X-Ray Reverberation Mapping of Ark 564 Using Gaussian Process Regression

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Abstract

Ark 564 is an extreme high-Eddington narrow-line Seyfert 1 galaxy, known for being one of the brightest, most rapidly variable soft X-ray active galactic nuclei (AGN), and for having one of the lowest temperature coronae. Here, we present a 410 ks NuSTAR observation and two 115 ks XMM-Newton observations of this unique source, which reveal a very strong, relativistically broadened iron line. We compute the Fourier-resolved time lags by first using Gaussian processes to interpolate the NuSTAR gaps, implementing the first employment of multitask learning for application in AGN timing. By simultaneously fitting the time lags and the flux spectra with the relativistic reverberation model RELTRANS, we constrain the mass at \( M \approx 3.7_{-1.4}^{+1.3} \times 10^6 M_{\odot} \), although additional components are required to describe the prominent soft excess in this source. These results motivate future combinations of machine learning, Fourier-resolved timing, and the development of reverberation models.

Unified Astronomy Thesaurus concepts: Accretion (14); Gaussian Processes regression (1930); Black holes (162); Astrostatistics techniques (1886); High energy astrophysics (739); X-ray active galactic nuclei (2035); Model selection (1912); Astrostatistics (1882)

1. Introduction

X-ray emission from active galactic nuclei (AGN) is powered by accretion onto a central supermassive black hole. The accretion disk emits thermally, producing UV seed photons that are Compton up-scattered to X-ray energies by a region of high-energy particles located close to the black hole known as the corona (Sunyaev & Trumper 1979). The Comptonized emission from the corona creates a direct coronal continuum in the X-ray spectrum. This emission then irradiates and is reprocessed by the inner accretion disk, producing correlated variability that is delayed on the order of the corona-to-disk light travel time (see Uttley et al. 2014; Cackett et al. 2021 for a recent review). This reprocessing produces the reflection component of the spectrum, including the iron K emission lines around 6.4–6.9 keV, the iron K edge around 7–8 keV, the broad Compton hump peaking near 20 keV, and a collection of fluorescent lines from iron and lower Z elements at softer energies (George & Fabian 1991; Ross & Fabian 2005).

In addition to the flux spectrum, the reflection features arise when plotting the time delays between correlated variability in each energy band to a common reference band (the lag-energy spectrum) (e.g., Fabian et al. 2009; Zoghbi et al. 2011; Kara et al. 2016). Features in the lag-energy spectrum associated with reverberation, namely, from the soft excess (De Marco et al. 2013) and the iron Kα line (Kara et al. 2016), have been detected in over 20 sources and have unlocked a new approach for probing AGN accretion flows.

In both the flux spectrum and the lag-energy spectrum, the shape and prominence of the relativistic reflection features vary significantly with the system’s geometry and physical properties (Fabian et al. 2000; Cackett et al. 2014). This has motivated increasingly sophisticated models to describe the reflection features observed in both types of spectra. Cackett et al. (2014) first fit the Fe Kα lines observed in NGC 4151 by calculating general relativistic transfer functions for reverberation for 28 combinations of height, spin, inclination, and reflection fraction. Since then, models have been developed for placing constraints on seven physical parameters of Mrk 335 by...
simultaneously modeling both the flux spectrum and lag-energy spectra in two frequency ranges (Mastroserio et al. 2020). These data were fit using the same model used in this paper, the relativistic reverberation mapping model RELTRANS, which models the direct coronal continuum as well as the reflection spectrum and time lags (Ingram et al. 2019; Mastroserio et al. 2021). The model also showed success in describing the time lags observed in five epochs during the hard-to-soft state transition of black hole X-ray binary MAXI J1820+070 by Wang et al. (2021), who, from modeling the reverberation, revealed that the corona extends vertically during the transition. Several previous studies (e.g., Zoghbi et al. 2020; Mastroserio et al. 2020; Wang et al. 2021), however, find discrepancies in the physics, namely, the height of the corona, inferred from modeling the time lags versus the flux spectra.

In this paper, we model the X-ray spectrum and time lags of well-known narrow-line Seyfert I (NLS1) Ark 564 by simultaneously fitting both the NuSTAR and XMM-Newton flux spectra and lag-energy spectra in three frequency ranges. Doing so with the same reverberation model allows us to probe model consistency and properties of the system by comparing how a single description for the accretion flow and central engine describes the flux spectra versus the time lags.

Most previous work on Ark 564 has focused on modeling the source’s flux spectrum (e.g., Giustini et al. 2015; Kara et al. 2017; Jiang et al. 2019), which exhibits features typical for an NLS1, including a strong soft excess and a steep spectral slope (Brandt et al. 1997). The first deep observation of the source with NuSTAR observatory (∼200 ks) revealed that Ark 564 also has one of the coolest coronas discovered to date, with an electron temperature of roughly 15 keV (Kara et al. 2017).

The Fourier frequency-resolved timing approach has been fruitful in understanding Ark 564 and other sources by isolating the time lags from variability occurring on different timescales (i.e., frequencies) due to distinct physical processes. Ark 564’s high-frequency soft lags were first discovered tentatively by McHardy et al. (2007). The soft lags were then confirmed by Legg et al. (2012) and then Kara et al. (2013), who also found evidence for the Fe K lag. The lowest frequency one can probe with this approach, however, is limited by the length of one’s longest continuous observation—a significant limit for data collected with instruments in low-Earth orbit. Due to NuSTAR’s data gaps from Earth occultations, however, we cannot probe long enough timescales to access the low-frequency hard lags, thought to be associated with the inward propagation of accretion rate fluctuations (Kotov et al. 2001; Arévalo & Uttley 2006).

In order to probe Ark 564’s low-frequency hard lags, Legg et al. (2012) corrected for the breaks between XMM-Newton observations by applying the maximum-likelihood method of Miller et al. (2010), which models the autocorrelations and cross correlation (and thus, the frequency-dependent time lags) by fitting the light curves. This approach was implemented by Zoghbi et al. (2013), who aimed to extend reverberation studies to the non-continuously sampled data (beyond XMM-Newton observations) due to Earth occultations. Kara et al. (2017) applied the maximum-likelihood method of Zoghbi et al. (2013) in order to access the NuSTAR low-frequency lags, but were unable to probe the reverberation lags at high frequencies due to limited statistics.

More recently, Gaussian process regression (GPR) has grown in popularity and has shown success in modeling the underlying probability distribution of sparse light curves of asteroids (Willecke Lindberg et al. 2021), AGN (Kelly et al. 2014; Wilkins 2019; Griffiths et al. 2021), and stars (Breuer & Stello 2009; Czekala et al. 2017; McAllister et al. 2017). Continuous realizations of the light curve can then be generated after modeling the observed variability, allowing for a probabilistic treatment of data generated in the gaps. Using this method, Wilkins (2019) recovers a simulated lag of 200 s from $5 \times 10^{-4}$ and $2 \times 10^{-3}$ Hz within a fractional error of 2% from simulated NICER observations of Ark 564 with low-Earth orbit data gaps. Unlike the approaches of Miller et al. (2010) and Zoghbi et al. (2013), Gaussian processes do not require any model assumptions for the cross correlation between energy bands—the models describing the variability in each light curve produce this on their own. The light curve in each energy band is treated as an independent entity, in the same way as when applying traditional Fourier techniques.

We present three new observations of Ark 564: two observations with XMM-Newton totaling 230 ks that are simultaneous with a longer exposure of 410 ks with NuSTAR, the latter being the longest single exposure of the observatory to date. Thanks to these new observations and the implementation of GPR to maximize the use of the NuSTAR data, we are able to probe the time lags in three distinct frequency ranges for both instruments spanning 0.01–0.9 mHz. The ability to simultaneously model six lag-energy spectra and the flux spectra is a combination of new data and the flexibility of the RELTRANS model.

This paper is organized as follows: our observations and data reduction are presented in Section 2. An introduction to Gaussian processes, multitask learning, and kernel functions for regression application to NuSTAR data is provided in Section 3. The basics of performing Fourier-resolved timing analysis on our GPR results are outlined in Section 4. We present the time lags and spectra, and physical constraints from fitting with a reverberation model in Section 5, which are discussed further in Section 6.

### 2. Observations and Data Reduction

Our analysis uses a combination of new and archival data of Ark 564 from the NuSTAR and XMM-Newton observatories, which are shown in Table 1. We present three new observations of Ark 564: 410 ks by NuSTAR (PI: E. Kara)—the observatory’s longest exposure yet—collected beginning 2018 November 28, as well as two 115 ks observations collected by XMM-Newton in early 2018 December (PI: E. Kara), partially simultaneous with the new NuSTAR observation. Light curves of these observations are shown in Figure 1, which show the source’s high variability. The $2-10$ keV flux of these new XMM-Newton observations is $1.4 \times 10^{-11}$ erg cm$^{-2}$ s$^{-1}$, and a

| Observatory | Obs. ID | Obs. Date | Exposure (s) |
|-------------|---------|-----------|--------------|
| NuSTAR      | 6801033002 | 2015-5-22 | 211209       |
|             | 68010301002 | 2018-6-9 | 38090        |
|             | 68010301004 | 2018-11-28 | 408958      |
| XMM-Newton  | 0830540101 | 2018-12-1 | 114900       |
|             | 0830540201 | 2018-12-3 | 114400       |

Table 1: Observations Used for This Analysis, with Columns Indicating the Observatory, Observation ID, Start Date of the Observation, and Exposure Time.
10–20 keV flux of $3.6 \times 10^{-12}$ erg cm$^{-2}$ s$^{-1}$ for the new NuSTAR observation. In addition to our new observations, we use all of the archival NuSTAR data for a total of 660 ks from NuSTAR: 210 ks collected on 2015 May 22, during which a $\sim$5 ks flare was observed (Kara et al. 2017), and 38 ks of data collected on 2018 June 9.

The NuSTAR data was reduced using the NuSTAR pipeline (NUPIPELINE). This consists of processing Level 1 data products with the NuSTAR Data Analysis Software (NUSTARDAS V2.0.0) and then creating and calibrating the Level 2 event files with CALDB version 20201130. We use a circular source region with a 50" radius and a circular background region with a 60" radius for both Focal Plane Module A and Focal Plane Module B (FPMA, FPMB) instruments. The FPMA and FPMB light curves are binned to 128 s bins and then added after background subtraction to improve signal to noise.

We find the NuSTAR spectra to be consistent (within a maximal deviation of 10%) across observations and thus combine spectra, resulting in a single spectrum per FPM. The energy bins of the spectra are grouped in order to oversample the instrument’s resolution by a factor of 3 and to have a signal to noise of at least 3$\sigma$ per bin.

For the XMM-Newton data, we focus spectral analysis on data from the EPIC-pn instrument (Strüder et al. 2001) due to the instrument’s larger effective area. We reduced the EPIC-pn data using the XMM-Newton Science Analysis System (SAS V18.0.0). We avoid background flares by constructing a good time interval filter using a background count rate cutoff of 0.4 counts s$^{-1}$ and avoid spurious detections using the conditions PATTERN $\leq$ 4 and FLAG $== 0$. We produce our spectra and light curves using circular source and background regions with a radius of 35". The light curves were extracted and corrected using the tools EVSELECT and EPICLCCCORR with a binning to 10 s bins. The spectra were extracted using the tools EVSELECT and BACKSCALE, with the redistribution matrices (RMF) and ancillary response files (ARF) being generated for each observation using the RMFGEN and ARFGEN tools. We evaluated the amount of pile-up per observation using the SAS task EPATPLOT. Minor pile-up does appear to be present in the XMM-Newton observations, particularly below 0.5 keV. As such, we do not fit below 0.5 keV in the flux spectra and time lags throughout our analysis. As a check, we find the spectra and time lags to be very consistent (well within error) when using an annular source region in an attempt to improve the pile-up versus a circular source region.

We also find an effect occurring above 7 keV, where there is an observed excess in both single and double events. The XMM-Newton spectra exceed the NuSTAR spectra at these energies by $\sim$20%, similar to the inconsistency between spectra reported by Kara et al. (2017). We find the effect does not improve when excising the bright center of the source with an annular source region. The discrepancy improves to $\sim$10% when implementing the XMM-Newton current calibration file (CCF) released on 2022 April 7,\textsuperscript{16} which includes the ABSCORRAREA correction to the effective area above roughly 4 keV, but most significantly affects the 7–10 keV band. Figure A1 shows the discrepancy before and after applying the correction to the effective area. We use the data that includes this correction for the entirety of our analysis. We note that, because of this discrepancy between XMM-Newton and NuSTAR, the equivalent width of the iron line is greater in NuSTAR than in XMM-Newton by a factor of $\sim$2 without the correction. We caution investigators modeling just the XMM-Newton spectra, as the inclusion of this 7–10 keV band will result in an artificially weak iron line.

Just as we did with the NuSTAR spectra, we combine the XMM-Newton spectra across observations after finding the maximum deviation of the spectra to be consistent within 15%. The spectra are binned in order to oversample the instrument’s resolution by a factor of 3 and to have a signal to noise of at least 3$\sigma$ per bin.

The ratio of the spectra to a simple power-law model is shown in Figure 2. Ark 564 shows a steep spectral slope as well as strong features associated with relativistic reflection, including a strong soft excess below 1 keV. The cutoff energy appears to be low, and the prominent iron K feature is broad, both in agreement with Kara et al. (2017).

3. Gaussian Processes

We aim to analyze and model Ark 564’s time lags, which we uncover using a Fourier approach that extracts the lags/leads of

\textsuperscript{16} CCF Release Note: https://xmmweb.esac.esa.int/docs/documents/CAL-SRN-0388-1-4.pdf.
is the expected contribution of noise to the variance of
random variables, any finite number of which have a
Gaussian distribution (Rasmussen & Williams 2006). In our
case, these random variables are simply the count rate values of
our time series, and the Gaussian process acts as a prior over a
function of count rates $f(t)$ at time $t$.

Following Wilkins (2019), we have a data vector of count rates $d$ at times $t$ from NuSTAR. We assume this data is a
 realization of a Gaussian process, meaning we assume the vector $d$ has been drawn from a multivariate Gaussian
distribution with mean function $m(t) = \mathbb{E}[f(t)]$ and the covariance between any two entries in the time vector is given by the
covariance function, formally known as the kernel function $k(t, t) = \mathbb{E}[(f(t) - m(t))(f(t') - m(t'))]$. To generate other
realizations of the data vector $d$, we denote by the data vector $d_*$, at different times $t_*$, we first need to define a model
for the mean function and one for the kernel function.

Our light-curve data is used as the training set that informs
these two functions, where training generally describes the
process of using our data to define these functions. As per
standard practice, we first standardize the training set data by
subtracting the mean from the light curves and dividing by the
standard deviation. As such, we assume that $m(t) = 0$.

The kernel function describes how the data deviates from the
mean function and is thus essential to an accurate description of
the observed variability. There are many functional forms for
the kernel function, but we consider only those that are sta-
tionary, meaning they depend only on the time difference
between points such that $k(t, t) = k(t' - t)$ is a function of a
single variable. Note that, in this stationary case, the kernel
$k(t' - t)$ is simply the autocorrelation function of the light
curve. Each form of the kernel function has different hyper-
parameters $\theta$ that encode a property of the variability, such as
length scales and amplitudes. We determine the values of the
kernel function’s hyperparameters through a process known as
hyperparameter optimization. This process consists of finding
the set of hyperparameter values that maximizes the probability
of the model given our training data, which is quantified by the
marginal likelihood (Rasmussen & Williams 2006). In practice,
however, it is common to instead minimize the negative log
marginal likelihood (NLML)

$$
-\log p(y|\theta) = \frac{1}{2} y^\top (K_\theta + \sigma_n^2 I)^{-1} y + \frac{1}{2} \log |K_\theta + \sigma_n^2 I| + \frac{n}{2} \log 2\pi,
$$

where $y = d - m(t)$ is the set of normalized observed count rate
values and the entries of the covariance matrix $K_\theta$ are
$k(i, j) = k(t_i, t_j|\theta)$, whose hyperparameters $\theta$ have been
optimized using $n$ training points. The kernel function $k(t, t')$ generates
the elements of the covariance matrix. $I$ is the identity matrix,
and $\sigma_n^2$ is the expected contribution of noise to the variance of
each data point. We note that treating the Poisson noise as
Gaussian is valid at high count rates, which is not the case for
our NuSTAR data above 14 keV. As a check, we rebin the
data to ensure >20 counts per bin before rerunning the Gauss-
ian processes. We find that the resulting time lags above

![Image](image_url)

Figure 2. NuSTAR spectra (black) from the new 410 ks observation and the XMM-Newton spectra from the first and second 115 ks observations (orange and purple, respectively) fit to a simple, steep ($\Gamma = 2.57$) power law with Galactic absorption.
14 keV remain within 1σ of those computed originally with the lower-count-rate time binning, which have larger uncertainties as well.

The first term in the NLML equation is the only term that features the training set data (our observed count rate values) and acts to motivate the model’s fit to the data. The second term punishes overly complex kernel functions, and the third term is a normalization constant. Since the Poisson noise affecting each point is uncorrelated, we account for noise in the model by adding a diagonal term (σ² I) to the covariance matrix.

In order to generate realizations of the light curves with no gaps with data points dᵢ, we make random draws of the conditional distribution (dᵢ|d) from the multivariate Gaussian distribution defined by the optimized kernel function and the observed data vector d (Equation (5) from Wilkins 2019):

\[
(x|y) \sim N(μ_x + K_{xy} K_y^{-1}(y - μ_y), K_x - K_{xy} K_y^{-1} K_{yx}),
\]

where \(x = dᵢ\) and \(y = d\) and \(μ\) is the mean of these vectors. \(K_{xy}\) denotes the covariances between elements of \(x\) and \(y\), which is calculated by evaluating the kernel function between our observed time bins \(t\) and the time bins \(tᵢ\) at which we draw light-curve realizations.

Rather than training a separate Gaussian process on each individual light curve, we simultaneously fit the model kernel function to the entire data set in each energy band. This informs the time lags between energy bands by adding a diagonal term to the covariance matrix.

Our approach using multitask learning assumes that our light curves modeled the variability of each observation independently (e.g., Wilkins 2019; Griffiths et al. 2021). Here, we train a shared set of hyperparameters by optimizing the summed NLML of all NuSTAR observations in each energy band of interest. This is equivalent to simultaneously fitting the model kernel function to the entire data set in each energy band.

Multitask learning has been shown to improve how effective the model is at predicting missing data, known as model generalization (Caruana 1997). Determining a single set of hyperparameters by training on all of our observations is especially advantageous for shorter observations, such as our 40 ks NuSTAR observation from 2018, which has far fewer data points to train its own set of hyperparameters. It is important that the Gaussian process models variability across a wide range of timescales, however, training a set of hyperparameters with only short observation biases against modeling longer-timescale variability (Caruana 1997).

Smaller training sets are also more likely to have multiple local optima similar in magnitude in the NLML function, corresponding to different and often unphysical interpretations of the data (Rasmussen & Williams 2006). While we perform optimization multiple times in an attempt to avoid such local optima, training using all observations largely mitigates this issue, resulting in local NLML optima now differing by orders of magnitude. Lastly, longer observations also have larger contributions to the total NLML and thus have a greater weight on the model as expected.

Our approach using multitask learning assumes that our light curves can be characterized by a single description of the observed variability on timescales up to the length of the observation, or, equivalently, a single, shared kernel function. This would require an assumption that there are no fundamental differences across observations regarding the underlying variability processes and the characteristic timescales that the hyperparameters describe. As is common practice in X-ray timing analysis, we assume stationarity of Ark 564, which is motivated by the general consistency in Ark 564’s power spectral density (PSD) across our observations. As a check, we compute the Lomb–Scargle periodogram of each NuSTAR observation in the frequency range of interest (0.01–0.9 mHz), and find that fitting each periodogram with a power law results in fit parameters that agree within 1σ. We find similar consistency when computing the PSDs above 0.3 mHz using the continuous NuSTAR data between the gaps and fitting each with a power law.

### 3.1. Multitask Learning for Hyperparameter Optimization

Previous applications of Gaussian processes for X-ray light curves modeled the variability of each observation independently (e.g., Wilkins 2019; Griffiths et al. 2021). Here, we train a shared set of hyperparameters by optimizing the summed NLML of all NuSTAR observations in each energy band of interest. This is equivalent to simultaneously fitting the model kernel function to the entire data set in each energy band.

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17. [https://scikit-learn.org/](https://scikit-learn.org/)
18. [http://github.com/wilkinsdr/pylag](http://github.com/wilkinsdr/pylag)
Table 2

| Kernel Form | NLML (Primary) | NLML (Reference) |
|-------------|----------------|------------------|
| SE          | 7182.4         | 5347.7           |
| Matérn -1/3 | 7059.3         | 5233.5           |
| Matérn -2/3 | 7090.3         | 5518.8           |
| RQ          | 7008.5         | 5202.0           |

Note. Lower NLML corresponds to a higher probability of the model given the training data.

3.2. Selecting the Kernel Function

Choosing a proper functional form for the kernel function is crucial to accurately model the observed variability, and has been found to affect the significance of lag detection (Griffiths et al. 2021). We consider three common forms for the kernel function to model the variability of Ark 564: the squared exponential (SE), rational quadratic (RQ), and Matérn kernel. We refer the reader to Wilkins (2019) for an introduction and details on these kernel function forms.

We minimize the NLML function to determine the set of hyperparameter values given our light curves. This process is performed separately in each energy range of interest and for the broader reference band. As such, we are interested in comparing how accurately each kernel form can model the variability in both the individual primary energy bands of interest and the reference band. This is commonly done by comparing the probability that the model describes the training data, i.e., the minimized NLML values for the best-fit kernel. As such, we average the minimized NLML values for the primary energy bands of interest, as well as for the reference band, shown in Table 2.

While we do find the choice of kernel form to impact lag detection, the effects of this choice are much smaller in our case than those found by Griffiths et al. (2021). This is likely due to the difference in data sampling/length of their Swift monitoring campaign versus our NuSTAR data. The uncertainties on the lowest-frequency lags are roughly constant across kernel forms (within roughly 20% on average and 10% for the high-frequency lags). The amplitude of the lag is even more consistent across kernel forms (within 15% for the lowest-frequency lags and 10% for the high-frequency lags). In summary, the time-lag results from using any of the investigated kernel forms are generally consistent in all three frequency ranges of interest.

We conclude that the RQ kernel best captures the variability of our light curves, given that this kernel results in the lowest optimized total NLML value, with the Matérn -1/3 kernel inching behind. Wilkins (2019) similarly finds the RQ kernel to be the most successful for lag recovery when simulating NICER light curves of Ark 564 with a 200 s lag and low-Earth orbit data gaps. The author concludes that the accuracy achievable with the RQ kernel is sufficient for analysis of data available from current missions. Our NLML results are also generally consistent with those from Griffiths et al. (2021), who found the RQ and Matérn -1/3 kernel functions to yield the most well-specified models for coarsely sampled, simulated X-ray light curves of Mrk 335.

4. Fourier-resolved Timing with Gaussian Processes

After training the Gaussian process and drawing continuous light-curve samples, we apply standard Fourier-resolved timing analysis, described further by Uttley et al. (2014), to determine the time delays between correlated variability in different energy bands with respect to a common reference band.

The lowest-frequency one can probe is limited by the length of the longest continuous light-curve segment (the length of the observation in an ideal case). The highest frequency attainable is set by the Nyquist frequency $f = 1/2Δt$ for sampling rate $Δt$, but dominating Poisson noise greatly lowers this limit in practice.

For two light curves $X(t)$, $Y(t)$ with corresponding Fourier transforms $\tilde{X}(f) = |\tilde{X}(f)|e^{iϕ_X}$ and $\tilde{Y}(f) = |\tilde{Y}(f)|e^{iϕ_Y}$, the cross spectrum $\tilde{C}(f)$ is given by

$$\tilde{C}(f) = \tilde{Y}^*\tilde{X} = |\tilde{X}(f)||\tilde{Y}(f)|e^{i(ϕ_X−ϕ_Y)},$$

Equation (2)

We convert the argument of the cross spectrum (the phase lag as a function of frequency) to a time lag by dividing by the frequency, resulting in the lag-frequency spectrum

$$τ(f) = \frac{\text{arg}(\tilde{C}(f))}{2πf}.$$  

Equation (3)

The lag-frequency spectrum allows us to probe correlated variability between two light curves as a function of timescale. A positive time lag at frequency $f$ indicates (by convention) that the variability process with corresponding timescale $1/f$ is first observed in light curve $X$ and is seen lagging in light curve $Y$. We refer to light curve $X$ as the primary energy band light curve, and light curve $Y$ to be the reference band light curve.

We create the cross spectrum between each primary energy band of interest and a common reference before averaging over a broader frequency bin to optimize the signal to noise, resulting in the lag-energy spectrum. We emphasize that we are interested in the relative lag between energy bins to gain information on correlated variability in different energy bands with respect to a common reference band, rather than the amplitude of the lags themselves.

The reference band is taken to be the broadest possible reference band (across all energies with good signal to noise) to minimize uncertainty associated with Poisson noise. We also subtract the primary energy band light curve from the reference band light curve to remove Poisson noise in the primary band that would be correlated with itself in the reference band. For XMM-Newton observations, we use the entire 0.5–10 keV energy range for the reference band, and 3–14 keV as the reference band for our NuSTAR light curves where the signal to noise is greatest.

In the case of our continuous XMM-Newton light curves, we compute these timing products immediately, without Gaussian processes. For each data-gap-ridden NuSTAR observation, we draw 5000 samples of both the primary energy band and the primary-band-subtracted reference band from the Gaussian process posterior. We calculate the cross spectrum and power spectra from each sample pair before averaging the spectra across the 5000 sample pairs, resulting in three final spectra required to calculate the time lag and associated uncertainty. Uncertainty on the lags is calculated from coherence as outlined by Uttley et al. (2014).

The lag-energy spectrum reveals how different energy bands contribute to correlated variability on different timescales, and is thus an important tool for studying the causal relationship.
between different spectral components (Uttley et al. 2014). We thus combine the Fourier products given that we have assumed stationarity of the source on the timescales spanned by our observations, motivated by the cross spectra and power spectra being consistent across observations. In each energy bin, we take all points in each observation’s cross spectra and pair of power spectra (the power spectra are used to calculate coherence and thus uncertainty on the lags) that fall in a frequency range of interest, average, and convert to a final time lag. This is particularly valuable for our NuSTAR observations to reduce the larger time-lag uncertainties imposed by Gaussian processes (see Section 4). Since there is no prior placed on correlations between energy bands, sampled data in the gaps will be uncorrelated with that in another energy band, resulting in lower coherence and thus larger errors. Ark 564 is one of the only sources with a low enough mass that allows us to perform the test of comparing the reverberation lags above ~0.03 mHz computed using Gaussian processes versus the immediately available continuous NuSTAR segments. The results from both approaches are consistent, as shown in Figure A2, but using Gaussian processes results in larger errors by roughly 40% on average below 10 keV.

We perform simulations similar to those of Wilkins (2019) to evaluate the effects of the Gaussian processes on time-lag recovery in the case of our specific observations. We simulate light curves with lengths, means, and standard deviations matching our observations using the method of Timmer & Koenig (1995). The reverberation light curves are generated by convolving the original light curves with a δ-function, shifting the light curves by 100 s (on the order of the observed Fe K lag). We introduce data gaps replicating those from the NuSTAR low-Earth orbit and generate Gaussian process realizations including data in the gaps. We find results consistent with Wilkins (2019): we are able to recover the 100 s lag within 5% at all frequencies in which reverberation is probed in this paper (0.06–0.9 mHz).

5. Results

The lowest-frequency lag-energy spectra (the top row of spectra in Figure 4) exhibit the canonical hard lags, which monotonically increase with energy. The intermediate frequency range (the middle row of spectra in Figure 4) similarly shows the hard lags, but begins to show faint signs of the high-frequency reverberation lags, namely, a potential Fe K lag in the 6–7 keV NuSTAR bin. Interestingly, in the intermediate frequency range of 0.06–0.2 mHz, we see that the hard lags change in slope and level out at 10 keV, which can be seen only in the NuSTAR band. This atypical change in slope in the hard lags could be related to the appearance of the Compton hump in

![Figure 4](image-url)
the spectra, or due to the particularly low electron temperature of the corona (10–20 keV).

The high-frequency spectra (the bottom row of spectra in Figure 4) show tentative evidence for the soft lag features associated with reverberation. A previous 500 ks XMM-Newton campaign of Ark 564 showed significant detections of a soft lag (Legg et al. 2012) and an Fe K lag at 99.94% significance (Kara et al. 2013), but in our shorter campaign, we do not make a significant detection of the iron K line. That said, the lags do increase from 4 to 10 keV and peak at 6–7 keV, consistent with previous results. We also see a broad feature centered at 0.8–0.9 keV in the high-frequency lags, which is consistent with a feature that we observe in the flux spectrum. The potential origin of the feature is discussed in Section 6.

While in practice, we will use the spectrum and the Fourier-resolved time lags to constrain model parameters, here we focus on the significance of reverberation in just the high-frequency lags. We perform a simple test for the statistical significance of the reverberation features by considering the null hypothesis that the observed lag spectra in the highest frequency range are comprised of only the continuum, modeled in RELTRANS as a pivoting power law (i.e., the boost parameter is set to 0 so no reverberation is included). For this test, we assume values for the parameters found from fitting the flux spectra alone. We compare the resulting best fit ($\chi^2/\nu = 1.36/10$, where $\chi^2$ denotes the reduced chi-squared for $\nu$ degrees of freedom) to that found when including nonzero boost with the pivoting power law. The latter model (i.e., including reverberation) results in a $\Delta \chi^2 = 3.89$ for one additional degree of freedom ($\chi^2/\nu = 1.01/9$), corresponding to a significance of 91.1% using an F-test.

The 0.2 mHz lower bound of the range of frequencies considered for reverberation (i.e., the highest frequency range) was selected due to limited NuSTAR statistics from employing Gaussian processes. Contributions from the hard lag at this lower frequency appear to be flattening the lag-energy spectrum below 2 keV. When we instead isolate higher frequencies, we find prominent soft lags from the soft excess consistent with those that have been seen previously in this source (Kara et al. 2013).

We model the XMM-Newton and NuSTAR flux spectra and lag-energy spectra simultaneously using the relativistic reverberation mapping model RELTRANS (Ingram et al. 2019). We fit six lag-energy spectra in total with the flux spectra: one lag-energy spectrum per observatory in each of three contiguous frequency ranges spanning the accessible frequency range (0.01–0.9 mHz). The low-frequency hard lags are modeled by a pivoting power-law component discussed by Mastroserio et al. (2018, 2021), which includes three additional free parameters per frequency range: $\phi_A$ (a normalization phase), $\phi_{AB}$ (phase difference between the spectral index and the normalization variability), and $\gamma$ (amplitude ratio between the spectral index and the normalization variability). $\phi_{AB}$ and $\gamma$ are tied between lag-energy spectra in the same frequency range, whereas the normalization phase $\phi_A$ is left untied.

We fit the flux and lag spectra (by minimizing the summed $\chi^2$) with reltransDCp, a flavor of RELTRANS that implements a physically motivated thermal Comptonization continuum using nthcomp (Zdziarski et al. 1996; Życki et al. 1999) to model the coronal emission with the parameters power-law photon index $\Gamma$ and electron temperature $kT_e$. The reflection in the model originates from the XILLVER grids (García et al. 2013). The model calculates the energy shifts and light-crossing delays, including general relativistic effects, of the X-rays emitted by a lamppost corona positioned on the spin axis of the central black hole. The X-ray reflection spectrum is computed using the most updated rest-frame reflection emission convolved with the general relativistic ray-tracing transfer function computed from the lamppost corona. The model correctly accounts for the instrument response from both instruments when computing the lag-energy spectrum. This version is also capable of probing the disk’s electron density up to $n_e = 20 \, \text{re}$. reltransDCp is not yet publicly available, but will be included in public releases in the future. The model is capable of fitting the time lags and the flux spectra by self-consistently modeling the direct coronal continuum and the corresponding reflection spectrum. We probe model consistency for describing the time lags and the flux spectra with a single model for the accretion disk by fitting these data products simultaneously, which was fruitful for Mastroserio et al. (2020). We present the resulting constraints on properties of the accretion disk and black hole, including a mass estimate from fitting the time lags. The fit parameters and model consistency are discussed further in Section 6.

Galactic absorption is accounted for in the blackbody component only, since it is already accounted for self-consistently within reltransDCp. The frozen fit parameters are the cosmological redshift (0.02468), the inner and outer radii of the disk (at the innermost stable circular orbit and 1000 $R_g$, respectively), and a maximum value for the spin, which is consistent with previously reported values (Walton et al. 2012; Tripathi et al. 2018; Jiang et al. 2019). The ionization of the disk ($\log(Z)$) is assumed to be constant.

Our initial best fit with reltransDCp alone gives a poor description ($\chi^2/\nu = 1.48/3068$) of the flux spectrum, especially the Fe K feature. The poor quality of the fit is shown by the data-to-model ratio shown in the top panel of Figure 5. The fit improves dramatically when excluding energies below 2 keV and refitting ($\chi^2/\nu = 1.01/2763$).

In order to model the soft excess below 2 keV, we include a phenomenological single-temperature blackbody component ($kT = 0.11$ keV) to the model using zbody, which contributes to the flux spectra but not the time lags. We account for Galactic absorption ($n_{b,Gal} = 5.3 \times 10^{20} \text{cm}^{-2}$; Kalberla et al. 2005) with tbabs, using abundances from Wilms et al. (2000). This model (tbabs+zbody+reltransDCp in XSPEC syntax) achieves a much more successful description of the flux spectra in particular when including the soft excess below 2 keV ($\chi^2/\nu = 1.21/3065$). All fit parameters except the source height of the lamppost corona, inclination, ionization, and boost remain within error with the inclusion of the blackbody. The boost factor adjusts the reflection fraction resulting from the assumed point-like lamppost corona, with values $>1$ causing a stronger reflection component than expected in the lamppost geometry and $<1$ returning a weaker-than-expected reflection (Ingram et al. 2019; Mastroserio et al. 2020). The model is driven to a higher source height from 2.1 to 10 $R_g$ to 10.3 $R_g$, lower inclination (from 36.7 to 0.8), lower ionization ($\log(\xi)$ from 3.3 to 3.16), and higher boost (from 0.61 to 0.49). These changes, in addition to a near-maximal iron abundance ($\sim 10$ times solar iron abundance) in both cases, are likely attempting to fit the aforementioned feature just below 1 keV in both the flux.
spectra and the time lags. Nonetheless, the new fit leaves residuals in the flux spectra throughout the soft excess, especially around the $\sim 1$ keV feature, as shown in the middle panel in Figure 5. The model continues to underestimate the Fe Kα line, even with maximal iron abundance.

Because we were unable to find an acceptable fit with just a blackbody soft excess component, we include a phenomenological Gaussian component using gauss to assist the model with the $\sim 1$ keV feature in the flux spectra, leaving the center and width of the Gaussian as free parameters. The feature is not a narrow line, and likewise, the Gaussian is broad ($\sigma = 0.18$) and is centered at 0.9 keV. The model (tbabs*(zbody+g gauss)+reltransDCp) includes the blackbody and again accounts for Galactic absorption on the Gaussian and blackbody components. Adding this Gaussian component dramatically improves the residuals around the reflection features, especially the soft excess, in the flux spectra. The fit on the time lags shows minor improvements, particularly in the intermediate frequency range. The resulting best fit of this final model is shown in Figure 6, with a fit statistic of $\chi^2 / \nu = 1.08/3062$. The fit is dominated by the flux spectra, with the flu and the time lags contributing a $\chi^2$ of 3265.13 (in 3026 bins) and 26.98 (in 66 bins), respectively. The best-fit parameters are comparable to those when fitting without the Gaussian, with the exception of iron abundance. The component removes the need for the reflection to replicate the $\sim 1$ keV feature with near-maximal iron abundance, lowering the iron abundance from 10 to 2.25 times solar iron abundance. We find that all of the best-fit parameters found when modeling the flux spectra above 2 keV with RELTRANS (without additional components) lie within 2$\sigma$ of those found when fitting 0.5–40 keV with the additional blackbody and Gaussian components, with most values consistent within 1$\sigma$.

Table 4 in the Appendix shows the fit parameters in these two cases.

While the Gaussian is phenomenological, similar features have been seen in other high-Eddington accretors, such as the NLS1 1H 1934-063 (Xu et al. 2022) and the extreme changing-look AGN 1ES 1927+654 (Masterson et al. 2022). We discuss further the potential physical origin of the feature near 1 keV in Section 6.

Warm absorbers have been seen previously in this source (Matsumoto et al. 2004; Giustini et al. 2015). When we fit the RGS spectra from 0.4–1.5 keV with a blackbody and power law, we see narrow absorption that is particularly strong around O VII and O VIII. Further modeling of the RGS data of the warm absorbers is beyond the scope of this paper, but we do see a broad excess from 0.8–1.5 keV, which is also seen in the EPIC-pn data. Additional future work is warranted on modeling these features.

The model is successful at reproducing both the hard and soft lags across the entire frequency range, except for residuals on the feature near 0.9 keV in the high-frequency XMM-Newton spectrum. The lag spectra are generally consistent with those computed from the XMM-Newton archival data, although minor changes in the high-frequency lags below 1 keV render the soft-excess lags to be less prominent than those found previously (Kara et al. 2013). Changes in the lag-energy spectra have been observed on month-long timescales in this source (see Figure 5 in Kara et al. 2013) and in other sources (e.g., Alston et al. 2020). Proposed causes include changes in the geometry of the corona, which we are unable to distinguish in our case: if the best-fit model from this paper is applied to the archival lags, a similar fit statistic is obtained (the reduced chi-squared increases by less than 0.2), with residuals on the high-frequency lags located below 1 keV in both cases.

The reported parameter values and their associated uncertainties are determined using a Monte Carlo Markov Chain (MCMC) analysis, using the Goodman–Weare algorithm in xspec. We ran three chains, each with a different initial distribution for the walkers to ensure that the walkers are not trapped in local extrema. Each chain consists of 200 walkers in total with 15,000 iterations each, with the walkers initially
either distributed (1) normally with mean and covariance information from the best fit, (2) normally with the same normal distribution but with the covariance rescaled by 0.2, or (3) uniformly about the best-fit parameters. For the chain with the first aforementioned initial distribution, we burn the first 25% of the iterations per walker, whereas the other two chains converge much faster and require a burn-in of only 10% of iterations. It is after this burn-in that we find each MCMC has converged based on a rapidly decaying autocorrelation function and the Geweke convergence measure for every free parameter.

We also find the posterior distributions from the first 10% and last 50% of the chains (excluding the burn-in period) are consistent, further indicating that the chain has converged in the first 10% of iterations. We lastly combine the chains, finding that the three chains converge to the same stationary distribution based on the Gelman–Rubin statistic for each parameter across the three chains. The median of the resulting posterior distributions and associated $1\sigma$ errors are shown in Table 3. The posterior distributions, made using the module CORNER (Foreman-Mackey 2016), for several fit parameters are shown in Figure 7.

The best-fit source height (9.6$_{-0.7}^{+0.7}$) is typical for a $10^6–10^7 M_\odot$ black hole (Chainakun et al. 2016; Kara et al. 2017; Mastroserio et al. 2020; Alston et al. 2020). We find the temperature for the corona to be low at 14.7$_{-1.0}^{+1.0}$ keV, consistent with the low coronal temperature reported by Kara et al. (2017). We find a relatively low electron density for the disk (log($n_e$/cm$^{-3}$) = 15.1$_{-0.7}^{+0.7}$). We were unable to find a better fit when requiring a higher value for the density, such as the density value for Ark 564 reported by Jiang et al. (2019) (log($n_e$/cm$^{-3}$) = 18.55), or by using a steppar over density.

Modeling the time lags allows one to also estimate the mass of the black hole, from which we find the mass of Ark 564 to be $2.3^{+2.6}_{-1.3} \times 10^6 M_\odot$. This constraint is consistent with Denney et al. (2009) (1.7 $\times 10^6 M_\odot$), Botte et al. (2004) (2.6 $\times 10^6 M_\odot$), and the upper limit found from optical reverberation mapping by Shemmer et al. (2001). Our estimate is also within error from the upper mass limit reported by Nikolajuk et al. (2009), which was determined from applying NLS1 corrections to mass estimates found using the scaling relation by Wang & Lu (2001) and Bian & Zhao (2003). By applying a bolometric correction of 20 from Marconi et al. (2004) to our observed 2–10 keV luminosity (2.40 $\times 10^{43}$ erg s$^{-1}$), this mass constraint corresponds to a bolometric luminosity of $L/L_{Edd} = 0.76–3.69$. As a result of fitting the lag-energy spectra in multiple frequency ranges, we do not see the degeneracy between black hole mass and corona height that has been observed when fitting lag-energy spectra in a single frequency range (Cackett et al. 2014; Ingram et al. 2019).

Figure 6. The XMM-Newton and NuSTAR flux spectra from 0.5–40 keV with the best-fit model (upper) and corresponding data-to-model ratio (lower). The total model (tbabs*(zbody+zgauss)+reltransDCp) is shown by a solid line, with model components tbabs*zbody (blackbody component fit to the soft excess), tbabs*zgauss, and reltransDCp shown by dashed–dotted, dotted, and dashed lines, respectively.

Table 3

| Parameter          | Time Avg. + Time Lags |
|--------------------|-----------------------|
| $h$ [R$_g$]        | 9.6$^{+0.7}_{-0.7}$   |
| $i$ (deg)          | 37.0$^{+1.0}_{-1.0}$   |
| $\Gamma$           | 2.48$^{+0.03}_{-0.03}$ |
| log($\xi$ (erg cm s$^{-1}$)) | 3.25$^{+0.03}_{-0.03}$ |
| $A_{Fe}/A_{Fe}$    | 2.3$^{+0.4}_{-0.4}$   |
| log($n_e$ (cm$^{-3}$)) | 15.1$^{+0.7}_{-0.7}$   |
| $1/B$ (boost)      | 0.50$^{+0.03}_{-0.03}$ |
| $kT_e$ (keV)       | 14.7$^{+0.7}_{-0.7}$   |
| Mass (10$^6 M_\odot$) | 2.3$^{+1.3}_{-1.3}$   |
| $\chi^2$/d.o.f.   | 1.08/3062             |
6. Discussion

We combined the flux and lag-energy spectra of our two new 115 ks XMM-Newton observations, as well as our new 410 ks NuSTAR observation with archival data, totaling 660 ks with NuSTAR and 230 ks with XMM-Newton. We apply the relativistic reverberation model RELTRANS to simultaneously model the flux spectra and six lag-energy spectra (one per observatory in each of three frequency ranges). The flux spectra required an additional blackbody and a Gaussian component in order to obtain a successful description of the soft excess, including an unknown feature at $\sim 1$ keV, which also appears in the time lags. Including additional components to describe the flux spectra that are not included in the time lags allows us to better understand how features in the flux spectra manifest in the time lags, unlike previous works that found notable tension between the reflection features in the flux spectra and lag-energy spectra (e.g., Zoghbi et al. 2020; Wang et al. 2021).

6.1. Fitting the Soft Excess

In Section 5, we were unable to adequately fit the flux spectra, especially the soft excess, with RELTRANS alone. The fit improves significantly by adding a blackbody component, which could be accounting for additional Comptonization off a warm corona (Petrucci et al. 2020). We continue to see residuals around 1 keV in both the flux spectra and the time lags. The final fit of the Ark 564 flux spectra by Chainakun et al. (2016) shows similar residuals from this $\sim 1$ keV feature. We found that including a broad Gaussian component to assist the model with this feature improved the fit residuals across the entire energy range and lowered the iron abundance from 10 to 2.25 times solar iron abundance. The best-fit parameters found from modeling the flux spectra above 2 keV with only RELTRANS are consistent with those found when fitting the entire spectrum with these additional components, with most values consistent within 1$\sigma$. Here, we discuss possible physical

Figure 7. Posterior distributions from the MCMC of fitting the time lags with the flux spectra. The plots on the diagonal show the histogram for each model parameter, dashed vertical lines corresponding to the median and 1$\sigma$ from the median. The off-diagonal plots are projections of the 2D distributions between any two parameters, with contours of equal probability. An enlarged 1D mass posterior is shown in the upper right.
interpretations for why a broad Gaussian centered near 1 keV allows us to fit the soft excess.

Super-solar iron abundances have been commonly found when fitting the reflection features (e.g., Dauser et al. 2012; Garcia et al. 2015; Mastroserio et al. 2020). Nonetheless, it has been suggested that such high iron abundance compensates for physics missing from the model in some cases. For instance, Tomsick et al. (2018) found that their inferred super-solar iron abundance was attempting to account for high-density effects when modeling the spectra of Cyg X-1. The broad ~1 keV residual could be related to the model unable to fit the smeared Fe L reflection feature, which peaks near 1 keV (Fabian et al. 2009), and would explain why the feature arises in the high-frequency time lags. This could be related to modeling reflection off a razor-thin disk, a geometry less apt for describing high-Eddington accretion flows, where radiation pressure is expected to increase the scale height of the disk (e.g., Begelman & Meier 1982; Sadowski 2011; Jiang et al. 2014; Sadowski et al. 2014; Taylor & Reynolds 2018; Lančová et al. 2019).

Unidentified broad features around 1 keV have been seen in CCD spectra of several high-Eddington accretors. For instance, the 1 keV feature looks very similar to that detected in the NLS1 AGN 1H 1934-063 by Xu et al. (2022), the extreme changing-look AGN 1ES 1927+654 by Masterson et al. (2022), as well as several ultraluminous X-ray sources (ULXs), especially those in the supersoft ultraluminous subclass of ULXs (e.g., NGC 247, NGC 6946, M1, and M101: Urruty & Soria 2016; Earnshaw & Roberts 2017; Pinto et al. 2021, respectively). Proposed solutions in these cases have included blueshifted O VIII ionization edges, or high-ionization Fe L or Ne IX-X absorption lines with velocities of ~0.1–0.2c indicative of an optically thick wind (Pinto et al. 2021). Indeed, previous studies of Chandra gratings observations of Ark 564 show blueshifted absorption lines consistent with a relativistic (~0.1c) outflow (Gupta et al. 2013).

It is possible that the residuals on the feature without the Gaussian is due to us not modeling the outflows, explaining why reflection alone fails to describe the feature and worsens the fit of the other reflection features in an attempt to do so. This could also explain why we do not see the time lags being affected by including these phenomenological components, suggesting these additional components do not contribute to the variability on the timescales probed here. Nonetheless, additional future work is required, which includes modeling of the warm absorbers/outflows.

6.2. Consistency between Time Lags and Time-averaged Spectra

We include two additional components to assist in describing the flux spectra only. We are unable to meaningfully add these components to the time-lag fit, as components to the time lags contribute nonlinearly. While this breaks the self-consistency of the simultaneous fit, we find that the inclusion of the blackbody to the flux spectra has minor effect on the time-lag fit, as shown in Figure 5. This could suggest that the blackbody does not contribute significantly to the correlated variability and thus the time lags. On the other hand, the time-lag residuals near 1 keV motivate that the Gaussian added to the flux spectra may also be required to describe the lags.

It has been found previously some physical parameter estimates inferred from the time lags do not agree with those inferred from the flux spectra, especially the height of the corona (Wang et al. 2021). When we model the flux spectra independently, the fit parameters are consistent with those found when we include the time-lag information, likely due to the fit statistics being dominated by the flux spectra. Fitting the time lags on their own comes with complications in such a high-dimensional parameter space as a result of the large uncertainties on the high-frequency NuSTAR time lags, which are exacerbated by the use of Gaussian processes. As a result, we freeze the temperature to the value from fitting the flux spectra. However, we still find statistically successful solutions with minimal height and very low inclination in which the model entirely smears out the Fe K feature when trying to fit the soft excess. Given that the Fe K lag has been detected in previous observations of this source (Kara et al. 2013), we ignore these solutions. Doing so results in a best-fit source height that is lower by roughly a factor of 3 than the value found from simultaneously fitting the lags with the flux spectra, which is a minor discrepancy given the uncertainties (3.6 ± 1.0hRg). This discrepancy is smaller than that found previously by Wang et al. (2021), who found this discrepancy in source height to be as large as a factor of 10. An independent fit to the time lags gives an inclination, photon index, and disk electron density consistent with that when fitting the data simultaneously with the additional components. The model requires a maximal iron abundance in addition to lower boost and ionization to counteract the smearing of the reverberation features.

7. Conclusions

We have simultaneously modeled the time lags and flux spectra of Ark 564 using the relativistic reverberation model RELTRANS. Here are our main results:

1. We present the first results on a long 410 ks NuSTAR observation of Ark 564, simultaneous with two new 115 ks XMM-Newton observations.
2. We implement multitask learning for the first time for AGN timing, using all of our light curves to train a single Gaussian process model for the observed variability in each energy band.
3. We detect the high-frequency time lags and attribute them to reverberation, and model them with the general relativistic ray-tracing model RELTRANS.
4. Through simultaneous modeling of both the XMM-Newton and NuSTAR flux spectra with the lag-energy spectra, we constrain the black hole mass to be 2.3^{+1.6}_{-1.3} × 10^6M_\odot.
5. An independent fit to the time lags gives an inclination, photon index, and disk electron density consistent with that when fitting the lags simultaneously with flux spectra.
6. We find that modeling the soft excess requires additional components, and we speculate that the complexity in modeling the soft excess is related to the high-Eddington nature of this source. This motivates future, intensive analysis, including modeling of the warm absorbers/outflows.

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Appendix

We find the XMM-Newton spectra exceeds the NuSTAR spectra by $\sim$20\% above 7 keV. The discrepancy improves to $\sim$10\% when implementing the XMM-Newton current calibration file (CCF) released on 2022 April 7. Figure A1 shows the discrepancy before and after applying the correction to the effective area. Figure A2 shows the high-frequency lag-energy spectra computed using Gaussian processes vs. the immediately available NuSTAR chunks. Both approaches give results consistent within error. Table 4 compares the best-fit parameters when simultaneously fitting the time lags with the flux spectra from 0.5–40 keV (which required additional blackbody and Gaussian components), vs. fitting 2–40 keV with only RELTRANS.

**Figure A1.** The new NuSTAR spectra (black) and XMM-Newton spectra before and after the release of the current calibration file, including the correction to the effective area (orange and purple, respectively) fit to a power law. Without the correction, the XMM-Newton spectra exceeds the NuSTAR spectra above roughly 7 keV by $\sim$20\%. This discrepancy nearly halves with the effective area correction.

**Figure A2.** Lag-energy spectra (0.3–0.9 mHz) computed from the NuSTAR data using Gaussian processes to generate realizations that include data in the low-Earth orbit gaps (black) vs. using the immediately available, continuous chunks (orange). Both approaches give comparable results, but Gaussian processes result in slightly larger uncertainties.

| Parameter | 0.5–40 keV | 2–40 keV |
|-----------|------------|----------|
| $h$ [R$_e$] | 9.6$^{+0.2}_{-0.3}$ | 9.7$^{+0.3}_{-0.2}$ |
| $i$ (deg) | 37.0$^{+1.0}_{-1.0}$ | 38.2$^{+1.2}_{-1.1}$ |
| $\Gamma$ | 2.48$^{+0.05}_{-0.04}$ | 2.47$^{+0.05}_{-0.02}$ |
| log($\xi$ (erg cm s$^{-1}$)) | 3.25$^{+0.03}_{-0.04}$ | 3.28$^{+0.09}_{-0.08}$ |
| $A_{bol}$/$A_{V_{00}}$ | 5.4$^{+0.3}_{-0.4}$ | 1.7$^{+0.6}_{-0.4}$ |
| log($n_e$ (cm$^{-3}$)) | 15.1$^{+0.2}_{-0.1}$ | 15.3$^{+0.4}_{-0.2}$ |
| 1/$\delta$ (boost) | 0.50$^{+0.02}_{-0.03}$ | 0.51$^{+0.07}_{-0.05}$ |
| $kT$ [keV] | 14.7$^{+1.0}_{-0.9}$ | 15.3$^{+1.1}_{-1.0}$ |
| Mass [$10^6 M_\odot$] | 2.3$^{+0.1}_{-0.1}$ | 3.5$^{+0.3}_{-0.3}$ |
| $\chi^2$/$\nu$ | 1.08/3062 | 1.01/2763 |

**Table 4**

Median and 1\sigma Uncertainties on the Fit Parameters for Simultaneously Fitting the Flux Spectra and Lag-energy Spectra from 2–40 keV with RELTRANS Alone versus Our Best 0.5–40 keV Fit. Including our Additional Blackbody and Gaussian Components

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