of O$_{\text{viii}}$ Ly$\alpha$, respectively. Using these fractional contributions, we computed the predicted emission-line fluxes from each component and the total flux. The former are computed by comparing the predicted O$_{\text{vii}}$ $f$ and O$_{\text{viii}}$ Ly$\alpha$ fluxes with the absorption-corrected fluxes, taking into account the fractional contributions of each component, in order to derive a scaling factor for each component. Then the remaining line fluxes are computed by multiplying the ratios of their fluxes to those of O$_{\text{vii}}$ $f$ or O$_{\text{viii}}$ Ly$\alpha$ by the derived scaling factors. The final values are listed in Table 1, along with the observed and absorption-corrected fluxes. The fits for the individual lines are good overall, with the predictions for most of the stronger lines (i.e., with fluxes $\gtrsim 3 \times 10^{-14}$ photons cm$^{-2}$ s$^{-1}$) within $\sim 30\%$ of the absorption-corrected values. The discrepancies include C $\alpha$ He$\beta$ and He$\delta$, which are relatively weak and in a region where determining the continuum level is nontrivial and N$_{\text{vii}}$ Ly$\alpha$ is somewhat underpredicted.

In addition to emission lines included in Table 1, we also compared the predicted and measured RRCs, using the same relative contributions from the two model components (see Table 4). Although we detected the O$_{\text{viii}}$ RRC, the feature is too heavily blended with the surrounding emission for us to have been able to determine the width and flux accurately. Overall, the predicted fluxes fit the measured values reasonably well. The model-predicted electron temperatures correspond to widths of $kT = 4.0$ eV and 44.4 eV for LOWION and HIGHTION, respectively. While the LOWION value is on the same order as the measured values of the He-like RRCs, the
3.2.2. Model-derived Covering Factors

Having obtained a reasonable fit to the RGS spectrum with our two-component model, we calculate the covering factors ($C_f$) for each component by comparing the emitting area, the ratio of the emission-line luminosities to their model-predicted fluxes, with the surface area of a sphere surrounding the central source. As we mentioned above, we assume that both LOWION and HIGHION are 50% from the source, which sets $n_{H}$ for each component for the value of $U$ for each component and thus the predicted emission-line fluxes. Based on our spectral fitting, the total luminosity of the O vii line emitted by LOWION is $2.5 \times 10^{40}$ erg s$^{-1}$. Dividing by the predicted flux, 0.215 erg cm$^{-2}$ s$^{-1}$, the total emitting surface area of LOWION is $\sim 10^{41}$ cm$^2$, which corresponds to a covering factor $C_f = 0.35$. Based again on our spectral fitting, for HIGHION, the total luminosity of O viii Lyγ is $1.5 \times 10^{40}$ erg s$^{-1}$, while the predicted flux is 0.051 erg cm$^{-2}$ s$^{-1}$, from which we derive an emitting surface of $2.5 \times 10^{41}$ cm$^2$ and $C_f = 0.84$. Although the covering factors are physically possible, in the sense that they are less than unity, the value for HIGHION requires that this component subtends a larger solid angle than the emission-line bicone, even if the bicone were filled (e.g., Das et al. 2006). We will revisit this point in Section 4.3.

3.2.3. UV and Optical Constraints on the X-Ray Emission-line Gas

Although the ionization parameters for both emission components are significantly higher than those determined for the UV and optical emission-line gas (e.g., Kraemer et al. 1998; Kraemer & Crenshaw 2000b), except for the “CORONAL” component of the hot spot (Kraemer & Crenshaw 2000a), the LOWION model predicts strong O vii $\lambda\lambda 1031.9, 1037.6$. Scaling the predicted flux by the emitting area determined from the O vii $f$, the predicted O vii luminosity is $\sim 1.9 \times 10^{41}$ erg s$^{-1}$, which corresponds to an observed flux $F_{O\,vi} \sim 1.0 \times 10^{-11}$ erg cm$^{-2}$ s$^{-1}$ (note that the contribution from HIGHION is more than two orders of magnitude less and hence can be ignored).

NGC 1068 was observed with the Hopkins UltraViolet Telescope (HUT), aboard the space shuttle Columbia (Kriss et al. 1992), through two circular apertures of 18” and 30”, hence encompassing the region of strong X-ray emission (e.g., Young et al. 2001). They measured $F_{O\,vi} = 3.74 \pm 3.1 \times 10^{-12}$ erg cm$^{-2}$ s$^{-1}$. While the emission-line fluxes reported by Kriss et al. were not corrected for extinction, based on the ratio of He ii $\lambda 1640$ (from HUT) to He ii $\lambda 4686$ (Koski 1978), they derived an extinction $E_{B-V} = 0.16$, assuming an intrinsic 1640/4686 ratio of 7.0 (Seaton 1978). Using the UV extinction curve in Seaton (1979), the corrected $F_{O\,vi} \approx 2.5 \times 10^{-11}$ erg cm$^{-2}$ s$^{-1}$, which indicates that LOWION contributes 40% of the O vi emission. Based on this, our model meets the constraints from the UV emission. Also, it is possible that some regions of UV and optical emission are undetectable owing to extinction (see discussion in Kraemer et al. 2011) but could be detected in the X-ray, in which case LOWION accounts for an even smaller fraction of the intrinsic UV emission.

Given the model parameters of the hot spot CORONAL component ($\log U = 0.23$; $\log N_{H} = 22.6$; Kraemer & Crenshaw 2000a), it could contribute to the overall X-ray emission. However, neither of our components has similar parameters. Furthermore, while CORONAL was optimized to match the observed [S xii] $\lambda 7611$, the peak ionization states are S ix and S xv for LOWION and HIGHION, respectively. Finally, forcing the inclusion of a component similar to CORONAL into the spectral fitting produced statistically unacceptable results. This suggests that the conditions that give rise to the [S xii] emission are not typical of the X-ray NLR as a whole.

4. DISCUSSION

4.1. Total Mass and Mass-loss Rates

Based on our model results and constraints on the covering factors of each component, we can determine the total mass of the X-ray emission-line gas, $M_{tot}$, for a given radial distance, $R$. Assuming that the gas lies in shells, the thickness of which are constrained by the model-derived values of $N_{H}$, the total mass is given by

$$M_{tot} = 4\pi R^{2} N_{H} \mu m_{p} C_{f},$$

(2)

where $m_p$ is the mass of a proton and the factor $\mu$ is the mean atomic mass per proton (we assume equal to 1.4, primarily from the contribution from helium). For our fiducial distance, $R = 50$ pc, and derived model parameters, we obtain $M_{tot} = 8.7 \times 10^{4} M_{\odot}$ and $4.7 \times 10^{5} M_{\odot}$ for LOWION and HIGHION, respectively. Note that, given the possibility that the emission-line gas lies at greater radial distance, $M_{tot}$ could be somewhat greater.

We estimate the mass-loss rates, $\dot{M}$, as follows (Crenshaw et al. 2003):

$$\dot{M} = 4\pi R N_{H} \mu m_{p} C_{f} \nu,$$

(3)

where $\nu$ is the outflow velocity. Using $\nu_{rad}$ in place of $\nu$, we obtain mass-loss rates of $\dot{M} \approx 3.8 \times 10^{-7} M_{\odot}$ yr$^{-1}$ and $0.6 M_{\odot}$ yr$^{-1}$ for the two components. Clearly, $\dot{M}$ would be greater if the gas were at a larger radial distance, as is the case for $M_{tot}$, or if the outflow velocities were greater than $\nu_{rad}$.

The derived values of $M_{tot}$ and $\dot{M}$ are roughly the same as those determined from the Chandra/HETG spectrum by Kallman et al. (2014), and, based on our estimate of $L_{bol}$, the...
latter is on the same order as that of the fueling rate. From the results of the STIS long-slit spectral analysis (Kraemer & Crenshaw 2000a, 2000b), we estimate that within a single slit the results of the STIS long-slit spectral analysis (Kraemer & Crenshaw 2000a). Therefore, UV gas with radial distance. However, given the uncertainties in the model parameters, these components are roughly in pressure equilibrium if colocated. In contrast, the predicted gas pressure for the UV/optical emission-line gas from the hot spot is $3.5 \times 10^{-7}$ dyn cm$^{-2}$ (based on the model parameters in Kraemer & Crenshaw 2000a). Therefore, UV/optical knots would not be pressure confined by the X-ray emission-line gas. In that case, one would expect to see a drop in the density of the optical/UV gas with radial distance. However, given the large pressure differential, the density drop would be much more rapid than observed (Kraemer & Crenshaw 2000b). This suggests other scenarios, such as creation/evaporation of clouds out of/into the X-ray medium (Krolik & Kriss 2001) or in situ acceleration of gas that has rotated into the illumination cone (Crenshaw et al. 2010a), rather than outflow and expansion of individual knots.

In Figure 6, we show the log$T$ – log$U/T_\odot$, or S-curve, plot generated with our assumed SED and abundances. Note that there is only one region with pronounced negative slopes, indicative of strong instabilities; the overall stability is the result of the high metal abundances in our models (see Bottorff et al. 2000). The inset shows that both components lie on stable, i.e., positive-sloped, sections of the S-curve. While HIGHION does lie close to an unstable region, given that the AGN is radiating close to its Eddington limit, it is unlikely that it will experience an ionizing flux increase that would drive it into instability.

### 4.3. Structure of the X-Ray NLR

As noted in Section 3.2.2, the model-derived covering factors are physically possible. However, it is difficult to reconcile such large values considering that the optical emission southwest of the nucleus is heavily attenuated by the disk of the host galaxy (Kraemer & Crenshaw 2000a) and that X-ray emission from the inner ~30 pc appears to be absorbed by gas outside the bicone (Kraemer et al. 2011). Hence, it is likely that there is more X-ray emission-line gas than that detected in the RGS spectra. If so, the covering factors could be significantly greater and could easily exceed unity for HIGHION.

Both HIGHION and LOWION are matter bounded, and in such cases, emission-line fluxes can be increased to an extent by increasing $N_H$. This would, correspondingly, decrease the required emitting surface areas and, hence, the covering factors. However, in the case of HIGHION, $N_H$ is constrained by the $\Delta R/R$ condition (see Section 3.2.1). One way around this is if the emission-line gas consists of a number of matter-bounded components at increasing radial distances. As an example, in Figure 7 we show the incident and transmitted continuum for HIGHION; clearly, there is no significant attenuation of the incident continuum, and hence highly ionized gas could exist in the “shadow” of a component similar to HIGHION, i.e., subtending the same solid angle with respect to the ionizing radiation. LOWION also produces weak attenuation. Assuming that density decreases with $R$, as observed with the optical emission-line
We analyzed an archival XMM-Newton/RGS spectrum of the Seyfert 2 galaxy NGC 1068, which was previously published by Kinkhabwala et al. (2002). In the process, we remeasured the emission-line fluxes, widths and radial velocities, and the fluxes and widths of RRCs and, overall, obtained similar values to those of Kinkhabwala et al. (2002). We generated photoionization models, using CLOUDY (Ferland et al. 2013), to fit the emission-line spectrum. Our main results are as follows.

1. Overall the X-ray emission lines have radial velocities blueshifted with respect to the systemic velocity of the host galaxy. The velocities and FWHM are roughly the same as that of \([\text{O} \text{iii}] \lambda 5007\), which suggests that the X-ray gas is part of the mass outflow through the NLR. Although there is evidence for two kinematic components, with the N vi and O vii lines having more negative radial velocities than the N vii and O viii lines, the differences are less than the measurement uncertainties.

2. Based on our preliminary modeling results, we determined the abundances of heavy elements in the emission-line gas to be overall 1.5\times solar. However, the carbon and nitrogen abundances are 3.2 and 6 times solar, respectively. One possibility is that an early period of star formation produced much of the excess carbon, which was followed by conversion of carbon into nitrogen in a more recent period. Kallman et al. (2014) also suggested nonstandard abundances for the emission-line gas but did not discuss possible connections with the star formation history.

3. We were able to fit most of the strong emission lines with two components, LOWION and HIGHION, characterized by log\(U = -0.05\) and 1.22 and log\(N_{\text{H}} = 20.85\) and 21.2, respectively. The LOWION produces most of the emission from He-like C, N, and O lines, while the HIGHION produces the H-like N, O, and Ne and most of the He-like Ne lines. The predicted electron temperature for LOWION is consistent with the measured widths of He-like RRCs; however, that of HIGHION is several times higher than that derived from the H-like RRCs, which we attribute to uncertainties in the width measurements. Overall, the emission lines and RRCs are consistent with photoionization, albeit with a small contribution from photoexcitation for the resonance lines.

4. The covering factors determined for LOWION and HIGHION were 0.35 and 0.84, which, while physically possible, are high given the likelihood that a fraction of the X-ray emission is undetected owing to absorption by material in the disk of the host galaxy or surrounding the NLR. However, the transparency of these components to the ionizing radiation leads to the possibility that there are multiple zones of highly ionized gas that subtend the same solid angle. The additional emission from these zones would reduce the covering factors.

5. Our estimated total mass and mass outflow rates for LOWION and HIGHION were 0.35 and 0.84, which, while physically possible, are high given the likelihood that a fraction of the X-ray emission is undetected owing to absorption by material in the disk of the host galaxy or surrounding the NLR. However, the transparency of these components to the ionizing radiation leads to the possibility that there are multiple zones of highly ionized gas that subtend the same solid angle. The additional emission from these zones would reduce the covering factors.

6. The ionization state and temperature of HIGHION are consistent with those of the scattering medium in which the polarized emission arises (Miller et al. 1991; Kraemer & Crenshaw 2000a), although its column density is an order of magnitude too small. However, if there are multiple zones, as noted in item 4, the total column density of high-ionization gas could be sufficient to produce the scattered light. The radial profile of the continuum radiation (Crenshaw & Kraemer 2000a) is consistent with such a scenario. Therefore, we suggest that the scattered emission arises in the X-ray emission-line gas, in agreement with Ogle et al. (2003).

Finally, the overall properties of NGC 1068, including a high mass accretion rate, supersolar abundances, large amounts of highly ionized gas and molecular gas (e.g., Riffel et al. 2014), and active star formation (Bruhweiler et al. 2001) may be connected to its stage of activity. That is, NGC 1068 is in an
early part of its active phase, at which time the AGN is being rapidly fueled, but before the inner nucleus has been cleared.

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