A sensitive search for unknown spectral emission lines in the diffuse X-ray background with XMM-Newton

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Abstract. The Standard Model of particle physics can be extended to include sterile (right-handed) neutrinos or axions to solve the dark matter problem. Depending upon the mixing angle between active and sterile neutrinos, the latter have the possibility to decay into monoenergetic active neutrinos and photons in the keV-range while axions can couple to two photons. We have used data taken with the X-ray telescope XMM-Newton for the search of line emissions. We used pointings with high exposures and expected dark matter column densities with respect to the dark matter halo of the Milky Way. The posterior predictive p-value analysis has been applied to locate parameter space regions which favour additional emission lines. In addition, upper limits of the parameter space of the models have been generated such that the preexisting limits have been significantly improved.

Keywords: X-rays, axions, dark matter theory, neutrino properties

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Contents

1 Introduction 1

2 Observations and data analysis 2
  2.1 Data selection 2
  2.2 SAS data reduction and analysis 3
  2.3 Instrumental background 6
  2.4 Fitting strategy 9
    2.4.1 Null hypothesis model 9
    2.4.2 Alternative hypothesis model 19
  2.5 Statistical methods 19
  2.6 Upper limits based on the $\Delta \chi^2$-statistics 20
  2.7 Combined model-dependent upper limits 21
    2.7.1 Constraints on $F_{\gamma}$ 22
    2.7.2 Constraints on $\sin^2(2\Theta)$ and $g_{\phi\gamma\gamma}$ 22
  2.8 Additional lines in the diffuse X-ray background 23

3 Discussion 25

4 Conclusion 26

1 Introduction

The $\Lambda$CDM\(^1\) model describes the universe on cosmological scales and requires a non-baryonic dark matter component [1]. The rotation curves of galaxies including the Milky Way [2, 3] reveal an unexpected flatness which can be explained by the gravitational influence of such a dark matter component. The dark matter is distributed as a spherical halo. The shape of the dark matter halo derived from the observations allows to interpret its constituents as non-relativistic and non-baryonic particles. One simple approach to describe the density distribution of the dark matter halo is an isothermal sphere.

Most of the dark matter particle models predict weak interactions of the dark matter with baryonic matter which opens an observation window to the dark matter component. These dark matter particle candidates fall into three groups with widely different rest masses: (1) weakly interacting massive particles (WIMPs), (2) ultra-light and cold weakly interacting slim particles (WISPs) and (3) warm dark matter particles with energies in the keV to MeV range like sterile neutrinos. This work investigates the predicted observable effects related to the particles of categories (2) and (3) by the search for unidentified emission lines in the spectra of the diffuse X-ray background which could originate in the decay of sterile neutrinos or the transition of axions into photons. Such a signal is expected if the particles with mass $m = O(\text{keV})$ are unstable on cosmological time-scales and decay into a two-particle final-state.

Previous publications have dealt with the observation of three major object classes to derive upper limits of parameter spaces of dark matter models: spiral galaxies [64, 71, 76], especially the Milky

\(^1\)The term $\Lambda$CDM is an abbreviation composed of the greek letter $\Lambda$ which stands for a cosmological constant and CDM which stands for "Cold Dark Matter".
Way \[62, 63, 65, 66, 75\], and M31 \[61, 62, 65, 67, 72, 73, 76\], dwarf spheroidals \[60, 63, 75\], galaxy clusters \[67, 68, 74\], and the diffuse galactic and extragalactic background \[67, 70, 77\]. The data of the X-ray telescopes XMM-Newton, Chandra and HEAO-1 have been primarily used for the analyses in these publications. The typical exposures and expected dark matter column densities are of the order of \(O(10 – 1000)\) ks and \(O(10^{28})\) keV cm\(^{-2}\), respectively. The detection of a unknown spectral emission line at an energy of 3.55 keV was claimed \[67, 68\] and gave rise to intensive discussions and further analyses \[59, 61–66, 78, 79\] as well as several theoretical interpretations \[23–58\].

A consensus on the origin of this line has not been established so far. Future X-ray missions as eRosita \[11\] and Athena \[12\] will likely have the chance to further investigate this topic.

In the aforementioned publications \[59, 61–66\] widely different statistical methods have been used which may not be optimal in coverage and sensitivity. This work presents an optimised data selection and statistical method. All available data sets of the X-ray telescope XMM-Newton \[4\] have been ranked by the exposure and the predicted dark matter column densities. The diffuse X-ray background spectra of the most promising data sets according to the ranking have been generated.

The posterior predictive p-value analysis \[14\] was chosen as the statistical method to determine a statistical measure which enabled us to favour a null hypothesis model describing the astrophysical parts of a spectrum or an alternative hypothesis model incorporating the null hypothesis model and an additional emission line, dependent on the parameter values of the models. This method works as a hypothesis test among spectral models of different degrees of freedom, e.g., an continuum model versus the same model plus an additive component (Gaussian emission line). This statistical method has the advantage that the underlying sampling distributions, generated by Monte-Carlo processes, are well-known, which is not true for the pure application of the F-test or the likelihood-ratio method.

Additionally, an upper limit of the parameters of an additional Gaussian-shaped spectral emission line have been calculated based on a \(\Delta \chi^2\)-distribution. This statistical distribution requires the aforementioned alternative hypothesis to be favoured or with other words, it requires the existence of such an additional emission line.

2 Observations and data analysis

2.1 Data selection

This work uses data sets up to the year 2013 taken with the EPIC PN detector \[5\] onboard the XMM-Newton satellite since it is the X-ray detector with the largest effective area available. Two features are directly relevant to the filtering of the most promising data sets:

1. The exposure time should be maximised to reach high signal-to-noise ratios (S/N) to derive the most sensitive limits of emission lines in general.

2. The direction of the pointed observations is directly linked to the model-dependent column density of the dark matter distribution.

We considered a Navarro-Frenk-White (NFW) dark matter profile \[15\] of shape and parameters \[16\]

\[
\rho_{\text{NFW}}(r) = \frac{\rho_0}{(r/r_0)(1 + r/r_0)^2} \quad \text{and} \quad \rho_0 = 0.4 \frac{\text{GeV}}{c^2} \text{ cm}^{-3}, \ r_0 = 21 \text{ kpc},
\]

as a model of the warm dark matter distribution of the Milky Way halo. The normalised product of the \(i\)th of \(N\) data sets obtained from the estimated or raw exposure \(t_{\text{exp}}^\text{est}\) and the dark matter column
density $S_{NFW;i}$, dependent on the integration length $s$ and the Galactic coordinates $(l_i, b_i)$, followed by equation (2.3), was chosen as the benchmark value:

$$b_{NFW;i} = \frac{S_{NFW;i} \cdot t_{\text{exp};i}}{\max_j (S_{NFW;1} \cdot t_{\text{exp};1}, \ldots, S_{NFW;j} \cdot t_{\text{exp};j}, \ldots, S_{NFW;N} \cdot t_{\text{exp};N})}, \quad i \in \{1, \ldots, N\},$$

(2.2)

where

$$S_{NFW}(s, l_i, b_i) = S_{NFW;i} = \int_0^\infty \rho_{\text{dm}}(s, l_i, b_i) \, ds,$$  

(2.3)

The highly time-varying instrumental and particle backgrounds encountered by XMM-Newton are not covered by this benchmark. Despite this disadvantage, the benchmark is acceptable because the most common dark matter distribution models of the dark matter halo of the Milky Way have a comparable spatial and angular shape and a density maximum matching the position of the Galactic center. In this work, the focus is set onto the presumed dark matter halo of our Milky Way. Table 1 presents the specifications of $N = 23$ data sets. The observation identities (ObsId) as well as the applied filters, the Galactic coordinates $(l_i, b_i)$, the estimated exposures $t_{\text{est};i}$ and the exposures after filtering (net exposures) $t_{\text{net};i}$ as well as the net fields of view (net fov) $\Omega_{\text{net};i}$, are shown next to the expected dark matter column densities $S_{NFW;i}$ based on the NFW-distribution. The very right column contains the final benchmark values $b_{NFW;i}$. The poor quality of a major part of the data sets in terms of a high contamination of instrumental and particle background by cosmic-ray induced fluorescence processes and/or soft proton clouds collected by the detectors (see section 2.2), respectively, led to a high reduction of the number of data sets used for analysis. In practice, the data sets with the highest benchmark values and net exposures above 22 ks, listed in table 1, have been used for further analysis.

2.2 SAS data reduction and analysis

The basic data reduction and analysis up to the generation of count spectra and their companion files have been achieved with the Scientific Analysis System (SAS, version 14.0.0)\(^3\) and the related Current Calibration Files (CCF)\(^4\) provided by the XMM-Newton Science Operations Center (XMM-SOC). The SAS data reduction and analysis can be classified into four major steps: reprocessing, time and spatial filtering, source detection and spectral analysis:

1. The reprocessing task, in particular the task $epproc$, has been applied with the default adjustments recommended by the SAS-team.

2. The time and spatial filtering of the data sets was performed by the script $espfilt$ from the ESAS\(^5\) software package. It filters flares in the light curves by cutting the tails of the count rate histogram generated from the light curve. The energy range has been set from 0.3 keV to 12 keV. For illustration, the light curves of the field of view and the corners of the data set with the observation identification 0604860301 ($i = 2$) are plotted in figure 1. The figure shows the filtered and unfiltered lightcurves of the field of view $\Omega_{\text{fov};i}$ of the PN-CCD and the out-of-fov or corner regions of the PN-CCD, respectively. The light curves of the corner area of the PN-CCD show smaller count rate levels than the lightcurves of the field of view $\Omega_{\text{fov};i}$ which

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\(^2\)The ‘Thin1’ and ‘Medium’ filters \(^5\) consist of 40 nm and 80 nm aluminium plus 160 nm polymide, respectively.

\(^3\)“Users Guide to the XMM-Newton Science Analysis System”, Issue 11.0, 2014 (ESA: XMM-Newton SOC).

\(^4\)The Current Calibration Files are dated February 3rd, 2015.

\(^5\)The XMM-ESAS software package is based on the software used for the background modeling described in [7].
Table 1. The table lists the observation IDs, coordinates and the estimated exposures $t_{\text{est}}$ and net exposures $t_{\text{net}}$, as well as the net fields of view $\Omega_{\text{fov,net}}$ of the data sets analysed in this publication. The model-dependent, predicted dark matter column densities $S_{\text{DM}}$ and the final benchmark values $b_{\text{NFW}}$ are also listed.

| Index | Object       | Obsid       | Filter | $l_i$ (degree) | $b_i$ (degree) | $t_{\text{est}}$ exp, $t_{\text{net}}$ | $\Omega_{\text{fov,net}}$ | $S_{\text{DM,net}}$ | $b_{\text{NFW,net}}$ |
|-------|--------------|-------------|--------|---------------|---------------|---------------------------------|--------------------------|---------------------|---------------------|
| 1     | V4046 Sgr    | 0604860201  | Medium | 359.66        | -7.26         | 123316.0, 62580.4                | 13.45                    | 164.38              | 0.86                |
| 2     | V4046 Sgr    | 0604860301  | Medium | 359.66        | -7.26         | 123419.0, 72761.8                | 13.78                    | 164.38              | 1.00                |
| 3     | V4046 Sgr    | 0604860401  | Medium | 359.66        | -7.26         | 123715.0, 72572.7                | 13.63                    | 164.38              | 1.00                |
| 4     | V4633 Sgr    | 0653550301  | Thin1  | 5.12          | -6.26         | 87320.0, 56167.0                 | 13.71                    | 158.87              | 0.75                |
| 5     | PDS 456      | 0501580201  | Thin1  | 10.38         | 11.14         | 92359.0, 49372.2                 | 12.46                    | 125.92              | 0.52                |
| 6     | PDS 456      | 0501580101  | Thin1  | 10.38         | 11.14         | 92359.0, 49372.2                 | 12.46                    | 125.92              | 0.52                |
| 7     | VV Sco       | 0555650301  | Medium | 352.63        | 19.86         | 105375.0, 40931.0                | 13.60                    | 108.61              | 0.44                |
| 8     | VV Sco       | 0555650201  | Medium | 352.63        | 19.86         | 105375.0, 40931.0                | 13.60                    | 108.61              | 0.44                |
| 9     | CNOC2 Field 1| 0603590101  | Medium | 50.98         | -42.00        | 82317.0, 34084.2                 | 13.58                    | 54.42               | 0.16                |
| 10    | OGLE 1999 BUL32 | 0152420101 | Medium | 2.45          | -3.53         | 49940.0, 28501.1                 | 12.22                    | 191.69              | 0.46                |
| 11    | MACHO 96 BLG 5 | 0305970101 | Thin1  | 3.21          | -3.10         | 107012.0, 48967.2                | 12.93                    | 189.78              | 0.78                |
| 12    | LH VLA 2     | 0554121301  | Medium | 148.46        | 51.42         | 55542.0, 22947.6                 | 13.56                    | 30.45               | 0.06                |
| 13    | RXJ2328.8+1453 | 0502430301 | Thin1  | 94.96         | -43.46        | 104910.0, 53772.2                | 13.53                    | 38.07               | 0.17                |
| 14    | CDFS         | 0555780101  | Thin1  | 223.46        | -54.40        | 133118.0, 34855.0                | 13.44                    | 31.92               | 0.09                |
| 15    | CDFS         | 0555780201  | Thin1  | 223.48        | -54.40        | 133118.0, 34855.0                | 13.44                    | 31.92               | 0.11                |
| 16    | CDFS         | 0555780301  | Thin1  | 223.47        | -54.41        | 123811.0, 50978.4                | 13.54                    | 31.92               | 0.14                |
| 17    | CDFS         | 0555780501  | Thin1  | 223.63        | -54.43        | 113004.0, 61887.7                | 13.62                    | 31.94               | 0.17                |
| 18    | CDFS         | 0555780601  | Thin1  | 223.64        | -54.43        | 118413.0, 48940.7                | 13.68                    | 31.94               | 0.13                |
| 19    | CDFS         | 0555780701  | Thin1  | 223.66        | -54.43        | 118415.0, 59393.9                | 13.59                    | 31.94               | 0.16                |
| 20    | CDFS         | 0555780801  | Thin1  | 223.62        | -54.44        | 120919.0, 47766.2                | 13.50                    | 31.94               | 0.13                |
| 21    | CDFS         | 0555780901  | Thin1  | 223.64        | -54.44        | 121518.0, 44934.8                | 13.52                    | 31.94               | 0.12                |
| 22    | CDFS         | 0555781001  | Thin1  | 223.65        | -54.44        | 125813.0, 58772.7                | 13.65                    | 31.94               | 0.16                |
| 23    | CDFS         | 0555782301  | Thin1  | 223.65        | -54.44        | 125714.0, 51584.6                | 13.64                    | 31.94               | 0.14                |

is mainly a scaling effect proportional to the regarded detector area. The difference of the raw and filtered light curves comprises flares originating in instrumental background effects which have an effect on both the field-of-view (fov) region and the out-of-fov region of the PN-CCD. Furthermore, a spatial filter has been applied via the task `evselect` to cut the events contributing to the hot columns, the bad pixels and the chip gaps of the PN-detector.

3. The source detection algorithm `vtpdetect`\[6\] \[8\] included in the CIAO analysis software \[9\] provided by the Chandra X-ray Center was applied in our analysis. The `vtpdetect` algorithm determines complex regions following isocontours of the detected sources instead of circular regions as does the standard SAS source detection. This approach results in a reduced contamination by the exclusion of sources. The energy range was of between 0.38 keV to 16.5 keV during the source detection to comprise a wide energy range in which astrophysical sources or instrumental artifacts can be located and be consequently detected by the means of the `vtpdetect`-algorithm. The parameter `coarse` defines the lower threshold of events to be inter-

\[6\] See “The Detect Reference Manual” (dated December 2006) for further information: http://cxc.harvard.edu/ciao/download/doc/detect_manual/.

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The figure shows lightcurves of the data set 0604860301 ($i = 2$), selected for the successive analysis. In particular, the red and black error bars represent the filtered lightcurve and the raw lightcurves of the net field of view $\Omega_{\text{net}} = 2$, respectively, while the green and blue error bars represent the filtered lightcurves and the raw lightcurves of the corner fields of view, respectively. The time bin size of the lightcurves is 50 s.

Interpreted as contributors to real sources and was set to 2 instead of 10. The number of false source events is equal the product of the parameter $\text{limit} = 10^{-6}$ times the number of background events. Note, the choice of parameters prioritises the detection of unresolved sources over the non-detection of misidentified sources.

The SAS source detection procedure was executed in addition to the aforementioned source detection algorithm $vtpdetect$ to obtain a conservative upper limit of the remaining source photons in the X-ray background, since the source detection algorithm $vtpdetect$ only outputs a value of the number of false source events per number of background events which does not allow to compute the individual contributions of the counts to the true source events, the false background events and the true background events in one go. Furthermore, the choice of such an upper limit is justified by the quality of the outcome of the $vtpdetect$-algorithm, which led to more precise result in each of the data sets contrary to the SAS source detection.

The energy range was set from 0.5 keV to 4 keV for all tasks involved in the SAS source detection. The task $\text{emask}$ masks all pixels of the detector which have an exposure below the fraction of the maximum exposure denoted by the parameter $\text{threshold}_1$. The latter was set to 0.1 instead of the default value of 0.3 to avoid excessive rejections of pixel on the detector and therefore photon counts in the event file. The minimum detection likelihood $\text{likemin}$ or $\text{mlmin}$ was adjusted down to 3 from 10 for the tasks $\text{eboxdetect}$, $\text{emldetect}$ and $\text{esensmap}$. 
The number of detection runs $n_{\text{runs}}$ of the command `eboxdetect` was increased from 3 to 4. This change was necessary to identify very faint or weak sources since the focus of this analysis lay on the diffuse X-ray background. Furthermore, the source selection radius $s_{\text{cut}}$ and the source cut-out radius $e_{\text{cut}}$ of the script `emldetect` were adjusted to 0.4 and 0.95, respectively. The latter two parameters represent the encircled energy as a fraction of the point spread function of the calibration. The column denoted by $N_{\text{source}}^{\text{X-ray}}$ in table 2 lists upper limits of the percentage of photons from the sources which possibly remained in the filtered background event file and are calculated as: \[ N_{\text{source}}^{\text{X-ray}} = \frac{100 (1 - e_{\text{cut}})}{N_{\text{background}}} N_{\text{source}}. \] This upper limit also applies to the `vtpdetect` results. Exemplary results of the two source detection algorithms applied on the data set corresponding to the observation identifier 0604860301 ($i = 2$) can be compared in figure 3.

4. The spectral analysis was applied with changes in the parameters of the tasks `rmfgen` and `arfgen`: the energy interval has been expanded from 0.05 keV to 20.48 keV and the number of energy bins has been increased to a range of 30 to 4096 bins to match the spectral resolution of the physical energy channels of the PN-detector.

The figure 2 visualises the raw event file (upper left panel) and the outcomes of the three successive analysis steps: the time and particle background filtering (upper right panel), the spatial filtering (lower left panel) and the source filtering (lower right panel) of the data set corresponding to the observation identifier 0604860301 ($i = 2$).

2.3 Instrumental background

The data taken with the X-ray telescope XMM-Newton suffer from both non-negligible instrumental and particle background contamination and electronic noise [10]. The satellite is frequently exposed to energetic cosmic radiation, varying in parts systematically and in parts randomly in orbit as well as clouds of low energy protons entering the telescope. Figure 4 shows the instrumental background spectrum applied in this analysis as red and blue error bars. The instrumental background spectrum shows emission lines due to fluorescence effects triggered by cosmic-ray interactions with the support structure of the PN-CCD and the detector material itself. The most dominant lines are identified as aluminum Al-K$_{\alpha}$ (1.49 keV), nickel Ni-K$_{\alpha}$ (7.48 keV), copper Cu-K$_{\alpha}$ (8.05 keV and 8.95 keV) and zirconium Zn-K$_{\alpha}$ (8.64 keV and 9.57 keV). The filter-wheel-closed event files provided by the XMM-SOC were used to generate the spectrum of the instrumental background for the PN-detector. The event file of the instrumental background is a merger of all data taken while the filter-wheel of the telescope was closed.\textsuperscript{7} Despite the closed filter wheel, the corresponding light curve shows flares induced by cosmic ray incidents. Therefore, it has been time-filtered with the similar time filtering procedure mentioned in section 2.2. This procedure led to a spectrum with a net exposure $t_{\text{net}}^{\text{exp, inst}}$ of 215 ks. The merged and time-filtered instrumental background continuum has been fitted\textsuperscript{8} simultaneously in the energy intervals (0.65; 1.10) keV, (1.675; 1.925) keV, (2.325; 4.350) keV, (4.75; 5.15) keV, (6.9; 7.15) keV, (9.2; 9.3) keV and (10.00; 13.25) keV with a polynomial of the form

\[ R(E) = \sum_{i=0}^{7} a_i \left( \frac{E}{\text{keV}} \right)^i. \]  

\textsuperscript{7}The corresponding event file in full-frame mode of the version dated 2013 was taken from the webpage of the XMM-SOC: http://xmm2.esac.esa.int/external/xmm_sw_cal/background/filter_closed/pn/index.shtml.

\textsuperscript{8}The method applied here is alike the fitting procedure used in the software package ESAS [7].
The above energy intervals have been selected to avoid spectral lines in the fitted energy range. The resulting goodness-of-fit is $\chi^2 = 1324.82$ with 1338 degrees of freedom (d.o.f.) and a probability value or p-value of 0.596 as well as best-fit coefficients $\vec{a} = (739.57, -2.26, 4.79 \cdot 10^{-3}, -5.86 \cdot 10^{-6}, 4.29 \cdot 10^{-9}, -1.85 \cdot 10^{-12}, 4.28 \cdot 10^{-16}, -4.09 \cdot 10^{-20})^T$ s$^{-1}$. The final model of the instrumental background continuum is composed of line-free measured intervals on the one hand and interpolated over intervals of the measured instrumental spectrum on the other hand, which exhibit strong lines. Figure 4 shows the final model of the instrumental background continuum as red error bars and red line segments. The fitted instrumental background spectrum has been normalised to each $i$th spectrum of the 23 astrophysical background spectra in the energy range of between 12.5 keV to 14 keV. We do not expect a significant number of photon or counts having an astrophysical origin in the aforementioned energy range but mainly a contribution of photons or counts with an instrumental
Figure 3. The panels show two source-filtered event files of the data set 0604860301 \((i = 2)\) taken with the PN detector in an energy range of 0.38 keV to 12 keV. The colour coding represents the number of X-ray photon counts per bin. The coordinates X and Y correspond to the sky pixel coordinates. The right panel (B) represents the output of the source filtering routine by the SAS and the left panel (A) shows the output of the \textsc{vtpdetect} source detection the CIAO software package. The two representations of the corresponding event files have been smoothed with a Gaussian kernel having a filter width of 0.25\(\sigma\).

origin in that energy range. The normalisation factor

\[ N_{\text{INST}} = \frac{R_{\text{background}}}{R_{\text{inst}}} \]  

composed of a ratio of the sums of the background and the instrumental photon counts in the energy range of between 12 keV and 14 keV,

\[ R_{\gamma \in \{\text{background, instrumental}\}} = \sum_{E_{\text{photon}}} \begin{cases} 1, & \text{if } 12.5 \text{ keV} \leq E_{\text{photon}} \leq 14 \text{ keV}, \\ 0, & \text{elsewhere}, \end{cases} \]  

is listed in table 2 for each individual data set. The effective area is close to zero in this energy regime, so that the fraction of the instrumental background photon counts dominates above 10 keV for each of the astrophysical background spectra. In a further step, the partially fitted and normalised instrumental source detection has been subtracted from the astrophysical background spectrum with the program XSPEC [6]. The equation describing the subtraction of photon counts of a channel or bin \(b\) by instrumental photon counts of the same channel or energy bin \(b\) used in this analysis is

\[ N_{b,\text{subtracted background}} = N_{b,\text{background}} - N_{b,\text{inst}} \cdot \frac{t_{\text{net exp}} \cdot \Omega_{\text{net fov}}}{t_{\text{net exp, inst}} \cdot \Omega_{\text{net fov, inst}}} \]  

with \(N_{b,\text{background}}\) and \(N_{b,\text{inst}}\) being the photon counts in the \(b\)th channel of the background spectrum and the instrumental background spectrum, respectively, and \(t_{\text{net exp}}\) and \(t_{\text{net exp, inst}}\) are the respective

\[^{9}\text{The program XSPEC V11 [6] has been used for the purpose of subtracting the individually scaled instrumental background spectra of the astrophysical spectra and of fitting the remaining spectra with multiplicative and/or additive combinations of predefined spectra.}\]
Figure 4. The model of the instrumental background continuum shows the measured line-free segments (red crosses with error bars) and the fitted gaps (red line segments) which have been dominated by spectral lines (blue error bars) in the primary spectrum. A polynomial of the 7th order has been applied to bridge the gaps.

net exposures, while $\Omega_{\text{net}}$ and $\Omega_{\text{net, inst}}$ are the corresponding net fields of view. The errors per bin or channel of a instrumental-background-subtracted spectrum have been calculated due to standard error propagation under the assumption that the errors of the counts per bin or channel of the initial spectrum and the instrumental background spectrum are individually distributed as a Gaussian function.

2.4 Fitting strategy

2.4.1 Null hypothesis model

The analysis focuses on possible additional emission lines in the diffuse X-ray background. This leads to a null hypothesis model $m_0$\textsuperscript{10} of a continuum with superposed line emission:

$$m_0 \left( n_{H,i}, \Gamma_i, N_{\text{pow};i}, T_i, N_{\text{brems};i}, E_{\text{line};ij}, \sigma_{ij}, F_{\text{photon};ij} \right) =$$

\begin{equation}
\sum_{i=1}^{N} \left( w_{\text{abs}} \left( n_{H,i} \right) \cdot \left( \text{pow} \left( \Gamma_i, N_{\text{pow};i} \right) + \text{brems} \left( T_i, N_{\text{brems};i} \right) \right) \right) \text{continuum emission}
\end{equation}

$$+ \left( \sum_{j=1}^{l} \text{gauss} \left( E_{\text{line};ij}, \sigma_{ij}, F_{\text{photon};ij} \right) \right) . \tag{2.9}$$

\textsuperscript{10}The models are folded with the corresponding response matrices and their auxiliary files during the fitting process to account for instrumental effects, e.g., the spectral energy resolution.
Firstly, the continuum emission of an $i$th data set is modelled as a powerlaw ‘pow’ dependent on dimensionless photon index $\Gamma_i$ and a normalisation $N_{\text{pow};i}$ and a thermal bremsstrahlung spectrum ‘brems’ dependent on a temperature $T_i$ and a normalisation $N_{\text{brems};i}$, both jointly attenuated by a photoelectric absorption component denoted as ‘wabs’, dependent on a hydrogen column $n_{H;i}$. Secondly, the line emission of such an $i$th data set is modelled by the sum of $L = 19$ astrophysical and instrumental emission lines, each of Gaussian shape dependent on the mean energy $E_{\text{line};ij}$, the line width $\sigma_{ij}$ and the flux normalisation $F_{\text{photon};ij}$ of a $j$th emission line.

The fitted Gaussian lines accounting for the line emission at energies of 0.58 keV (O VII), 0.67 keV (O VIII), 0.76 keV (Fe XVII), 0.84 keV (Fe XVII), 0.93 keV (Ne IX), 1.04 keV (Ne IX), 1.37 keV (Mg XI) and 2.34 keV (Si XIII) are considered to be of an astrophysical origin while the instrumental Gaussian emission lines are located at energies of 1.49 keV (Al-K\text{\alpha}), 1.87 keV (Si-K\text{\alpha}), 4.54 keV (Ti-K\text{\alpha}), 5.43 keV (Cr-K\text{\alpha}), 6.42 keV (Fe-K\text{\alpha}), 7.48 keV (Ni-K\text{\alpha}), 8.04 keV (Cu-K\text{\alpha}), 8.08 keV (Cu-K\text{\beta} and Zn-K\text{\alpha}), 8.90 keV (Cu-K\text{\alpha}) and 9.58 keV (Zn-K\text{\alpha}). All 23 data sets listed in table 1 have been fitted simultaneously in an energy range from 0.38 keV to 12 keV by the application of a fitting procedure using the program XSPEC. During the fitting procedure all astrophysical components of the model $m_0$ have been treated independently. We investigated any systematical differences by independently fitting the astrophysical parameters even for observations of the same fields of view. The resulting differences are well consistent with the assumed statistical uncertainties which gives confidence in the procedure. The quality of the resulting best-fit reaches a goodness-of-fit of $\chi^2 = 52519.26$ while having 52529 degrees of freedom (d.o.f.) and a p-value = 0.5111. These values indicate a stable and good fit. No additional systematic uncertainties have been considered. The intrinsic widths $\sigma_{ij}$ of the astrophysical lines have been frozen to zero\textsuperscript{11} in contrast to the instrumental Gaussian emission lines. The forward-folding of the model with the related response matrix during the fitting process expands the corresponding line widths $\sigma_{ij}$ to the energy-dependent spectral resolutions. Some of the astrophysical lines have not been detected in all data sets.

\textsuperscript{11}A Gaussian line width of zero is interpreted as the width of one energy channel or 0.005 keV by Xspec.
| Object       | ObsId       | $w$  | $N_{\text{abs}}^{\text{X-ray}}$ | $N_{\text{INST}}$ | Absorption | Bremsstr. | Bremsstr. | Powerlaw | Powerlaw |
|--------------|-------------|------|---------------------------------|---------------------|------------|-----------|-----------|----------|----------|
|              |             |      |                                  |                     |            |           |           |          |          |
|              |             |      |                                  |                     |            |           |           |          |          |
|              |             |      |                                  |                     |            |           |           |          |          |
|              |             |      |                                  |                     |            |           |           |          |          |
|              |             |      |                                  |                     |            |           |           |          |          |
| V4046 Sgr    | 0604860201  | 0.10 | 1.18                            | 0.19                | 1.59 ± 0.17 | 2.78 ± 0.15 | 60.80 ± 14.11 | 1.01 ± 0.04 | 14.66 ± 0.64 |
| V4046 Sgr    | 0604860301  | 0.12 | 1.23                            | 0.23                | 1.59 ± 0.16 | 2.78 ± 0.14 | 61.66 ± 13.45 | 1.04 ± 0.03 | 14.66 ± 0.63 |
| V4046 Sgr    | 0604860401  | 0.12 | 1.17                            | 0.22                | 1.60 ± 0.16 | 2.79 ± 0.15 | 59.81 ± 13.24 | 1.09 ± 0.04 | 13.75 ± 0.64 |
| V4633 Sgr    | 0653550301  | 0.09 | 0.07                            | 0.15                | 2.11 ± 0.19 | 3.02 ± 0.20 | 66.22 ± 16.90 | 1.19 ± 0.05 | 14.90 ± 0.97 |
| PDS 456     | 0501580201  | 0.08 | 2.10                            | 0.18                | 2.26 ± 0.30 | 3.43 ± 0.40 | 24.65 ± 9.84  | 1.05 ± 0.05 | 13.04 ± 0.97 |
| PDS 456     | 0501580101  | 0.06 | 3.34                            | 0.14                | 2.30 ± 0.33 | 3.47 ± 0.47 | 28.03 ± 12.77 | 1.11 ± 0.06 | 15.99 ± 1.37 |
| VV Sco      | 0555650303  | 0.04 | 0.69                            | 0.12                | 2.26 ± 0.30 | 2.41 ± 0.18 | 104.94 ± 40.87 | 1.00 ± 0.06 | 11.55 ± 0.81 |
| VV Sco      | 0555650201  | 0.05 | 0.68                            | 0.14                | 2.02 ± 0.27 | 2.44 ± 0.18 | 85.49 ± 31.04 | 1.03 ± 0.05 | 13.96 ± 0.90 |
| CNOCS2 Field | 0603590101  | 0.02 | 0.61                            | 0.10                | 0.56 ± 0.28 | 2.15 ± 0.21 | 24.04 ± 11.25 | 0.92 ± 0.05 | 14.68 ± 0.87 |
| OGLE 1999 BUL 32 | 0152420101  | 0.05 | 0.02                            | 0.05                | 2.59 ± 0.32 | 2.69 ± 0.26 | 98.80 ± 43.47 | 1.82 ± 0.06 | 32.09 ± 2.38 |
| MACHO 96 BLG 5 | 0305970101  | 0.09 | 0.07                            | 0.10                | 2.58 ± 0.19 | 3.12 ± 0.22 | 86.07 ± 22.45 | 1.55 ± 0.05 | 33.02 ± 1.94 |
| LH VLA 2     | 0554121301  | 0.01 | 0.11                            | 0.07                | 1.66 ± 0.49 | 1.83 ± 0.21 | 54.99 ± 39.35 | 1.09 ± 0.08 | 14.40 ± 1.32 |
| RXJ2328.8+1453 | 0502430301  | 0.02 | 0.06                            | 0.13                | 1.01 ± 0.31 | 2.63 ± 0.31 | 13.13 ± 6.39  | 0.80 ± 0.05 | 10.77 ± 0.65 |
| CDFS         | 0555780101  | 0.01 | 0.17                            | 0.10                | 1.09 ± 0.37 | 2.41 ± 0.34 | 18.23 ± 10.93 | 1.00 ± 0.07 | 11.20 ± 0.93 |
| CDFS         | 0555780201  | 0.01 | 0.15                            | 0.12                | 0.94 ± 0.32 | 2.46 ± 0.30 | 16.00 ± 8.25  | 0.91 ± 0.05 | 12.71 ± 0.82 |
| CDFS         | 0555780301  | 0.02 | 0.14                            | 0.14                | 0.87 ± 0.29 | 2.71 ± 0.33 | 13.04 ± 5.96  | 0.77 ± 0.05 | 10.76 ± 0.67 |
| CDFS         | 0555780501  | 0.02 | 0.12                            | 0.12                | 0.92 ± 0.26 | 2.89 ± 0.33 | 11.83 ± 4.81  | 0.70 ± 0.05 | 10.00 ± 0.61 |
| CDFS         | 0555780601  | 0.02 | 0.11                            | 0.14                | 1.33 ± 0.29 | 2.47 ± 0.26 | 22.52 ± 10.00 | 0.81 ± 0.05 | 11.24 ± 0.74 |
| CDFS         | 0555780701  | 0.02 | 0.26                            | 0.17                | 1.07 ± 0.26 | 2.49 ± 0.24 | 18.19 ± 7.40  | 0.79 ± 0.05 | 11.24 ± 0.63 |
| CDFS         | 0555780801  | 0.02 | 0.13                            | 0.14                | 1.21 ± 0.31 | 2.53 ± 0.28 | 19.10 ± 9.00  | 0.80 ± 0.05 | 11.23 ± 0.74 |
| CDFS         | 0555780901  | 0.01 | 0.12                            | 0.13                | 1.17 ± 0.33 | 2.21 ± 0.24 | 23.95 ± 12.35 | 0.93 ± 0.05 | 12.73 ± 0.82 |
| CDFS         | 0555781001  | 0.02 | 0.16                            | 0.17                | 1.08 ± 0.27 | 2.55 ± 0.27 | 17.51 ± 7.51  | 0.84 ± 0.05 | 12.77 ± 0.71 |
| CDFS         | 0555782301  | 0.02 | 0.12                            | 0.15                | 1.10 ± 0.29 | 2.51 ± 0.26 | 17.91 ± 7.86  | 0.78 ± 0.05 | 11.53 ± 0.69 |

**Table 2.** The table above lists the best-fit values of the absorbed bremsstrahlung and the powerlaw components.
\begin{table}
\centering
\begin{tabular}{|l|c|c|c|c|c|c|c|c|c|}
\hline
Object & ObsId & \(w\) & \(N_{\text{X-ray}}\) & \(N_{\text{INST}}\) & \(F_{\text{photon}}^{\text{O VII}}\) & \(F_{\text{photon}}^{\text{O VIII}}\) & \(F_{\text{photon}}^{\text{Fe XVII}}\) & \(F_{\text{photon}}^{\text{Ne IX}}\) \\
\hline
V4046 Sgr & 0604860201 & 0.10 & 1.18 & 0.19 & 10.26 ± 0.24 & 6.44 ± 0.26 & 4.08 ± 0.25 & 5.39 ± 0.24 & 3.65 ± 0.15 \\
V4046 Sgr & 0604860301 & 0.12 & 1.23 & 0.23 & 10.72 ± 0.23 & 6.63 ± 0.25 & 4.10 ± 0.24 & 5.64 ± 0.23 & 3.60 ± 0.14 \\
V4046 Sgr & 0604860401 & 0.12 & 1.17 & 0.22 & 10.15 ± 0.22 & 6.28 ± 0.25 & 4.00 ± 0.24 & 5.39 ± 0.23 & 3.55 ± 0.15 \\
V4633 Sgr & 0653550301 & 0.09 & 0.07 & 0.15 & 9.59 ± 0.23 & 6.04 ± 0.29 & 5.32 ± 0.28 & 6.57 ± 0.25 & 4.09 ± 0.17 \\

PDS 456 & 0501580201 & 0.08 & 2.10 & 0.18 & 3.85 ± 0.15 & 2.73 ± 0.19 & 2.30 ± 0.19 & 3.16 ± 0.18 & 2.08 ± 0.12 \\

PDS 456 & 0501580101 & 0.06 & 3.34 & 0.14 & 4.47 ± 0.21 & 3.10 ± 0.23 & 2.90 ± 0.23 & 3.88 ± 0.20 & 2.26 ± 0.15 \\
VV Sco & 0555650301 & 0.04 & 0.69 & 0.12 & 8.46 ± 0.31 & 5.16 ± 0.38 & 3.44 ± 0.37 & 4.15 ± 0.36 & 2.89 ± 0.19 \\
VV Sco & 0555650201 & 0.05 & 0.68 & 0.14 & 9.68 ± 0.28 & 6.47 ± 0.36 & 3.99 ± 0.34 & 4.38 ± 0.32 & 3.08 ± 0.19 \\

CNOC2 Field 1 & 0603590101 & 0.02 & 0.61 & 0.10 & 6.96 ± 0.31 & 1.14 ± 0.21 & – & – & 0.52 ± 0.12 \\

OGLE 1999 BUL 32 & 0152420101 & 0.05 & 0.02 & 0.05 & 7.82 ± 0.30 & 4.07 ± 0.35 & 2.53 ± 0.42 & 4.96 ± 0.45 & 4.01 ± 0.23 \\

MACHO 96 BLG 5 & 0305970101 & 0.09 & 0.07 & 0.10 & 8.09 ± 0.23 & 3.77 ± 0.28 & 3.70 ± 0.28 & 6.59 ± 0.26 & 4.57 ± 0.18 \\

LH VLA 2 & 0554121301 & 0.01 & 0.11 & 0.07 & 3.83 ± 0.30 & – & – & – & – \\

RXJ2328.8+1453 & 0502430301 & 0.02 & 0.06 & 0.13 & 2.95 ± 0.24 & 0.77 ± 0.23 & – & – & 0.15 ± 0.08 \\

CDFS & 0555780101 & 0.01 & 0.17 & 0.10 & 2.90 ± 0.23 & – & – & – & – \\

CDFS & 0555780201 & 0.01 & 0.15 & 0.12 & 2.60 ± 0.20 & – & – & – & 0.15 ± 0.09 \\
CDFS & 0555780301 & 0.02 & 0.14 & 0.14 & 2.78 ± 0.19 & – & – & – & – \\
CDFS & 0555780501 & 0.02 & 0.12 & 0.18 & 2.96 ± 0.17 & – & – & – & – \\
CDFS & 0555780601 & 0.02 & 0.11 & 0.14 & 2.91 ± 0.19 & – & – & – & 0.17 ± 0.09 \\
CDFS & 0555780701 & 0.02 & 0.26 & 0.17 & 2.92 ± 0.18 & – & – & – & 0.13 ± 0.08 \\
CDFS & 0555780801 & 0.02 & 0.12 & 0.14 & 3.20 ± 0.20 & – & – & – & 0.24 ± 0.10 \\
CDFS & 0555780901 & 0.01 & 0.12 & 0.13 & 3.49 ± 0.21 & – & – & – & 0.25 ± 0.09 \\
CDFS & 0555781001 & 0.02 & 0.16 & 0.17 & 3.41 ± 0.19 & – & – & – & 0.12 ± 0.08 \\
CDFS & 0555782301 & 0.02 & 0.12 & 0.15 & 2.99 ± 0.19 & – & – & – & 0.17 ± 0.09 \\
\hline
\end{tabular}
\end{table}

To be continued on the next page.
| Object          | ObsId     | $w$ | $N_{\text{X-ray}}^{\text{X}}$ | $N_{\text{DIST}}$ | $F_{\text{phot}}^{\text{X}}$ | $F_{\text{phot}}^{\text{X}}$ | $F_{\text{phot}}^{\text{X}}$ | $F_{\text{phot}}^{\text{X}}$ |
|-----------------|-----------|-----|---------------------|-------------------|---------------------|---------------------|---------------------|---------------------|
| V4046 Sgr       | 0604860301| 0.12| 1.23                | 0.22              | 1.45 ± 0.09         | 0.44 ± 0.06         | 3.89 ± 0.08         | –                   |
| V4046 Sgr       | 0604860401| 0.12| 1.17                | 0.22              | 1.45 ± 0.09         | 0.44 ± 0.06         | 3.89 ± 0.08         | –                   |
| V4633 Sgr       | 0653550301| 0.09| 0.07                | 0.15              | 1.91 ± 0.11         | 0.35 ± 0.06         | 3.28 ± 0.07         | –                   |
| PDS 456         | 0501580201| 0.08| 2.10                | 0.18              | 0.78 ± 0.08         | 0.30 ± 0.06         | 3.37 ± 0.09         | 0.32 ± 0.05         |
| MACHO 96 BLG 5  | 0305970101| 0.09| 0.07                | 0.10              | 2.80 ± 0.12         | 0.46 ± 0.07         | 2.29 ± 0.07         | 0.48 ± 0.06         |
| LH VLA 2        | 0554121301| 0.01| 0.11                | 0.07              | –                   | –                   | 6.03 ± 1.01         | –                   |
| RXJ2328.8+1453  | 0502430301| 0.02| 0.06                | 0.13              | –                   | –                   | 5.06 ± 0.10         | –                   |
| CDFS            | 0555780101| 0.01| 0.17                | 0.10              | –                   | 0.31 ± 0.13         | 5.78 ± 0.16         | 0.26 ± 0.11         |
| CDFS            | 0555780201| 0.01| 0.15                | 0.12              | –                   | 0.30 ± 0.12         | 5.78 ± 0.15         | 0.37 ± 0.10         |
| CDFS            | 0555780301| 0.02| 0.14                | 0.14              | –                   | 0.44 ± 0.09         | 5.76 ± 0.11         | 0.27 ± 0.09         |
| CDFS            | 0555780501| 0.02| 0.12                | 0.18              | –                   | 0.31 ± 0.07         | 6.01 ± 0.10         | 0.14 ± 0.08         |
| CDFS            | 0555780601| 0.02| 0.11                | 0.14              | –                   | 0.41 ± 0.09         | 6.20 ± 0.12         | 0.25 ± 0.09         |
| CDFS            | 0555780701| 0.02| 0.26                | 0.17              | –                   | 0.34 ± 0.07         | 6.15 ± 0.10         | 0.29 ± 0.09         |
| CDFS            | 0555780801| 0.02| 0.13                | 0.14              | –                   | 0.24 ± 0.07         | 6.52 ± 0.11         | 0.47 ± 0.10         |
| CDFS            | 0555780901| 0.01| 0.12                | 0.13              | –                   | 0.52 ± 0.14         | 6.03 ± 0.17         | 0.22 ± 0.10         |
| CDFS            | 0555781001| 0.02| 0.16                | 0.17              | –                   | 0.51 ± 0.11         | 6.42 ± 0.13         | 0.34 ± 0.09         |
| CDFS            | 0555782301| 0.02| 0.12                | 0.15              | –                   | 0.40 ± 0.13         | 6.26 ± 0.15         | 0.12 ± 0.09         |

To be continued on the next page.
| Object         | ObsId       | w | $N_{\text{X-ray}}^s$ | $N_{\text{INST}}$ | $F_{\text{phot}}$ | $F_{\text{phot}}$ | $F_{\text{phot}}$ | $F_{\text{phot}}$ |
|---------------|-------------|---|----------------------|-------------------|------------------|------------------|------------------|------------------|
|               |             |   |                      |                   |                  |                  |                  |                  |
| V4046 Sgr     | 0604860201  | 0.10 | 1.18 | 0.19 | 0.08 ± 0.05 | 0.45 ± 0.05 | 0.22 ± 0.06 | 6.07 ± 0.19 |
| V4046 Sgr     | 0604860301  | 0.12 | 1.23 | 0.23 | 0.10 ± 0.04 | 0.32 ± 0.05 | 0.29 ± 0.06 | 5.99 ± 0.17 |
| V4046 Sgr     | 0604860401  | 0.12 | 1.17 | 0.22 | 0.11 ± 0.04 | 0.41 ± 0.05 | 0.28 ± 0.06 | 6.47 ± 0.18 |
| V4633 Sgr     | 0653550301  | 0.09 | 0.07 | 0.15 | 0.20 ± 0.05 | 0.46 ± 0.05 | 0.31 ± 0.06 | 5.22 ± 0.17 |
| PDS 456       | 0501580201  | 0.08 | 2.10 | 0.18 | –            | 0.37 ± 0.05 | 0.33 ± 0.06 | 5.39 ± 0.16 |
| PDS 456       | 0501580101  | 0.06 | 3.34 | 0.14 | –            | 0.46 ± 0.06 | 0.25 ± 0.07 | 5.98 ± 0.27 |
| VV Sco        | 0555650301  | 0.04 | 0.69 | 0.12 | 0.17 ± 0.06 | 0.52 ± 0.07 | 0.25 ± 0.09 | 6.98 ± 0.22 |
| VV Sco        | 0555650201  | 0.05 | 0.68 | 0.14 | 0.14 ± 0.06 | 0.56 ± 0.07 | 0.28 ± 0.08 | 7.06 ± 0.23 |
| CNOC2 Field 1 | 0603590101  | 0.02 | 0.61 | 0.10 | 0.33 ± 0.09 | 0.67 ± 0.10 | 0.37 ± 0.12 | 9.63 ± 0.37 |
| OGLE 1999 BUL 32 | 0152420101 | 0.05 | 0.02 | 0.05 | –            | 0.23 ± 0.05 | 0.08 ± 0.06 | 2.66 ± 0.15 |
| MACHO 96 BLG 5 | 0305970101 | 0.09 | 0.07 | 0.10 | 0.08 ± 0.04 | 0.27 ± 0.05 | 0.30 ± 0.06 | 3.52 ± 0.13 |
| LH VLA 2      | 0554121301  | 0.01 | 0.11 | 0.07 | 0.43 ± 0.12 | 0.86 ± 0.13 | 0.60 ± 0.15 | 9.36 ± 0.41 |
| RXJ2328.8+1453 | 0502430301 | 0.02 | 0.06 | 0.13 | 0.21 ± 0.07 | 0.48 ± 0.08 | 0.30 ± 0.09 | 8.48 ± 0.24 |
| CDFS          | 0555780101  | 0.01 | 0.17 | 0.10 | 0.24 ± 0.09 | 0.70 ± 0.10 | 0.27 ± 0.12 | 8.81 ± 0.32 |
| CDFS          | 0555780201  | 0.01 | 0.15 | 0.12 | 0.31 ± 0.09 | 0.68 ± 0.10 | 0.25 ± 0.11 | 8.35 ± 0.31 |
| CDFS          | 0555780301  | 0.02 | 0.14 | 0.14 | 0.21 ± 0.08 | 0.55 ± 0.09 | 0.33 ± 0.10 | 8.22 ± 0.29 |
| CDFS          | 0555780501  | 0.02 | 0.12 | 0.18 | 0.24 ± 0.07 | 0.59 ± 0.08 | 0.53 ± 0.10 | 9.05 ± 0.27 |
| CDFS          | 0555780601  | 0.02 | 0.11 | 0.14 | 0.23 ± 0.08 | 0.68 ± 0.09 | 0.39 ± 0.11 | 8.80 ± 0.30 |
| CDFS          | 0555780701  | 0.02 | 0.26 | 0.17 | 0.26 ± 0.07 | 0.60 ± 0.08 | 0.40 ± 0.10 | 9.17 ± 0.30 |
| CDFS          | 0555780801  | 0.02 | 0.13 | 0.14 | 0.33 ± 0.08 | 0.82 ± 0.10 | 0.55 ± 0.11 | 9.64 ± 0.33 |
| CDFS          | 0555780901  | 0.01 | 0.12 | 0.13 | 0.35 ± 0.09 | 0.80 ± 0.10 | 0.59 ± 0.11 | 9.24 ± 0.33 |
| CDFS          | 0555781001  | 0.02 | 0.16 | 0.17 | 0.38 ± 0.08 | 0.80 ± 0.09 | 0.49 ± 0.10 | 9.41 ± 0.27 |
| CDFS          | 0555782301  | 0.02 | 0.12 | 0.15 | 0.26 ± 0.08 | 0.80 ± 0.09 | 0.51 ± 0.11 | 9.26 ± 0.31 |

To be continued on the next page.
| Object     | ObsId    | w  | $N_{X\text{-ray}}$ | $N_{\text{inst}}$ | $F_{\text{photon}}$ | $F_{\text{photon}}$ | $F_{\text{photon}}$ | $F_{\text{photon}}$ |
|------------|----------|----|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
|            |          |    |                   |                   | $10^{-4}$ cm$^{-2}$ | $10^{-4}$ cm$^{-2}$ | $10^{-4}$ cm$^{-2}$ | $10^{-4}$ cm$^{-2}$ |
| V4046 Sgr  | 0604860201 0.10 1.18 0.19 | 51.25 ± 0.53 | 7.98 ± 0.51 | 7.36 ± 0.56 | 10.38 ± 0.32 | 4.22 ± 0.37 |
| V4046 Sgr  | 0604860301 0.12 1.23 0.23 | 52.76 ± 0.50 | 7.91 ± 0.53 | 7.24 ± 0.33 | 10.82 ± 0.37 | 3.69 ± 0.33 |
| V4046 Sgr  | 0604860401 0.12 1.17 0.22 | 53.19 ± 0.47 | 7.43 ± 0.69 | 7.63 ± 0.36 | 11.05 ± 0.37 | 3.10 ± 0.29 |
| V4633 Sgr  | 0653550301 0.09 0.07 0.15 | 45.64 ± 0.41 | 6.76 ± 1.05 | 6.10 ± 0.52 | 9.21 ± 0.49 | 1.87 ± 0.27 |
| PDS 456   | 0501580201 0.08 2.10 0.18 | 46.28 ± 0.48 | 6.50 ± 0.59 | 6.68 ± 0.54 | 8.93 ± 0.31 | 3.36 ± 0.31 |
| PDS 456   | 0501580101 0.06 3.34 0.14 | 52.92 ± 0.54 | 7.10 ± 0.52 | 7.38 ± 1.05 | 10.13 ± 0.56 | 2.54 ± 0.35 |
| VV Sco    | 0555560301 0.04 0.69 0.12 | 58.81 ± 0.90 | 7.87 ± 0.63 | 9.00 ± 0.60 | 11.28 ± 0.40 | 2.89 ± 0.43 |
| VV Sco    | 0555560201 0.05 0.68 0.14 | 61.09 ± 0.84 | 8.16 ± 0.65 | 9.54 ± 0.92 | 12.05 ± 0.51 | 3.06 ± 0.38 |
| CNO2 Field 1 | 0603590101 0.02 0.61 0.10 | 78.99 ± 1.07 | 11.31 ± 0.91 | 11.21 ± 0.61 | 15.99 ± 0.55 | 4.64 ± 0.59 |
| OGLE 1999 BUL 32 | 0152420101 0.05 0.02 0.05 | 23.88 ± 0.46 | 3.71 ± 0.38 | 2.92 ± 0.22 | 4.71 ± 0.22 | 0.70 ± 0.20 |
| MACHO 96 BLG 5 | 0305970101 0.09 0.07 0.10 | 32.85 ± 0.31 | 5.92 ± 0.64 | 3.76 ± 0.20 | 6.15 ± 0.24 | 1.26 ± 0.20 |
| LH VLA 2  | 0554121301 0.01 0.11 0.07 | 84.08 ± 1.03 | 12.89 ± 1.95 | 9.60 ± 0.77 | 15.98 ± 0.92 | 1.77 ± 0.55 |
| RXJ2328.8+1453 | 0502430301 0.02 0.06 0.13 | 71.93 ± 0.79 | 7.52 ± 0.63 | 10.48 ± 0.43 | 13.83 ± 0.39 | 2.93 ± 0.33 |
| CDFS      | 0555780101 0.01 0.17 0.10 | 75.15 ± 1.10 | 9.26 ± 0.86 | 10.97 ± 0.60 | 14.48 ± 0.55 | 2.19 ± 0.42 |
| CDFS      | 0555780201 0.01 0.15 0.12 | 78.29 ± 0.75 | 13.70 ± 1.28 | 9.61 ± 0.58 | 15.29 ± 0.62 | 3.48 ± 0.40 |
| CDFS      | 0555780301 0.02 0.14 0.14 | 77.36 ± 0.70 | 11.92 ± 1.23 | 9.82 ± 0.58 | 15.27 ± 0.60 | 3.25 ± 0.36 |
| CDFS      | 0555780501 0.02 0.12 0.18 | 80.90 ± 0.67 | 11.07 ± 1.10 | 10.71 ± 0.55 | 15.89 ± 0.54 | 4.30 ± 0.35 |
| CDFS      | 0555780601 0.02 0.11 0.14 | 83.02 ± 0.73 | 13.74 ± 1.35 | 10.34 ± 0.60 | 15.76 ± 0.65 | 3.14 ± 0.39 |
| CDFS      | 0555780701 0.02 0.26 0.17 | 81.31 ± 0.75 | 11.71 ± 0.97 | 10.51 ± 0.56 | 16.36 ± 0.51 | 4.01 ± 0.35 |
| CDFS      | 0555780801 0.02 0.13 0.14 | 87.24 ± 0.83 | 11.75 ± 1.27 | 10.78 ± 0.67 | 16.81 ± 0.65 | 3.76 ± 0.40 |
| CDFS      | 0555780901 0.01 0.12 0.13 | 81.84 ± 0.81 | 12.51 ± 1.28 | 11.22 ± 0.66 | 16.49 ± 0.63 | 3.89 ± 0.41 |
| CDFS      | 0555781001 0.02 0.16 0.17 | 84.51 ± 0.76 | 11.56 ± 1.12 | 10.63 ± 0.67 | 16.12 ± 0.59 | 3.74 ± 0.37 |
| CDFS      | 0555782301 0.02 0.12 0.15 | 85.00 ± 0.77 | 11.66 ± 1.12 | 11.82 ± 0.60 | 16.59 ± 0.58 | 3.09 ± 0.38 |

Table 3. This table shows the best-fit values of the normalisations $F_{\text{photon}}$ of spectral emission lines in the null hypothesis model $m_0$. The mean energies $E_{\text{line}}$ of the spectral lines with Gaussian shape as well as their physical origins are presented in the first two rows. The observation identification (ObsId), the radial distance $\phi$ and the weightings $w$ of the additional line comprised in the alternative hypothesis model $m_1$ are also listed.
Figure 5. The panels A and B show the measured spectrum of an individual data set (observation identifier: 0604860301, \(i = 2\)) as black error bars and its fitted model in an energy range from 0.38 keV to 2 keV (upper panel) and from 2 keV to 12 keV (lower panel) as red lines, respectively, while the blue error bars show the instrumental background model. The fitted model is composed of two continuum components consisting of a bremsstrahlung component ‘brems’ and a powerlaw component ‘pow’, both attenuated by an absorption component ‘wabs’, plus 19 instrumental and astrophysical Gaussian emission lines ‘gauss’. The best-fit values are specified in tables 2 and 3. The panels B and D show the residuals per energy bin in values of \(\chi = \text{sgn}(\text{Data} - \text{Model}) \sqrt{\text{Data} - \text{Model}}^2\).

The instrumental background subtracted spectrum, the related best-fit model, the normalised instrumental background spectrum and the spectrum of the detected sources, all related to the data set having the observation identifier 0604860301 \((i = 2)\) are exemplarily plotted in the panels A and C of figure 5. The x-axis is the energy scale in keV and the y-axis indicates the photon counts. The
Figure 6. The panels A and B show the modelled spectrum $m_0$ of each of the 23 data sets in energy ranges of 0.38 keV to 2 keV (upper panel) and of 2 keV to 12 keV (lower panel), respectively. The fitted model consists of two continuum components consisting of a powerlaw component ‘pow’ and a bremsstrahlung component ‘brems’, both attenuated by an absorption component ‘wabs’, plus 19 instrumental and astrophysical Gaussian emission lines ‘gauss’. The best-fit values are specified in tables 2 and 3.

panels B and D show the residuals among the model $m_0$ and the data in units of $\chi = \text{sgn}(\text{Data} - \text{Model}) \sqrt{(\text{Data} - \text{Model})^2}$.

The resulting fitted values of the continuum component of the null hypothesis model $m_0$ are listed in table 2. Table 3 contains the normalisations $F_{\text{photon}}$ of the 19 Gaussian emission lines denoted as ‘gauss’ within the null hypothesis model $m_0$. Normalisations have been ignored (denoted by ‘‘..’’ in table 2 and 3) if the square root of the diagonal elements contained in the covariance matrix of the Levenberg-Marquardt fit were equal or higher than their central value. The absorption is given as the hydrogen column density $n_H$ and acts on the powerlaw and the bremsstrahlung components. The powerlaw is represented as the dimensionless photon index $\Gamma$ and its normalisation $N_{\text{pow}}$. The bremsstrahlung component is defined by the temperature $T$ in units of [keV] and its normalisation $N_{\text{brems}}$. Additionally, table 3 contains the mean energy $E_{\text{line}}$ and the normalisation values $F_{\text{photon}}$ of the all 19 Gaussian-shaped spectral emission lines with an astrophysical and an instrumental origin, respectively. The line energies are given as mean values since their variations are in the order of $O(eV)$. The photon fluxes $F_{\text{line}}$ of the instrumental lines are consistent with the overall activation of the telescope and its detectors by cosmic rays and soft proton clouds. The best-fit model $m_0$ of all 23 data sets are plotted in figure 6. The panels A and B show the modelled counts per bin of the astrophysical background spectra in energy ranges from 0.38 keV to 2 keV and from 2 keV to 12 keV, respectively.

The residuals distributions per energy bin in figure 7, panels A and B as well as the accumulated residual distribution of all energy bins, presented in figure 7, panel C, have a recognisable shift of their
Figure 7. The panels A and B show the residuals $\chi$ among the best-fit model and its underlying data sets in energy regimes of 0.38 keV to 2 keV (upper panel) and 2 keV to 12 keV (middle panel), respectively. The red curves indicate the $\pm 1\sigma$ levels of the residual distributions in each energy bin. The panel C presents the accumulated residual distribution of all energy bins. A normal distribution is also plotted for comparison.

means towards positive values. This bias of the residuals $\chi = \text{sgn}(\text{Data} - \text{Model}) \sqrt{[\text{Data} - \text{Model}]^2}$ can be explained by a non-vanishing contribution of photon counts from astrophysical sources in the normalisation range among the instrumental background model and the astrophysical spectra contrary to the assumption made in section 2.3.
2.4.2 Alternative hypothesis model

Accordingly, an alternative hypothesis model $m_1$ taking account of the alternative hypothesis is basically defined on the null hypothesis model $m_0$ and an additional Gaussian emission line $L_\gamma$ dependent on the mean energy $E_{\gamma;n}$, the line width $\sigma_{\gamma;i}$ as well as the flux normalisation $F_{\gamma;m}$ and its weighting factor $w_i$. The contribution of the flux normalisation $F_{\gamma}$ of the additional emission line is thereby distributed over all $23$ data sets:

$$m_1 \left( n_{H;i}, \Gamma_i, N_{\text{pow};i}, T_i, N_{\text{brems};i}, E_{\text{line};i,j}, \sigma_{ij}, F_{\text{photon};i,j}, E_{\gamma;n}, \sigma_{\gamma}, F_{\gamma;m} \right) =$$

$$m_0 \left( n_{H;i}, \Gamma_i, N_{\text{pow};i}, T_i, N_{\text{brems};i}, E_{\text{line};i,j}, \sigma_{ij}, F_{\text{photon};i,j} \right) + \sum_{i=1}^{23} L_{\gamma} \left( E_{\gamma;n}, \sigma_{\gamma}, w_i F_{\gamma;m} \right).$$

(2.10)

(2.11)

The flux normalisation $F_{\gamma}$ corresponding to the $i$th data set in the alternative hypothesis model $m_1$ is weighted by the factor

$$w_i = \frac{S_{\text{NFW};i} \cdot t_{\text{net}}^{\text{exp};i} \cdot \Omega_{\text{net};\text{fov};i}}{\sum_{k=1}^{23} \left( S_{\text{NFW};k} \cdot t_{\text{net}}^{\text{exp};k} \cdot \Omega_{\text{net};\text{fov};k} \right)}, \quad \sum_{i=1}^{23} w_i = 1,$$

(2.12)

to take the NFW model-dependent dark matter column density $S_{\text{NFW};i}$, the field of view $\Omega_{\text{net};\text{fov};i}$ and the exposure $t_{\text{net}}^{\text{exp};i}$ of each individual observation into account. The weightings $w_i$ are listed in table 2 as well as table 3.

The additive component $L_{\gamma} \left( E_{\gamma;n}, \sigma_{\gamma}, w_i F_{\gamma;m} \right)$ has been fitted to every point $\left( E_{\gamma;n}, F_{\gamma;m} \right)$ in a two-dimensional parameter grid spanned by discrete values of the line energies $E_{\gamma;n}$ and the flux normalisations $F_{\gamma;m}$,

$$G_2 \left( n, m \right) = \begin{pmatrix}
(E_{\gamma;1}, F_{\gamma;m}) & \ldots & (E_{\gamma;n}, F_{\gamma;m}) \\
\vdots & \ddots & \vdots \\
(E_{\gamma;1}, F_{\gamma;1}) & \ldots & (E_{\gamma;n}, F_{\gamma;1})
\end{pmatrix},$$

(2.13)

while the width $\sigma_{\gamma}$ has been fixed at zero as described in section 2.4.1. The limits in the two dimensions of the grid $G_2$ range from $0.38$ keV to $12$ keV on a linear energy axis $E_{\gamma}$ and from a total flux of $10^{-9}$ photons cm$^{-2}$ s$^{-1}$ to $10^3$ photons cm$^{-2}$ s$^{-1}$ on a logarithmic axis $F_{\gamma}$. The resolution was set to $151 \times 151$ grid points, wherein the resulting energy resolution is approximately $76.95$ eV, which is slightly above the energy resolution of the PN-detector of about $80$ eV.

2.5 Statistical methods

The posterior predictive $p$-value analysis in combination with the application of the $F_B$-statistics [13] as test statistics, was applied as a hypothesis test to test whether the null hypothesis model $m_0$ or the alternative hypothesis model $m_1$ is favoured, dependent on the position in the grid $G_2$. It is important to notice that these two models have differing degrees of freedom ($\Delta\text{d.o.f.} = 2$). In order to compare the model $m_0$ with the model $m_1$ two conditions have to be fulfilled [14]:

1. The null hypothesis model $m_0$ and the alternative hypothesis model $m_1$ must be nested so that the set of parameter values of one of the models is a subset of the set of parameter values of the other model.

2. The minimum values of the parameters of the additive model component $L_{\gamma}$ are not allowed to lie on the boundary of the set of allowed parameter values.
The first condition is true for the models $m_0$ and $m_1$, but the second condition is not obviously matched because the physically allowed minimum value of the flux of the additive emission line is zero. The $F_{\text{Bevington}}$-statistics [13] is defined as

$$F_{\text{Bevington}} = F_B = \frac{\chi_0^2 - \chi_1^2}{\chi_1^2} \tag{2.14}$$

and represents a measure to discriminate whether the null hypothesis model $m_0$ and its measure of goodness-of-fit $\chi_0^2$ or the alternative hypothesis model $m_1$ and its measure of goodness-of-fit $\chi_1^2$ should be favoured, by computing the difference of $\chi_0^2$ and $\chi_1^2$ divided by the reduced $\chi_1^2$, which is defined as $\chi_1^2$ divided by its number of degrees of freedom $\nu_1$. The alternative hypothesis model $m_1$ will be preferred in the case of positive $F_B$-values ($\chi_0^2 > \chi_1^2$) and vice versa. Therefore, the $F_B$-statistics has been applied to test for an additional emission line, e.g. described by a Gaussian function dependent on the flux $F_{\gamma;m}$, the line width $\sigma_\gamma$ and and a line energy $E_{\gamma;n}$. Since the aforementioned second condition would not be fulfilled if the flux $F_{\gamma;m}$ of the additional emission line is equals zero, the $F_B$-statistics is per se not a valid test statistics in the present scenario. Nonetheless, the $F_B$-statistics can still be applied if embedded into the framework of the posterior predictive p-value analysis as further described in the following steps [14]:

1. $D = 500$ data sets are simulated from the null hypothesis model $m_0$ with the command ‘fakeit’ in XSPEC while using the original binning, effective areas, response matrices and background models.

2. The null hypothesis model $m_0$ and the alternative hypothesis model $m_1$ are simultaneously fitted to each of the $D$ simulated data sets and the corresponding $F_B$-values are calculated from the resulting $\chi_0^2$ and $\chi_1^2$ values [13], respectively.

3. The approximate q-value (defined as $q = 1 - p$, while $p$ being the p-value) of a grid point $(E_{\gamma;n}, F_{\gamma;m})$ with $n, m \in \{1, \ldots, 151\}$, is determined by adding up all $F_B$-values of the simulated $F_B$-distributions up to the measured $F_B$-value as

$$q(E_{\gamma;n}, F_{\gamma;m}) = 1 - \sum_{k=1}^{D=500} \text{Ind}(\frac{F_{\text{Monte-Carlo}}^B(E_{\gamma;n}, F_{\gamma;m}) > F_{\text{Measured}}^B(E_{\gamma;n}, F_{\gamma;m})}{D}). \tag{2.15}$$

The abbreviation “Ind” denotes the indicator function

$$\text{Ind}(F_{\text{Monte-Carlo}}^B(E_{\gamma;n}, F_{\gamma;m}) > F_{\text{Measured}}^B(E_{\gamma;n}, F_{\gamma;m})) = \begin{cases} 1, & \text{if } F_{\text{Monte-Carlo}}^B(E_{\gamma;n}, F_{\gamma;m}) > F_{\text{Measured}}^B(E_{\gamma;n}, F_{\gamma;m}), \\ 0, & \text{if } F_{\text{Monte-Carlo}}^B(E_{\gamma;n}, F_{\gamma;m}) \leq F_{\text{Measured}}^B(E_{\gamma;n}, F_{\gamma;m}). \end{cases} \tag{2.17}$$

The $\Delta \chi^2$-statistics was rejected as a hypothesis test in the present work because of its inherent mathematical issues in the context to test for additive model components.

### 2.6 Upper limits based on the $\Delta \chi^2$-statistics

The basic hypothesis which allows the application of the $\Delta \chi^2$-statistics is the existence of an additional component or an emission line $L_\gamma$ or, with other words, the acceptance of the alternative
hypothesis model $m_1$ formulated in the section 2.4.2. This includes that the additional emission line $L_{\gamma} (E_{\gamma;n}, \sigma_{\gamma_i}, w_i, F_{\gamma;m})$ exhibits a flux normalisation greater zero. The value of $\Delta \chi^2$ is defined as the difference between a $\chi^2$ value and a local minimum in the $\chi^2$ space, both contained in a $l$th region of a number of $N_l$, $l \in \{1, \ldots, N_l\}$ detected closed regions $C_l$ in which the null hypothesis model $m_0$ was rejected by the posterior predictive p-value analysis, such that a 90% confidence level has to fulfill the condition\(^\text{12}\)

$$\Delta \chi^2_l (E_{\gamma;n}, F_{\gamma;m})_{90\%} = \chi^2_l (E_{\gamma;n}, F_{\gamma;m}) - \min_l \left( \chi^2_l (E_{\gamma;n}, F_{\gamma;n}) \right) = 4.61. \quad (2.19)$$

Eventually, the resulting set of $\Delta \chi^2_l (E_{\gamma;n}, F_{\gamma;m})_{90\%}$-values has been evaluated to determine the 90% confidence limits of the same points in the grid $G_2 (n, m)$, namely $(E_{\gamma;n}, F_{\gamma;m})$, of the closed regions $C_l$ in which the null hypothesis model was rejected. The combined application of the posterior predictive p-value analysis as a hypothesis test for additional emission lines and, in case of a rejection of the null hypothesis model $m_0$, the successive determination of flux limits with help of the $\Delta \chi^2$-statistics, proved to be a powerful tool to uncover spectral emission lines.

### 2.7 Combined model-dependent upper limits

In some dark matter models, particles with a mass $m_{dm}$ are proposed which are theoretically allowed to undergo two-body-decays to generate X-ray photons with an energy of $E_{\gamma} = \frac{m_{dm}}{2}$ in natural units, with $m_{dm}$ being the mass of the dark matter particle [17, 18, 20]. The decay rate of such a process contains the decay width $\Gamma_{dm}$ as the inverse of the decay time and is defined as

$$\epsilon_{dm} = \frac{1}{4\pi} \frac{E_{\gamma} \Gamma_{dm}}{m_{dm}}. \quad (2.20)$$

The expected intensity $I_{dm}$ is the product of the decay measure and the model-dependent dark matter column density $S_{dm}$ which, moreover, is an integral of a dark matter density distribution $\rho_{dm}$ over the distance $s$:

$$I_{dm}(s) = \epsilon_{dm} S_{dm}(s) = \frac{\Gamma_{dm}}{8\pi} \int_0^{\infty} \rho_{dm}(s) ds. \quad (2.21)$$

The upper limits of the flux of both statistical methods applied in this work have been used to constrain the parameter spaces of two theoretically proposed dark matter particles, the sterile neutrino and the axion. Both particles are theoretically allowed to decay into X-ray photons. The decay rate of the Majorana sterile neutrino [18, 19] as a warm dark matter particle of mass $m_{\nu_s}$ is

$$\Gamma(\nu_R \rightarrow \gamma \nu_L) = \Gamma_{\nu_s} = \frac{9\alpha G_F^2}{16 \pi^4} \sin^2(2\Theta) m_{\nu_s}^5 \approx 1.38 \cdot 10^{-32} \text{s}^{-1} \left( \frac{\sin^2(2\Theta)}{10^{-10}} \right) \left( \frac{m_{\nu_s}}{\text{keV}} \right)^5, \quad (2.22)$$

with $\alpha$ being the fine structure constant and $G_F$ denotes the Fermi constant. The Dirac sterile neutrino would have half the decay rate of the Majorana sterile neutrino. The decay rate of an axion, which would be a cold dark matter particle [22, 37] with mass $m_\phi$ is

$$\Gamma(\phi \rightarrow \gamma \gamma) = \Gamma_{\phi} = \frac{64\pi}{g_{\phi \gamma \gamma}^2 m_\phi^3} \approx 7.69 \cdot 10^{-26} \text{s}^{-1} \left( \frac{g_{\phi \gamma \gamma}}{10^{-10} \text{GeV}^{-1}} \right)^2 \left( \frac{m_\phi}{\text{eV}} \right)^3. \quad (2.23)$$

\(^{12}\)See the Xspec Manual: https://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/manual/XspecSpectralFitting.html
The intensity $I_{dm}$ is composed of the flux $F_\gamma$ divided by the field of view $\Omega_{\text{fov}}^{\text{net}}$, while the energy flux is the product of the normalisation $F_\gamma$ (photons per cm$^2$ per s) of the additional emission line $L_\gamma$ and the energy of the line $E_\gamma$:

$$I_{dm} = E_\gamma \cdot F_\gamma \cdot (\Omega_{\text{fov}}^{\text{net}})^{-1}. \quad (2.24)$$

The upper limits for the mixing angle $\sin^2(2\Theta)$ of the sterile neutrinos are constrained via the mixing angle by

$$\sin^2(2\Theta) \leq \left( \frac{E_\gamma \cdot F_\gamma}{6.9 \cdot 10^4 \text{keV cm}^{-2} \text{s}^{-1}} \right) \left( \frac{S_{dm}}{10^{27} \text{keV cm}^{-2}} \right)^{-1} \left( \frac{\Omega_{\text{fov}}^{\text{net}}}{4\pi \text{str}} \right)^{-1} \left( \frac{m_{\nu_s}}{\text{keV}} \right)^{-5}. \quad (2.25)$$

The coupling of the axion is constrained by

$$g_{\phi \gamma \gamma}^2 \leq \left( \left( \frac{E_\gamma \cdot F_\gamma}{3.8 \cdot 10^{30} \text{keV cm}^{-2} \text{s}^{-1}} \right) \left( \frac{S_{dm}}{10^{27} \text{keV cm}^{-2}} \right)^{-1} \left( \frac{\Omega_{\text{fov}}^{\text{net}}}{4\pi \text{str}} \right)^{-1} \left( \frac{m_{\phi}}{\text{keV}} \right)^{-3} \right) \text{GeV}^{-2}. \quad (2.26)$$

The combined upper limits of the coupling $\sin^2(2\Theta)$ can be calculated from the combined upper limits of the flux normalisation $F_\gamma$. The total coupling between active and sterile neutrinos of $N = 23$ data sets dependent on a point $(E_{\gamma;n}, F_{\gamma;m})$ contained in the grid $G_2(n, m)$ is

$$\sin^2(2\Theta)_{\text{total}}(E_{\gamma;n}, F_{\gamma;m}) = \sum_{i=1}^{23} \left( \frac{w_i \cdot E_{\gamma;n} \cdot F_{\gamma;m}}{6.9 \cdot 10^4 \text{keV cm}^{-2} \text{s}^{-1}} \right) \left( \sum_{p=1}^{23} \left( \frac{S_{\text{NFW}p}}{10^{27} \text{keV cm}^{-2}} \cdot \frac{\Omega_{\text{fov}p}^{\text{net}}}{4\pi} \right)^{-1} \left( \frac{2E_{\gamma;n}}{\text{keV}} \right)^{-5} \right). \quad (2.27)$$

The very same procedure leads to the combined upper limit of the coupling constant of the axions:

$$g_{\phi \gamma \gamma, \text{total}}^2(E_{\gamma;n}, F_{\gamma;m}) = \left( \sum_{i=1}^{23} \left( \frac{w_i \cdot E_{\gamma;n} \cdot F_{\gamma;m}}{3.8 \cdot 10^{30} \text{keV cm}^{-2} \text{s}^{-1}} \right) \left( \sum_{p=1}^{23} \left( \frac{S_{\text{NFW}p}}{10^{27} \text{keV cm}^{-2}} \cdot \frac{\Omega_{\text{fov}p}^{\text{net}}}{4\pi} \right)^{-1} \left( \frac{2E_{\gamma;n}}{\text{keV}} \right)^{-3} \right) \text{GeV}^{-2}. \quad (2.28)$$

**2.7.1 Constraints on $F_\gamma$**

A q-value of 0.998$^{13}$ has been chosen to discriminate the parameter space of an additional emission line into regions in which the null hypothesis model $m_0$ is favoured, $(q \leq 0.998)$, and in which the alternative hypothesis model $m_1$ is preferred, $(q > 0.998)$. Figure 8 shows the results of the posterior predictive p-value analysis. The panel contains the q-values calculated by equation (2.16) for every parameter pair $(E_{\gamma;n}, F_{\gamma;m})$ of the additional emission line in the two-dimensional grid $G_2$ represented by the x-axis and the y-axis, respectively. The scaling of the colour coding is defined by the colour bar on the right side next to the panel. The contours $C_\gamma$ of a q-value of 0.998 are presented in the panel as red solid lines. A $\Delta \chi^2$-value of 4.61 is plotted for a comparison (orange curve). The emission line detected by [68] at an energy of $3.51 \pm 0.03 \text{keV}$ and a normalisation of $3.9^{+0.6}_{-1.0} \cdot 10^{-6} \text{cm}^{-2} \text{s}^{-1}$ is indicated by a green-coloured error bar.

**2.7.2 Constraints on $\sin^2(2\Theta)$ and $g_{\phi \gamma \gamma}$**

The upper limits of the publications Watson et al. [72], Malyshev et al. [63], and Horiuchi et al. [69], represent a 95% confidence level with regard to a Monte-Carlo-generated distribution, a 90% confidence level, and a 90% confidence level or $\Delta \chi^2 = 4.61$, respectively. The plotted upper limits

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$^{13} q = 1 - \frac{1}{5} = 1 - \frac{1}{m} = 0.998.$
Figure 8. As the result of the posterior predictive p-value analysis, the q-values and the combined $q = 0.998$ confidence regions (red curve), on the grid $G_2$ for every parameter pair $(E_\gamma, m)$ of the additional Gaussian emission line $L_\gamma$, are plotted in this figure. The energy regime ranges from 0.38 keV to 12 keV and the flux normalisation regime ranges from $10^{-9}$ photons cm$^{-2}$ s$^{-1}$ to $10^{3}$ photons cm$^{-2}$ s$^{-1}$. The colour coding and its related colour bar on the right next to the two-dimensional plot shows the level of the q-values. A $\Delta \chi^2$-value of 4.61 (90% confidence level) is plotted for a comparison. The emission line detected by [68] at an energy of $3.51 \pm 0.03$ keV and a normalisation of $3.9^{+0.6}_{-1.0} \cdot 10^{-6}$ cm$^{-2}$ s$^{-1}$ is indicated by an orange error bar.

of Abazajian et al. [20] and Adhikari et al. [21] are composed of superpositions of several upper limits which have specifically been taken from the publications [73, 75–77, 80–89] and [63, 69, 72–77, 80, 84, 86–88, 90–100], respectively. The emission line candidate is located at a photon energy of $3.51 \pm 0.03$ keV and features an active-sterile neutrino coupling of $6.7^{+1.7}_{-1.0} \cdot 10^{-11}$ cm$^{-2}$ s$^{-1}$. It is denoted by a green error bar in the plot 9 and 10, respectively.

2.8 Additional lines in the diffuse X-ray background

The most dominant contour features have centroids in the areas closed by the $q = 0.998$ contour regions $C_l$ with energies and normalisations presented in table 4. The most-likely physical origins are also listed in table 4. The $q = 0.998$ regions at 0.38 keV and above 10 keV are not closed and could be consequences of badly constrained fits because of low effective areas at this energies.

The authors of [68] claim an emission line at a photon energy of $3.51 \pm 0.03$ keV and a normalisation of $3.9^{+0.6}_{-1.0} \cdot 10^{-6}$ cm$^{-2}$ s$^{-1}$ in case of a non-frozen energy parameter during their fitting procedure.

\[ q = 0.998 \]

\[ \Delta \chi^2 = 4.61 \]

\[ q = 0.998 \]

\[ \text{Bulbul et al., 2014} \]
Figure 9. The $q = 0.998$ confidence regions of the active-sterile neutrino coupling $\sin^2(2\Theta)^{\text{total}}(E_{\gamma,n}, F_{\gamma,m})$ calculated from the $q = 0.998$ confidence regions of the total flux normalisation $F_\gamma$ in a sterile neutrino mass regime from 0.76 keV to 24 keV. The results of this work are compared to the upper limit results of the publications Watson et al. [72], Abazajian et al. [20], Malyshev et al. [63], Horiuchi et al. [69] and Adhikari et al. [21] as well as the detected emission line in [68]. The shaded regions are excluded. A $\Delta \chi^2$-value of 4.61 is plotted as a orange line for comparison. The emission line detected by [68] at an energy of 3.51 ± 0.03 keV and an active-sterile neutrino coupling of $6.7^{+1.7}_{-1.0} \cdot 10^{-11}$ cm$^{-2}$ s$^{-1}$ is indicated by a black error bar.

and a normalisation of $2.5^{+0.6}_{-0.7} \cdot 10^{-6}$ cm$^{-2}$ s$^{-1}$ for a fixed energy at 3.57 keV. The emission line is located in the $q \leq 0.998$ region of this work as shown in figure 9. In summary, our results do not show any hints towards the existence of a spectral emission line at the energy claimed by [68].

The centroids of $N_l = 12$ closed $q > 0.998$ confidence regions $C_l$ found within this work (see table 4) are located at energies which allow standard explanations of their physical origins. The most likely physical origins are also presented in table 4. The centroid energies above 10 keV can be explained by the small effective area of the detector in that energy regime and the consequential low constraints on the fit. The $q > 0.998$-regions $C_l$, in which the null hypothesis model $m_0$ is rejected, mostly overlap with the corresponding regions of the $\Delta \chi^2$-space in which a minimum $\Delta \chi^2_{\text{min},l}$ exists. The centroids of both regions corresponding to the two statistical methods used in this work have been listed in table 4. The 90%-errors of the centroids in the $\Delta \chi^2$-space have been computed along each of the axes $E_\gamma$ and $F_\gamma$ by searching for the closest values to a local minimum $\Delta \chi^2_{\text{min},l}$ of each region $C_l$ by fulfilling the condition

$$\Delta \chi^2_{90\%} = \Delta \chi^2_{\text{min},l} + 4.61.$$  

Unfortunately, it is not possible to resolve the photon fluxes of the centroids into the individual contributions of the 23 data sets involved in the analysis because of the joint fitting and the consequential unified statistical handling of the data sets.
The $q = 0.998$ confidence regions of the active-sterile neutrino coupling $g_{\phi\gamma\gamma,\text{total}}(E_{\gamma;n}, E_{\gamma;m})$ calculated from the upper limits of the total flux normalisation in an axion mass regime from 0.76 keV to 24 keV. The results of this work are compared with the detected emission line [68]. A $\Delta \chi^2$-value of 4.61 is plotted as a orange line for comparison. The emission line detected by [68] at an energy of $3.51 \pm 0.03$ keV is indicated by a black error bar.

3 Discussion

A new type of analysis of X-ray background spectra has been carried out to search for unknown astrophysical or dark matter dependent emission lines. The application of a more rigorous and tailored statistical method in form of the posterior predictive p-value analysis was part of this work. The instrumental background continuum model was built from the merger of all filter-wheel-closed (FWC) data of the PN-detector available up to the year 2013 and scaled and subtracted from the astrophysical spectra. The subtraction of the instrumental background spectrum has its drawback in increasing the errors of the counts per energy bin of the resulting spectrum because of the necessary propagation of errors. It is important to note that the FWC data set used in this analysis is a merger of several single data sets from observation dates distributed over the operating duration of the satellite XMM-Newton. Therefore, the utilised FWC spectrum represents a time average of the energy distribution of the instrumental background. Unfortunately, the corner spectra were not applicable due to low numbers of counts because of the small chip area involved and additional instrumental emission lines which are not present in the field of view spectra. An alternative method would have been the combined fitting of the spectra by astrophysical and instrumental models in a single step. It is important to note that the instrumental model would not be allowed to be folded by the response matrix during the fitting process in such a scenario.

The results presented here were also achieved by the posterior predictive p-value analysis proposed by [14] which is well fitted to find confidence regions in parameter spaces of additional model.
components by the exertion of an hypothesis test. This allows to probe the parameter space of an additive component like a Gaussian curve for unidentified emission lines in spectra. The confidence regions found in the energy-flux parameter space of an additional line have been transferred to two popular dark matter models, namely, the sterile neutrino and the axion, both under the assumption of the NFW dark matter halo distribution.

The application of the posterior predictive p-value analysis as an hypothesis test to find regions in the parameter space which favour the alternative model \( m_1 \) unveiled several emission lines, having origins that can be explained by astrophysical or instrumental origins. Nonetheless, the incorporation of further data sets of additional astrophysical objects should be undertaken in the future to gain more confidence in the exclusion of parameter spaces of the aforementioned dark matter models.

### 4 Conclusion

In summary our search for unknown emission lines in the diffuse X-ray background exceeds previous searches. We did not find new lines, in particular the famous 3.55 keV line has not been seen. Notably, it has been shown that the posterior predictive p-value analysis can be successfully applied to scan parameter spaces of alternative hypothesis models incorporating additive components. The application of this method is not restricted to the X-ray regime but quite the contrary. Future ap-

| Posterior predictive p-value | \( \Delta \chi^2 \) | Physical origin |
|-----------------------------|-----------------|-----------------|
| \( E_{\gamma} \) | 10\(^{-4}\) cm\(^{-2}\) s\(^{-1}\) | \( E_{\gamma} \) | 10\(^{-4}\) cm\(^{-2}\) s\(^{-1}\) | \( \Delta \chi^2 \) |
| keV | | keV | | |
| 1.07 | 0.000590 | - | - | - | Ne X/Na-K\(_o\) |
| 1.85 | 0.000304 | - | - | - | Si-K, instrumental |
| 2.01 | 0.000687 | - | - | - | Al XIII and/or Si XIV |
| 2.54 | 0.918683 | 2.47\(^{+0.07}_{-0.10}\) | 0.21\(^{+0.10}_{-0.11}\) | -16.6 | S XV at 2.45 keV |
| 3.26 | 0.000619 | - | - | - | Ar XVIII at 3.31 keV |
| 5.88 | 0.166257 | 5.88\(^{+0.05}_{-0.02}\) | 0.17\(^{+0.10}_{-0.11}\) | -11.8 | Mn, instrumental line |
| 6.77 | 0.366257 | 6.81\(^{+0.42}_{-0.21}\) | 0.14\(^{+0.14}_{-0.13}\) | -6.0 | Fe XXV at 6.7 keV |
| - | - | 7.04\(^{+0.10}_{-0.11}\) | 0.21\(^{+0.12}_{-0.15}\) | -8.0 | Influence of iron K-edge at 7.04 keV |
| 7.81 | 0.645020 | 7.82\(^{+0.04}_{-0.05}\) | 0.30\(^{+0.28}_{-0.28}\) | -5.4 | Ni XXVII at 7.79 keV |
| 8.35 | 0.007506 | - | - | - | Residuals of Zn-K\(_o\) and Cu-K\(_o\), instrumental |
| 9.17 | 0.003528 | - | - | - | Au, instrumental |
| 9.53 | 0.008391 | - | - | - | Residual of Zn-K\(_o\), instrumental |
| 10.89 | - | 10.14\(^{+0.15}_{-0.11}\) | 0.91\(^{+0.62}_{-0.49}\) | -14.1 | - |
| 10.89 | - | 10.52\(^{+0.11}_{-0.09}\) | 1.32\(^{+0.71}_{-0.66}\) | -17.5 | - |
| 10.89 | - | 10.92\(^{+0.09}_{-0.04}\) | 1.91\(^{+1.05}_{-0.76}\) | -24.0 | - |
| 11.30 | - | 11.38\(^{+0.34}_{-1.37}\) | 1.32\(^{+1.25}_{-1.27}\) | -5.0 | - |
| 11.57 | - | 11.40\(^{+0.26}_{-1.45}\) | 1.32\(^{+1.42}_{-1.27}\) | -5.0 | - |

*Table 4.* The table lists the centroidal energies \( E_{\gamma} \) and normalisations \( F_{\gamma} \) of closed \( q = 0.998 \) and \( \Delta \chi^2 = 4.61 \) contour regions \( C_1 \) as well as the possible physical origins. Only regions with \( \Delta \chi^2 \)-values equal or lower than zero have been taken into account.
applications of this method have the potential to efficiently uncover parameter regions of additional components worthy to be the target of further researches.

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