Modeling of the Quasar Main Sequence in the Optical Plane

Swayamtrupta Panda1,2, Bożena Czerny1,2, Tek P. Adhikarī2, Krzysztof Hryniewicz2, Conor Wildy1,
Joanna Kuraszkiewicz3, and Marzena Śniegowska1,4

1 Center for Theoretical Physics (PAN), Al. Lotników 32/46, 02-668 Warsaw, Poland; spanda@camk.edu.pl
2 Nicolaus Copernicus Astronomical Center (PAN), ul. Bartycka 18, 00-716 Warsaw, Poland
3 Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA
4 Warsaw University Observatory, Al. Ujazdowskie 4, 00-478 Warsaw, Poland

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Abstract

The concept of the quasar main sequence is very attractive since it stresses correlations between various parameters and implies the underlying simplicity. In the optical plane defined by the width of the Hβ line and the ratio of the equivalent width of the Fe II to Hβ observed objects form a characteristic pattern. In this paper we use a physically motivated model to explain the distribution of quasars in the optical plane. Continuum is modeled as an accretion disk with a hard X-ray power law uniquely tight to the disk at the basis of observational scaling, and the broad-line region distance is determined also from observational scaling. We perform the computations of the Fe II and Hβ line production with the code CLOUDY. We have only six free parameters for an individual source, maximum temperature of accretion disk, Eddington ratio, cloud density, cloud column density, microturbulence, and iron abundance, and only the last four remain as global parameters in our modeling of the whole sequence. Our theoretically computed points cover well the optical plane part populated with the observed quasars, particularly if we allow for supersolar abundance of heavy elements. Explanation of the exceptionally strong Fe II emitter requires stronger contribution from the dark sides of the clouds. Analyzing the way our model covers the optical plane, we conclude that there is no single simple driver behind the sequence, as neither Eddington ratio nor broadband spectrum shape plays the dominant role. Also, the role of the viewing angle in providing the dispersion of the quasar main sequence is apparently not as strong as expected.

Key words: accretion, accretion disks – galaxies: active – quasars: emission lines – radiative transfer

1. Introduction

Quasars, or, more generally, active galactic nuclei (AGNs), are complex objects having a supermassive black hole located at the center of a galaxy accreting matter. In high Eddington ratio (λedd) sources, inflowing matter forms an accretion disk along with a surrounding medium in the form of a hot corona and a wind. In radio-loud (jetted) AGNs we also see a collimated outflow. Further out, the broad-line region (BLR) and the dusty/molecular torus are located, completing the picture. It is thus not surprising that active galaxies come in a variety of types. If we concentrate on sources with a clear view of the nucleus (Type 1 sources), they should display considerable variety, taking into account that the spectral morphology is affected by the black hole mass, accretion rate, black hole spin, and viewing angle. This last aspect is important even for Type 1 objects owing to flattened geometry of some elements (disk and BLR). Extinction and departures from stationarity further complicate the picture.

The search for a quasar main sequence has been undertaken in recent decades with surprising success. The study of Boroson & Green (1992) used principal component analysis to show that a single parameter corresponding to Eigenvector 1 (EV1) is responsible for a significant fraction of the dispersion, 29.2% of the total variance, in the studied quasar sample. In their analysis, EV1 represented a combination of 13 properties measured for each source, including several line equivalent widths (EWs), line shape parameters, absolute magnitude, and the broadband index αox. This line of study was further pursued by several authors (Dultzin-Hacyan & Ruano 1996; Sulentic et al. 2000; Boroson 2002; Kuraszkiewicz et al. 2009). In recent studies, instead of a full EV1, a reduced EV1 was used, with four elements (Sulentic et al. 2009; Marziani et al. 2014; Sulentic & Marziani 2015). The optical plane version was just based on two quantities: the ratio of the EW of the Fe II complex, measured in the 4434–4684 Å wavelength range, to Hβ range, Reβ, and the FWHM of Hβ (Shen & Ho 2014). The quasar main sequence is thus well established, although it is not as narrow as the stellar main sequence in the Hertzsprung–Russell diagram (Sulentic et al. 2000, 2001).

The key question is why such a sequence forms at all. Quasars are complex objects; their central engine is described by black hole mass, accretion rate (or Eddington ratio), and black hole spin, and its properties are also affected by the viewing angle. The BLR itself is a complex extended region. It is not simple to identify just a single underlying parameter, although papers devoted to the quasar main sequence attempted to identify the actual driver of the sequence. Boroson & Green (1992) have postulated that the key parameter is the Eddington ratio, with Shen & Ho (2014) tracing this to the black hole mass distribution among quasars. Additional dependence on extinction has also been reported (Kuraszkiewicz et al. 2009). Bonning et al. (2007) mentioned the possibility that the key parameter is the maximum temperature of the accretion disk or, equivalently, the peak of the spectral energy distribution (SED) since the shape of the incident continuum should be responsible for both the continuum and emission-line properties. Here we start from the generic approach: we model realistically the SED and the BLR setup, and we calculate the line emissivity using the code CLOUDY, version C17 (Ferland et al. 2017), and we compare them to the distribution of Reβ in the high-quality data subsample of the objects studied by Shen & Ho (2014). As our leading parameters we use the maximum disk temperature and...
the Eddington ratio instead of the black hole mass and accretion rate, with the aim of seeing whether any of the previously proposed main sequence indeed plays a dominant role in the optical plane coverage.

2. Model

We model the emission of the Fe II and Hβ lines as functions of physically motivated parameters of an active nucleus. The problem of Fe II emission and its ratio to Hβ has a long history. Fe II emission was first identified in the spectrum of the quasar 3C 273 by Wampler & Oke (1967) and in Seyfert galaxy I Zw I by Sargent (1968). Osterbrock (1976) studied in detail Mrk 376, a source with strong and broad Fe II emission. The width of the Balmer lines in this source is broad (FWHM of 5000 km s$^{-1}$). He identified the likely emission mechanism as the resonance fluorescence, and from the observed SED shape in this source he estimated the Fe II-to-Hβ ratio as $\sim 1$, but he mentioned that the estimate might not be accurate since the Balmer decrement does not agree with photoionization calculations.

The details of the Fe II excitation are still not fully known since modeling was not quite satisfactory (e.g., Collin & Joly 2000; Baldwin et al. 2004a). The importance of the hard X-rays, as proposed by Davidson & Netzer (1979), is also not clear (e.g., Wilkes et al. 1987; Boroson 1989; Zheng & O’Brien 1990; Shastri et al. 1994; see also Wilkes et al. 1999). Microturbulence or additional collisional excitation seems to be required (e.g., Baldwin et al. 2004a). The ratio of the optical Fe II to Hβ was successfully modeled by Joly (1987), where high-density ($10^{10.5}$–$10^{22}$ cm$^{-3}$), high column density ($10^{23}$–$10^{25}$ cm$^{-2}$), and low-temperature clouds are assumed (6000–8000 K). They also stressed the need for shielding of the region from the observed power-law continuum in order to have a low degree of ionization, which reduces Hβ. The ionization potentials of hydrogen are very similar, which makes modeling the broad range of the ratio of Hβ and Fe II transitions difficult.

In the present paper we use the current version of the code CLOUDY (Ferland et al. 2017), which incorporates the required local processes. We assume that the emission of both Fe II and Hβ comes from the same region. There are strong arguments that the emission regions of Fe II and Hβ are actually related. Both Fe II and Hβ belong to low-ionization lines (LILs) according to classification of Collin-Souffrin et al. (1988). Both Fe II and Hβ respond to the variations of the continuum. By analyzing NGC 7603 spectra, Kollatschny et al. (2000) found optical Fe II to vary with a similar amplitude to the Balmer lines. In Vestergaard & Peterson (2005) it was concluded that in NGC 5548 Fe II varied with an amplitude of 50%–75% of that of Hβ, while they also attempted to measure the Fe II delays. Their estimate (few hundred days for Fe II) remained highly uncertain. In Kuehn et al. (2008) a measurement of the reverberation response time of 300 days for Fe II lines in Ark 120 implied an origin in a region several times farther away from the central source than Hβ. Similar results were reported in Barth et al. (2013), Rafert et al. (2013), and Chelouche et al. (2014). However, reliable reverberation of optical Fe II lines done by Hu et al. (2015) for a sample of nine AGNs found that the detected lags were comparable to Hβ. The FWHMs of both show significant correlation (Cracco et al. 2016), although for high Eddington ratios a kinematic shift is visible (Hu et al. 2008), while others have found no such systematic redshift (Sulentic et al. 2012).

2.1. Incident Continuum

We parameterize the incident continuum as two power laws with low- and high-energy cutoffs. The optical/UV power law represents the emission from the accretion disk, where most of the energy is dissipated. This component forms the big blue bump (Czerny & Elvis 1987; Richards et al. 2006). The slope of the power law $\alpha_{\text{opt}}$ is assumed to be $1/3$ (in convention $F_\nu \propto \nu^{\alpha}$, consistent with the theory of accretion disks; Shakura & Sunyaev 1973), supported by polarimetric observations of quasars (Kimishimo et al. 2008) and broadband data fitting (Capellupo et al. 2015). The high-frequency cutoff, $\nu_0$, is the basic parameter that we vary in our model, i.e., we assume that the accretion disk luminosity can be described by the formula

$$\nu L_\nu = A\nu^{4/3} \exp(-\nu/\nu_0).$$

(1)

This parameter is directly related to the maximum temperature in the accretion disk, $T_{\text{max}}$. If we use the Newtonian approximation of the disk from Shakura & Sunyaev (1973), there is a simple relation between the maximum temperature and global parameters of the accretion flow

$$T_{\text{max}} = 1.732 \times 10^{19} \left(\frac{M}{M_\odot}\right)^{1/4} [K].$$

(2)

where the black hole mass, $M$, and the accretion rate, $\dot{M}$, are expressed in cgs units (see, e.g., Panda et al. 2017). The disk maximum temperature is also related to the peak of the spectral energy distribution (SED) of a Shakura–Sunyaev disk on the $\nu/F_\nu$ plot

$$\frac{h\nu_{\text{max}}}{kT_{\text{max}}} = 2.464.$$  

(3)

Here $h$ is the Planck constant and $k$ is the Boltzmann constant. The simplified shape of the spectrum given by Equation (1) peaks at the frequency $4\nu_0/3$. Therefore, combining these two factors, we finally obtain the convenient parameterization of the disk shape in the form

$$\nu L_\nu = A\nu^{4/3} \exp(-\nu/1.853kT_{\text{max}}).$$

(4)

In the case of an accretion disk around a rotating black hole, the relativistic corrections are very important, the position of the innermost stable circular orbit strongly depends on spin, and the relations between the $T_{\text{max}}$ and the global parameters of the accretion flow are more complex, and in that case more advanced back-modeling is necessary, as done by Thomas et al. (2016). However, for the purpose of the current work we only consider nonrotating black holes, which are well parameterized by the proposed prescription (see Figure 1) and are characterized by only two free parameters: black hole mass ($M$) and accretion rate ($\dot{M}$).

The normalization of the optical/UV power law in Equation (1) is given by the values of the black hole mass and accretion rate

$$A = 1.33 \times 10^{-20}(M\dot{M})^{2/3} \text{[erg s}^{-1}\text{Hz}^{-4/3}]$$

(5)

under the assumption of the viewing angle 60°. Adopting such a viewing angle relates the integrated spectrum to the source bolometric luminosity. Small corrections due to an on average...
smaller viewing angle of \( \sim 40^\circ \), due to the obscuration by the dusty torus (Lawrence & Elvis 2010), are not an important factor.

AGNs emit part of the energy in the form of the hard X-ray emission. We parameterize this component again as a power law with a low- and high-energy cutoff. The high-energy cutoff is set at 100 keV as in most fitting packages (e.g., OPTXAGN—standard AGN shape in CLOUDY; Done et al. 2012; Thomas et al. 2016). Observational data show a dispersion in this quantity from about 50 keV to over 200 keV, but the measurements are still rare (for a compilation of measurements from NuSTAR, see Fabian et al. 2015).

The relative normalization of the X-ray component with respect to UV is found from the universal scaling law recently discovered by Lusso & Risaliti (2017),

\[
\log L_X = 0.610 \log L_{UV} + 0.538 \log v_{FWHM} + 3.40, \tag{6}
\]

where \( L_{UV} \) is a monochromatic luminosity \( \nu L_{\nu} \) measured at 2500 Å and \( L_X \) is measured at 2 keV. The importance of the X-ray component decreases with the increase of the UV flux, as illustrated in Figure 1. Equation (6) gives us the value of the broadband index \( \alpha_{\text{OX}} \) measured between 2500 Å and 2 keV. In Figure 2 we show the range of this index covered in our computations.

However, in order to use this formula, we actually need the line \( v_{FWHM} \), which depends on the cloud location. We need this distance also for calculation of the line emissivity.

### 2.2. Distance to the BLR

To determine the distance to the BLR clouds, we use the observationally established relation from Bentz et al. (2013). We choose the version Clean from their Table 14,

\[
\log R_{\text{BLR}} = 1.555 + 0.542 \log L_{44,5100} \text{ [light days]}, \tag{7}
\]

where the luminosity at 5100 Å is measured in units of \( 10^{44} \text{ ergs s}^{-1} \).

Thus, the shape of the incident radiation with its normalization provides us with the distance to the BLR. The value of the black hole mass gives the required line width

\[
v_{\text{FWHM}} = \left( \frac{GM}{R_{\text{BLR}}} \right)^{1/2}, \tag{8}
\]

where we adopt the virial factor 1 for the BLR clouds. This is indeed a simplified approach since the virial factor seems to be a function of the measured line width but the average value is actually close to 1 (Mejía-Restrepo et al. 2018), which is enough for our current purpose.

Thus, for the two parameters characterizing the SED (e.g., normalization and the maximum disk temperature, or, equivalently, \( M \) and \( \dot{M} \)) all the other parameters required to do the radiative transfer calculation are uniquely determined.

### 2.3. Radiative Transfer

We calculate H/\( \beta \) and optical Fe II emission performing the computations with the CLOUDY code (Ferland et al. 2017, version 17). We use the incident radiation and the distance to the BLR as described above. We adopt a traditional single-cloud approximation (e.g., Mushotzky & Ferland 1984). This is a reasonable approach since we are interested in a single line ratio, so going to the more complex locally optimized cloud (LOC) model of Baldwin et al. (1995a) is not necessary. In addition, the BLR extension is not large, and the outer-to-inner ratio is estimated to be of order of 4–5 (Koshida et al. 2014). In CLOUDY computations we assume the plane-parallel...
geometry, which provides emission both from the illuminated side of the cloud and from the dark side of the cloud, in equal proportions. We assume that the density inside the cloud is constant. This is again an approximation since the clouds in the vicinity of the nucleus are expected to be in pressure equilibrium in order to survive at least in the dynamical timescale (e.g., Różańska et al. 2006). Some models based on radiation pressure confinement suggested that the density gradient in the cloud must be steep (Stern et al. 2014; Baskin & Laor 2018). However, at least in a significant fraction of sources that show the presence of the intermediate-line region instead of a well-separated BLR and NLR, the local density at the cloud surface must be high, and the density gradient is rather shallow (Adhikari et al. 2016, 2018a). We assume two additional free parameters of the cloud: density, $n$, and hydrogen column density, $N_H$.

$H\beta$ flux is taken from the code output, and FeII emission is calculated by summing up all the FeII lines in the range from 4434 to 4684 Å, as defined in Shen & Ho (2014). The parameter $R_{Fe}$ is calculated as the ratio of these two numbers.

2.4. Summary of the Model Parameters

For convenience, we decided to use the following parameters to present our results: $T_{\max}$, $L/L_{\text{Edd}}$, $n$, and $N_H$. Here $L/L_{\text{Edd}}$ is defined using the Eddington accretion rate value $1.26 \times 10^{38} (M/M_\odot)$, and to calculate the Eddington accretion rate, we used the Newtonian accretion disk efficiency $1/12$ (Shakura & Sunyaev 1973). For the Eddington ratio, we choose values between 0.01 and 1. We cannot consider higher values since then the slim disk effects would be important (Abramowicz et al. 1988; Wang et al. 2014). At lower accretion rates inner optically thin flow likely replaces the cold geometrically thin disk, which leads to modification of both the SED (Narayan & Yi 1994; Nemmen et al. 2014) and the BLR itself (e.g., Czerny et al. 2004; Balmaverde & Capetti 2015). In general, we consider the range of the $T_{\max}$ between $1.6 \times 10^4$ and $5 \times 10^5$ K, appropriate for the AGN big blue bump. The corresponding range of the black hole masses depends on the adopted Eddington ratio. We give example values in Table 1. We assume that the viable range of masses is between $10^6 M_\odot$ and $3 \times 10^9 M_\odot$ for low-redshift sources with a detected $H\beta$ line. Thus, not all of the $T_{\max}$ range is realistic for a given choice of the Eddington ratio, and we include this effect in our plots. Therefore, the allowed range of the $T_{\max}$ for a given Eddington ratio is further constrained by the limits on the black hole mass to be between $10^6 M_\odot$ and $5 \times 10^9 M_\odot$. For the cloud density $n$, we choose values from $10^{10}$ to $10^{12}$ cm$^{-3}$, appropriate for the LIL part of the BLR. The column density was assumed to vary from $10^{22}$ to $10^{24}$ cm$^{-2}$. We assume a constant-density cloud profile, but we address the issue of the constant-pressure clouds in the discussion. We also allow for the turbulent velocity since the need for a velocity of order of $10-20 \text{ km s}^{-1}$ is evident from the previous studies of the Fe II production (Bruhweiler & Verner 2008).

Finally, AGNs can have a range of metallicities, and most studies have found that the abundances are actually at least solar and mostly supersolar (factor of 1–10; Hamann & Ferland 1999; Tortosa et al. 2018), even for high-redshift quasars (by a factor of 5–10; e.g., Simon & Hamann 2010). In our computations we either assumed the standard chemical composition, which is the default in CLOUDY, or we allowed for an increase in Fe abundance. In the first option the default values are provided by CLOUDY, and in this case (see Table 7.1 of CLOUDY manual) C and O abundances come from photospheric abundances of Allende Prieto et al. (2001, 2002), while N, Ne, Mg, Si, and Fe are from Holweger (2001), and the Fe is taken from Holweger (2001). If we now specify a solar abundance, Fe is taken from the GASS model (Grevesse et al. 2010), and in this option we also consider supersolar abundance.

3. Results

We aim at reproducing the observed quasar optical plane from the physically motivated model of an accretion disk with a corona illuminating the BLR. Computations for a single quasar required assuming only the black hole mass and accretion rate (or alternatively, disk maximum temperature and the Eddington ratio), cloud number density, cloud column density, turbulent velocity, and metallicity. For a whole quasar population, we fix the black hole mass range at $10^6 M_\odot$–$3 \times 10^9 M_\odot$, and the bolometric luminosity range was chosen to be from 0.01 to 1.0. The global model of the optical plane is then set by the remaining parameters.

The choice of the Eddington ratio range may be particularly important, so we checked the distribution of this parameter in the Shen et al. (2011a) quasar sample. The mean value of the Eddington ratio in the full Shen & Ho (2014) catalog and in the subsample is close to 0.1, as demonstrated in Figure 3. The mean value of the black hole mass in the Shen et al. (2011a) catalog is $log M = 8.4$ if we limit ourselves to objects with measured $H\beta$, i.e., for redshift $z$ below $\sim 0.75$ (Panda et al. 2018, in preparation), and the corresponding value of $log T_{\max}$ is about 4.80.

Since modeling Fe II emission caused significant problems in the past, we first compare the model predictions for the mean values of the black hole mass and Eddington ratio in the sample with values measured by Shen et al. (2011a) and Shen & Ho (2014).

The mean and the median in the whole Shen et al. (2011a) catalog for objects with measured $R_{Fe}$ are 0.97 and 0.70, respectively, but if we limit ourselves only to the high-quality subsample with low measurement errors, then the corresponding values drop to 0.64 and 0.38 (Śniegowska et al. 2018). Our value from the model, for the mean quasar parameters, is in the range of 0.2–0.5, depending on the local density of the clouds. For the median Eddington ratio in the sample, 0.1, low-density clouds predict too faint Fe II, but for a density of $10^{12}$ cm$^{-3}$ and a column density of $10^{24}$ cm$^{-2}$, the obtained value is $\sim 0.3$, if no turbulence and only solar metallicity is assumed. If we allow for a turbulence of order of 10–20 km s$^{-1}$, then $R_{Fe}$ rises to 0.32–0.35. Increasing the Fe II abundance by a factor of 3, combined with the turbulent velocity of 10 km s$^{-1}$, increases $R_{Fe}$ up to 0.9. Thus, even with very moderate increase of metallicity we reproduce well the mean value of $R_{Fe}$ in the optical plane. This itself is interesting since we have only a few arbitrary parameters ($T_{\max}$, $\lambda_{\text{Edd}}$, $n_{H\beta}$).
and $N_{\text{HI}}$, and in this case two of them are actually fixed by observations.

Thus, on average, we do not need any additional strong turbulent heating to explain the typical $R_{\text{Fe}}$ ratios. Simple radiative reprocessing works well, which is consistent with the possibility of the reverberation mapping of $H\beta$ and Fe II. Thus, our relatively simple model works well for the average quasar parameters. We only need rather large densities and column densities, $10^{12}$ cm$^{-3}$ and $10^{24}$ cm$^{-2}$, respectively.

With this knowledge, we choose large cloud density and column density and a broad range of metallicity, and we calculated the results for the quasar sample. We overplotted the expected trends on the observational optical plane of EV1. We use the values $R_{\text{Fe}}$ and FWHM as obtained from the computations for the range of densities and Eddington ratios (see Figure 4). The model well covers the optical plane occupied by the data points. Some of the trends are consistent with expectations. Large values of the FWHM of $H\beta$ correspond to lower values of the Eddington ratio. This simply reflects the relation between the accretion rate, black hole mass, line width, and SED peak position. Curves for solar abundance cover the region occupied by quasar majority, but the high $R_{\text{Fe}}$ (above 1) appear only from the objects with assumed supersolar Fe II abundance.

The effective rise in the Fe II strength with increasing metallicity occurs with a caveat—the models shift rightward when compared with the optical plane coverage, and thus they only predict the trend for objects with very high FWHM (see Figure 4). Thus, it is not enough just to increase the metallicity to very high values to cover the high Fe II emitters; rather, it

Figure 3. Left: distribution of the $\lambda_{\text{Edd}}$ from Shen et al. (2011a) (in red). The error-limited sample (in turquoise) is shown underneath the whole distribution. The fitted Gaussian has $x = -0.769176, \sigma = 0.42134285$. Right: enlarged version of the error-limited sample. The fitted Gaussian has $x = -0.93127483, \sigma = 0.40046898$.

Figure 4. Quasar optical plane: comparison of vFWHM–$R_{\text{Fe II}}$ obtained from the photoionization simulations with observations (Shen et al. 2011a). We consider three cases of $\lambda_{\text{Edd}} = 0.01, 0.1, \text{ and } 1.0$ and three values of the Fe II abundance, solar, 3 times solar, and 10 times solar, for a fixed cloud density $n_{\text{H}} = 10^{12}$ cm$^{-3}$, column density $10^{24}$ cm$^{-2}$, and turbulent velocity $10$ km s$^{-1}$. The complete sample from the observations (105,783 objects) is shown in gray. The error-limited sample (4989 objects) is shown in gold. The black points with error bars represent the average for the selected bins based on the $R_{\text{Fe II}}$ values for the error-limited sample.
needs to be coupled with other parameters in such a way as to cover the region of large $R_{\text{Fe}}$ and small FWHM. On the other hand, this region is mostly populated by objects with low data quality (gray dots in Figure 4), and high-quality data points there (yellow dots) are rare.

The dependence on the Eddington ratio is as not simple as postulated by Boroson (2002). The Eddington ratio does not change monotonically along the main sequence; it actually changes rather perpendicularly to it, and the impression of the overall increase of the Eddington ratio comes from the fact that most strong Fe II emitters have narrow lines, and high Eddington ratio objects in our model concentrate toward the bottom of the diagram. Therefore, the Eddington ratio cannot be identified as a single driver of the quasar main sequence in the optical plane.

We thus test the dependence of the Fe II emissivity on the SED shape since this is another potentially promising driver of the quasar main sequence. With this aim we show the dependence of the $R_{\text{Fe}}$ on the disk maximum temperature. If $T_{\text{max}}$ is actually the expected driver, this dependence should be monotonic. The results of the computations for a range of Eddington ratios, densities, and turbulent velocities are shown in Figure 5. We see that the dependence in general is nonmonotonic, particularly for moderate and high Eddington ratios. At the lowest Eddington ratios it is almost monotonic, but the direction of the change depends critically on the local density of the clouds.

The decrease of the Fe II emissivity with the rise of $T_{\text{max}}$ happens since, for a fixed Eddington ratio, the distance to the BLR rises more slowly than the bolometric luminosity of the accretion disk, and the incident flux increases. In addition, the contribution of the hard X-ray power law also decreases, contributing to this overall trend. The cloud becomes more ionized, and the hydrogen ionization front visible for cold clouds disappears. To illustrate this phenomenon, we plot two examples of the emissivity profiles of H/$\beta$ and the 10 strongest Fe II transitions (see Figure 6). These plots also show why large cloud density is required for efficient production of the Fe II: less dense clouds are more highly ionized, and Fe II production is less efficient. Also, the role of the column density is clear: iron emission forms predominantly inside and at the back (dark side) of the cloud. We did not consider higher column densities than $10^{24}$ cm$^{-2}$.

4. Discussion

We constructed a simple but realistic model representing the physics of the line formation in AGNs with the aim of reproducing the quasar main sequence. Our model is parameterized by the disk maximum temperature, $T_{\text{max}}$, $\lambda_{\text{edd}}$, and the local cloud density ($n$). These values allow the building of broadband SEDs of AGNs, the determination of BLR locations, the emissivity of optical Fe II lines and H/$\beta$ from the CLOUDY code, and the calculation of H/$\beta$ line widths. Allowing for a realistic range of values, we analyzed the coverage of the optical FWHM versus $R_{\text{Fe}}$ plane by the model and the observational data from the quasar sample. The mean values from the model and the data are consistent under the assumption of solar metallicity, if we assume a cloud density of $10^{12}$ cm$^{-3}$, a column density of $10^{22}$ cm$^{-2}$, and a turbulent velocity of 10–20 km s$^{-1}$. For the same parameters, we represent well the whole optical plane if we allow for enhanced metallicity in some of the clouds. This is necessary to explain the extreme Fe II emitters.

It is very interesting that we are able to reproduce the Fe II emissivity under the assumption of purely radiative processes in the clouds. In the past, the need for additional collisional heating to achieve efficient Fe II production was postulated (Joly 1987; Netzer 2001; Baldwin et al. 2004b). Radiative driving of Fe II emission is strongly supported by the measured time delays of Fe II with respect to the continuum (Hu et al. 2008). It is also important to note that we assume a single production zone for Fe II and H/$\beta$, and the clouds responsible for the line emission have universal density and column density. Clearly, accurate modeling of the line ratios in specific objects requires a more complex approach, with a range of radii and densities (e.g., Moloney & Shull 2014; Costantini et al. 2016), and such modeling is frequently done within the LOC model (Baldwin et al. 1995b). However, apparently the statistical distribution concentrates around the values based on simple and direct estimates. The universal column density in our model is roughly consistent with predictions of the thermal instability in the irradiated medium introduced by Krolik et al. (1981) and later discussed in a number of papers (e.g., Begelman et al. 1983; Rozanska & Czerny 1996; Krolik & Kriss 2001; Krongold et al. 2003; Danehkar et al. 2018). The local density in turn is roughly consistent with the radiation pressure confinement of the BLR clouds nicely discussed by Baskin & Laor (2018) in the introduction to their paper. The self-consistency of the picture indicated that we are now making considerable progress in the understanding of the BLR physics, going beyond the predominantly parametric models.

Some of the parameters cannot be derived yet from the basic constraints, such as turbulent velocity and metallicity. Also, the geometrical setup is not yet firmly set from the first principles, although a major step forward has been done with the development of the dust-based model of BLR formation (Czerny & Hryniewicz 2011a; Czerny et al. 2015, 2017; Baskin & Laor 2018). We thus discuss below the particular aspects connected with these parameters.

4.1. Turbulence

The emitting medium is most likely turbulent, and the turbulence decreases the optical depth of the clouds for lines. Fe II emissivity is quite sensitive to this value (e.g., Bruhweiler & Verner 2008). Therefore, we performed tests of the influence of the turbulence velocity on the calculated $R_{\text{Fe}}$, varying it between 0 and 100 km s$^{-1}$. Overall, the Fe II emissivity increases, but the trend is not monotonic. The emissivity rises with the rise of the turbulent velocity up to 20 km s$^{-1}$, and a further increase in the velocity leads to a decrease of Fe II production apart from the low-temperature tail (see Figure 5). Thus, the turbulence in the range 10–20 km s$^{-1}$ is generally favored for more efficient Fe II production, as such values are actually favored in detailed fitting of specific objects (e.g., Bruhweiler & Verner 2008; Marziani et al. 2013; Hryniewicz et al. 2014; Średzińska et al. 2017).

4.2. Constant-pressure Clouds

In the computations above we assumed a constant-density model, traditionally adopted in the computations of the BLR clouds (Davidson 1977). However, physically it is not justified, particularly for such thick clouds since they are irradiated from
the side exposed to the radiation flux from the central region, while the other side of the cloud is relatively cold. Such a cloud cannot be in hydrostatic equilibrium and would be rapidly destroyed. Therefore, a more appropriate description of the cloud structure is to assume a constant pressure throughout the cloud, as discussed for narrow-line region clouds (e.g., Davidson 1972), warm absorbers (e.g., Różańska et al. 2006; Adhikari et al. 2015), and BLR clouds (e.g., Baskin et al. 2014a). The effect is particularly strong for low local density clouds, but for high-density clouds at BLR distances the compression is relatively less important, by a factor of a few (Adhikari et al. 2018a). Nevertheless, the effect may be noticeable. We thus calculated an example of the constant-pressure cloud corresponding to the most typical values for the observational sample: $\log T_{\max} = 4.8$, $\lambda_{\text{Edd}} = 0.1$, $\log n = 12$ at the cloud illuminated surface, and $\log N_H = 24$. The results are shown in Table 2. The value of $R_{\text{Fe}}$ calculated for such a cloud was somewhat higher than for a constant-density cloud, if the turbulent velocity was neglected, and the effect decreased with the rise of the turbulence velocity. Thus, for such dense clouds, constant-density and constant-pressure models give very similar results.

4.3. Closed Geometry and Enhanced Contribution of the Cloud Dark Sides

Clouds are irradiated from one side, and the dark sides of the clouds have a different proportion in H$\beta$ and Fe II emission. In the computations shown throughout this paper we used a plane-parallel geometry, and the line intensity was calculated from the Intrinsic line intensities section of the main CLOUDY output. These include the combined emission from the dark and the bright sides of the cloud. This approach is justified if an observer is not highly inclined, clouds do not shield each other, the reprocessing of the emission of one cloud by the other cloud is negligible, and the geometrical thickness of the BLR is relatively small. With these approximations, we see on average the same total illuminated and dark surfaces of all clouds. However, if any of these assumptions are violated, the obtained $R_{\text{Fe}}$ ratio will be different. Such extreme setups might be
responsible for the extreme Fe II emitters that were recovered in Section 3 only for supersolar metallicity.

Thus, another possibility is that the abundances are always solar but the BLR is so geometrically thick that it covers most of the quasar sky, and the number of clouds so large that the reprocessing is important. To check this option, we calculated one cloud model using the closed geometry. We assumed the same cloud parameters as in Section 2. In this case the increase of the $R_{\text{Fe}}$ is not very large since two effects counteract. One is that we now see basically the dark sides of the clouds, but the other is that multiple scattering increases the local incident flux and the cloud ionization. In addition, in order not to heavily absorb the continuum, we need a gap in the cloud distribution just along the line of sight to the innermost part of the accretion disk.

The second possibility is similar to the one above, but with the cloud number not as high, so the cross-illumination of clouds can be neglected. Again, in this case we see more of the dark sides of the clouds than of the bright sides. Such a picture has been used by Ferland et al. (2009), where the Fe II emission has been modeled as coming from infalling clouds. In this case we calculated separately the $R_{\text{Fe}}$ values for the bright side and for the dark side of the cloud, by using a plane-parallel approximation, but with the sphere command to store just the outward line emission, and the inward emission has been calculated as a difference between total (intrinsic) and outward line flux:

$$\Delta R_{\text{Fe II}} = R_{\text{Fe II (dark)}} - R_{\text{Fe II (bright)}}.$$  

The results are given in Table 3. In the case of the same cloud ($log\ T = 5$, log $n = 12$, log $N_{\text{H}} = 24$), we obtain $R_{\text{Fe}} = 0.2883$ for the bright side and $R_{\text{Fe}} = 0.2782$ for the dark side. Thus, if the clouds cover the nucleus densely, we do not see an enhancement in the Fe II production since the intercloud scattering increases the overall ionization. The situation is different if we calculate emission from the dark sides of the clouds in a standard plane geometry, when no such intercloud scattering is present. In such a geometry, the Fe II emission from

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**Figure 6.** Emissivity profile for two clouds as a function of the cloud depth measured from the illuminated surface. Since the plot is logarithmic, we plot depth times emissivity to show clearly the location of the emission peak. For a low-temperature cloud the hydrogen ionization front is visible and Fe II emission dominated at the dark side of the cloud.

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### Table 2

Fe II Strength Comparison between Constant-density (CD) and Constant-pressure (CP) Single Clouds with Microturbulence Effect ($log\ T_{\text{max}} = 5$, log $M/M_\odot = 8.5787$)

| $v_{\text{turb}}$ (km s$^{-1}$) | $R_{\text{Fe II}}$ (CD) | $R_{\text{Fe II}}$ (CP) | $\Delta R_{\text{Fe II}}$ |
|-------------------------------|--------------------------|--------------------------|--------------------------|
| 0                             | 0.305                    | 0.350                    | 0.044                    |
| 10                            | 0.421                    | 0.434                    | 0.013                    |
| 20                            | 0.364                    | 0.355                    | -0.008                   |

**Note.**

$\Delta R_{\text{Fe II}} = R_{\text{Fe II (CP)}} - R_{\text{Fe II (CD)}}$. 

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Notes.

a Int. = Intrinsic; Bri. = Bright; values are integrated intensities in erg cm\(^{-2}\) s\(^{-1}\).

b See Equation (9).

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**Table 3**

Open versus Closed Geometry—Contribution from the Dark Side of the Cloud

| \(R_{Fe} \) | Intrinsic | Bright | \(H\beta\) (Int.)\(^{a}\) | \(H\beta\) (Bri.) | Fe II (Int.) | Fe II (Bri.) | Dark\(^{b}\) |
|---------|-----------|-------|----------------|----------------|-------------|-------------|-------|
| open    | 0.143     | 0.133 | \(10^{44.016}\) | \(10^{44.010}\) | \(10^{43.173}\) | \(10^{43.133}\) | 0.278 |
| closed  | 0.285     | 0.288 | \(10^{44.142}\) | \(10^{43.972}\) | \(10^{43.597}\) | \(10^{43.432}\) | 0.278 |

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**Figure 7.** Effect of changing abundances starting from solar (\(Z_\odot\)) to \(10 \times Z_\odot\). Here, we have shown for the case with the maximum Fe II strength obtained \(\lambda_{eff} = 0.01\), \(n_H = 12\) [cm\(^{-3}\)], and \(v_{def} = 10\) km s\(^{-1}\) (left panel). In the right panel the same effect is shown for three cases of abundances (\(Z/3Z_\odot\) = 1, 3, and 10) with changing Eddington ratios (log \(\lambda_{eff} = 0.01, 0.1\), and 1).

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**Table 4**

Effect of Changing Abundances on the Obtained Values of \(R_{Fe}\)

| \(v_{def}\) (km s\(^{-1}\)) | \(R_{Fe}\) (def) | \(R_{Fe}\) (Z\(_\odot\)) | ratio (col2/col3) | \(R_{Fe}\) (3 Z\(_\odot\)) | Ratio (col5/col2) | Ratio (col5/col3) | \(R_{Fe}\) (10 Z\(_\odot\)) | Ratio (col8/col2) | Ratio (col8/col3) |
|--------------------------|----------------|----------------|-----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
| 0                        | 0.305          | 0.329          | 1.077           | 0.595          | 1.948          | 1.809           | 1.030          | 3.374          | 3.132          |
| 10                       | 0.421          | 0.462          | 1.096           | 0.907          | 2.153          | 1.964           | 1.634          | 3.882          | 3.540          |
| 20                       | 0.364          | 0.399          | 1.097           | 0.792          | 2.179          | 1.987           | 1.475          | 4.059          | 3.702          |

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the dark side of the cloud measured with respect to \(H\beta\) is enhanced by a factor of 6. So, in rare cases, when we see predominantly the dark sides of the clouds, we can reproduce \(R_{Fe}\) values as high as a few, required to explain the extreme data points without postulating supersolar metallicity.

**4.4. Metallicity**

The proper coverage of the optical plane, including the right corner occupied by the extreme Fe II emitters, required allowing for supersolar abundances, although the average quasar parameters were well represented without (see Section 3). The increase of the abundances simply enhances the Fe II emissivity, shifting the theoretical curves to the right in the optical plane (see Figure 4). The same effect is seen if the parameter \(R_{Fe}\) is studied directly as a function of the maximum disk temperature. We show the corresponding plots in Figure 7.

Upon using the GASS model (at \(Z_\odot\)), we find an increase in the Fe II strength by 7%–9% in all three cases of changing microturbulence compared to the default case for solar metallicity. The Fe II strength increases by 95%–118% and by 237%–406% when the metallicity \((Z)\) is increased to 3 and 10 \(Z_\odot\), respectively (Table 4). In this case only the most extreme values of \(R_{Fe}\) (above 4) are not accounted for and might require that we see predominantly dark sides of the clouds (see Figure 7).

**4.5. Extreme EV1 Objects**

In Śniegowska et al. (2018) 27 objects were selected for study from the Shen et al. (2011a) catalog, but after careful analysis only six objects were confirmed as strong Fe II emitters. Three of these sources had broad \(H\beta\) lines, with FWHM above 4500 km s\(^{-1}\), mean black hole mass \(log M = 8.9\), and Eddington ratio of about 0.01, while the other three had very narrow \(H\beta\) (below 2100 km s\(^{-1}\)), mean black hole mass \(log M = 7.5\), and Eddington ratio above 0.3. The first family of quasars is consistent with high expected values of \(R_{Fe}\) since the typical maximum temperature in this case is about 20,000 K. The second group has the temperatures of the order of \(2 \times 10^5\) K, and from the model computations the expected values of \(R_{Fe}\) are low, particularly for high Eddington ratio sources. The model predicts only the further rise of \(R_{Fe}\) if the temperatures are well above \(10^6\) K. This cannot happen within the frame of the blackbody representation of the big blue bump.
If the emission of Fe II and Hα microturbulence region, as assumed in the current paper, the ratio used from Bentz et al. emission is relatively more efficient if the BLR is located closer in, with all the other parameters fixed. This suggests that future studies should include the radial stratification of the BLR, but it is not simple since the results would depend on the weighted emissivity as a function of radius. Additionally, continuum is variable and BLR responds to it after a delay. One needs to take present-day continuum luminosity and line width that traces radius corresponding to continuum luminosity from the past. Single-epoch spectra, as in the Sloan Digital Sky Survey, do not trace this effect, which introduces some bias. Study of the full BLR structure is beyond the scope of the current work.

### 4.6. Effect of BLR Size

The inner radius of the BLR cloud that has been used in this paper follows Bentz et al. (2013) (Section 2.2). However, the BLR is actually extended. Here we test the effect of changing the radius from 0.3R_{Bentz} to 5R_{Bentz}. The lower limit (0.3R_{Bentz}) used has been set corresponding to maximum disk temperature (∼2000 K) expected from the BLR model based on dust presence in the disk atmosphere (Czerny & Hryniewicz 2011b). The upper limit is set assuming that R_{out} ∼ 5R_{Bentz} comes from the dust reverberation studies of the torus (Koshida et al. 2014). The results for one such case are shown in Figure 8. There is a monotonic behavior of the Fe II strength with respect to changing BLR radius. In a single-zone approximation Fe II emission is relatively more efficient if the BLR is located closer in, with all the other parameters fixed. This suggests that future studies should include the radial stratification of the BLR, but it is not simple since the results would depend on the weighted emissivity as a function of radius. Additionally, continuum is variable and BLR responds to it after a delay. One needs to take present-day continuum luminosity and line width that traces radius corresponding to continuum luminosity from the past. Single-epoch spectra, as in the Sloan Digital Sky Survey, do not trace this effect, which introduces some bias. Study of the full BLR structure is beyond the scope of the current work.

### 4.7. Viewing Angle

In our model we did not include the range of viewing angles toward the nucleus. As pointed out by many authors (Zhang & Wu 2002; Collin et al. 2006; Shen & Ho 2014), BLR is not flat. If the emission of Fe II and Hβ comes roughly from the same region, as assumed in the current paper, the ratio R_{Fe II} is not affected, but the measured Hβ width is expected to depend on the viewing angle, i. In type 1 sources this viewing angle is never very large; otherwise, the torus shields the view of the nucleus. The frequently adopted range of the viewing angles is thus between 0° and 45°. Marziani et al. (2001) and others have tried to connect the observational plane with the source orientation and Eddington ratio. The line width, in turn, depends on both sin i and the turbulent (random) velocity field. Thus, the FWHM can be affected by a factor of 2 for the BLR thickness of order of 0.3 (see Equation (8) in Collin et al. 2006), and a similar effect was determined in the studies of the virial factor trends (Mejía-Restrepo et al. 2018). Thus, the vertical extension of the covered area can be increased by a factor of less than 2 if this effect is included. On the other hand, we see from our modeling that the spread in the vertical direction is mostly caused by the coupling between the model parameters and the Fe II production efficiency. We intend to look into the effects of the orientation on the main sequence more carefully in our subsequent work.

### 4.8. Correlation between the Eddington Ratios and the Black Hole Masses

In our approach we have not yet explicitly connected the Eddington ratios to the black hole masses in the observed sample. If we plot the quality-controlled sample of 4989 objects from the original Shen et al. (2011b) study, the Eddington ratio and the black hole masses in the current optical plane can be constrained with

$$\log \lambda_{\text{Edd}} = -1.05 \log M_{\text{BH}} + 7.15,$$

where $M_{\text{BH}}$ is considered in $M_{\odot}$. This is shown in the left panel of Figure 9. If the analysis to model the black plane is to be contained within the limits of this boundary defined between the Eddington ratio and the black hole mass, then we cover a much lesser portion of the optical plane than before (see right panel of Figure 9). Still, with this additional constraint, we cover 4903 out of the 4989 objects, i.e., over 98% of the total subsample. Indeed, as shown in Figure 9, we require deeper observations to exploit the lower regime of the log $\lambda_{\text{Edd}} - \log M_{\text{BH}}$ in the context of the quasar optical plane.

### 5. Conclusions

We model the quasar main sequence using a realistic description of the quasar broadband spectra, assuming the distance to the BLR as known from reverberation measurements and calculating the line emission using CLOUDY, version C17. We show the following:

1. Mean quasar parameters are well reproduced by our single-zone constant-density model and solar abundance, particularly if we take into account the turbulent velocity of order of 10–20 km s^{-1}.
2. High-density clouds ($n \sim 10^{12}$ cm^{-3}) allow good coverage of the optical plane; such densities are consistent with the radiation pressure confinement of the BLR clouds (Baskin et al. 2014b; Adhikari et al. 2018b).
3. High values of $R_{Fe II}$ (>1) require higher abundance of iron and/or enhanced contribution from the cloud dark sides; in the second option very large solid angles of the BLR in these sources are required.
4. The range of viewing angles is only partially responsible for the dispersion in the quasar main sequence; most of the dispersion comes from a range of black hole masses and accretion rates.
5. The dependence of the $R_{Fe II}$ ratio on either the Eddington ratio or on the maximum disk temperature is not monotonic.

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Software: The results in this paper are mainly attributed to the photoionization code CLOUDY (Ferland et al. 2017). The authors would like to acknowledge the use of data analysis software TOPCAT (Taylor 2005).

Appendix

The atomic data available for radiative transfer are still under development and are far from satisfactory. This is reflected in the changes of the atomic data available in the CLOUDY code.
At the beginning of the project we made some runs using the CLOUDY code version C13 (Ferland et al. 2013), but finally we changed to version C17 (Ferland et al. 2017), and all results given here were obtained with the newest code. We always used the option species "Fe II+" levels = all for most accurate computations of the Fe II emission, as stressed in CLOUDY’s Hazy 1st Manual. We show the comparison of the two code versions in Figure 10. In general, the new code returns higher Fe II, so the net values of $R_{Fe}$ are lower in the newest version of CLOUDY.

The use of the option species "Fe II+" levels = all in version 17 is critical, since without it the Fe II emissivity is ∼50% higher than without this option. This option uses all the FeII transitions, including the Vernier et al. (1999) Fe II model, while if the option is not on, only a simplified old model of Wills et al. (1985) is adopted to speed up the computations.

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