Chapter 1
High-resolution spectral analysis

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Abstract SPEX[1] is an X-ray spectral fitting package that is optimised for analysing high-resolution astrophysical X-ray spectra observed by the current (e.g., XMM-Newton, Chandra) and future (e.g., XRISM, Athena, HUBS) X-ray observatories. Since the 1970s, SPEX code and its large atomic database have been continuously developed at SRON Netherlands Institute for Space Research[2]. At the time of writing, the latest version of SPEX is 3.07.01 that was released in August 2022 [8]. SPEX provides plasma models in different conditions, such as collisional ionisation equilibrium and photoionisation equilibrium, which can well describe the plasma properties in various kinds of astrophysical environments. This chapter will provide some basic commands and threads to fit high-resolution X-ray spectra of a nearby Seyfert 1 galaxy under the photoionisation equilibrium with SPEX.

Note:
The goal of this chapter is to setup the pion model (a photoionisation equilibrium model) for the soft X-ray absorption features in a nearby (z = 0.00386) Seyfert 1 galaxy observed with XMM-Newton observations (EPIC-pn and RGS). A simulated spectrum was used because this thread merely intends to show the setup of the pion model.

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[1] The user can download different versions of SPEX software from SPEX Zenodo page (https://doi.org/10.5281/zenodo.1924563) and install the entire program following the instructions in SPEX GitHub page (https://spex-xray.github.io/spex-help/getstarted/install.html).

[2] https://www.sron.nl

1.1 Introduction

Active galactic nuclei (AGN) accrete matter onto a central supermassive black hole (SMBH) to produce intense broadband radiation, which can ionise and drive away the surrounding matter in form of outflows, such as warm ionised and cold molecular outflows [6]. Many observational proofs have implied that outflows might play an important role in affecting the star formation, evolution, and even environment of their host galaxies, also known as AGN feedback [9]. Therefore, investigating properties of outflows might significantly help us to understand the formation of AGN outflows and their feedback efficiency to the host galaxy.

Warm absorbers (WAs) [5, 1] are one type of warm ionised outflows [13], which can be detected via absorption features along the line of sight in the ultraviolet (UV) and soft X-rays [14]. WAs have the outflow velocities from about one hundred to several thousand km s^{-1} [7, 3] and they might originate in the accretion disk [4, 11], broad line region (BLR) [16, 20], or dusty torus [10, 2]. Until now, WAs have been found in about 50% of nearby AGN [17, 19, 12].

`SPEX` is an X-ray spectral fitting package that is optimised for analysing high-resolution astrophysical X-ray spectra observed by the current and future X-ray observatories. Currently, `SPEX` is the only code that allows for the spectral energy distribution (SED) and the ionisation balance to be fitted simultaneously, while all other codes have to pre-calculate the ionization balance on a given SED. The `pion` model of `SPEX` is a robust and self-consistent photoionisation code that can simultaneously calculate the thermal/ionisation balance and the plasma spectrum in the photoionisation equilibrium. In addition, `SPEX` has a large atomic database that has been continuously developed at SRON Netherlands Institute for Space Research since 1970s. These characteristics make `SPEX` a powerful tool to study the physical properties of plasma in different astrophysical conditions. In this chapter, for the high-resolution X-ray spectra of a nearby Seyfert 1 galaxy, we aim to use `SPEX` to simultaneously fit the continuum spectra and the absorption features caused by WAs (described by the `pion` model) to obtain relevant physical parameters.

1.2 Preparation

The user can use the following two methods to convert OGIP spectra and response files into `SPEX` format:

- The `trafo`[3] program in `SPEX` software, which asks questions interactively;
- The `ogip2spex`[4] script of the `SPEX` Python tools (`pyspextools`[5]), which works with command-line arguments to gather all the input and is easy for scripting.

[3] https://spex-xray.github.io/spex-help/getstarted/runtrafo.html?highlight=trafo

[4] https://spex-xray.github.io/pyspextools/tutorials/ogip2spex.html

[5] https://spex-xray.github.io/pyspextools/

To follow the thread in this chapter, the user can download the example files (simulated_PN.spo, simulated_PN.res, simulated_RGS.spo, simulated_RGS.res) here[6]. The user can also make all the following analysis through `Pyspex`[7] module which offers a Python interface to the `SPEX` program.

1.3 Start `SPEX`

Start `SPEX` in a linux terminal window:

```
user@linux: > spex
Welcome user to SPEX version 3.07.01

NEW in this version of SPEX:
02-08-2022 Fixed issue with optimal binning

Currently using SPEXACT version 2.07.00. Type 'help var
calc' for details.
SPEX>
```

1.4 Load data

Use `data`[8] command to load the spectra and response files of EPIC-pn and RGS data for a nearby (z = 0.00386) Seyfert 1 galaxy:

```
SPEX> data simulated_PN simulated_PN
SPEX> data simulated_RGS simulated_RGS
```

1.5 Plot data and save the plotting

Use `plot`[9] command to open the graphic device xs (xserver) and plot the data that are loaded in Section 1.4 on this device:

[6] https://doi.org/10.5281/zenodo.7241267
[7] https://spex-xray.github.io/spex-help/pyspex.html
[8] https://spex-xray.github.io/spex-help/reference/commands/data.html
[9] https://spex-xray.github.io/spex-help/reference/commands/plot.html

```
SPEX> plot dev xs
SPEX> plot type data
```

Set the x-axis plot in the unit (`ux`) of keV, on a log scale (`log`), and ranging (`rx`) from 0.3 to 13 keV:

```
SPEX> plot ux kev
SPEX> plot x log
SPEX> plot rx 0.3:13
```

Set the y-axis plot in the unit (`uy`) of Counts s^{-1} $Å^{-1}$, on a linear scale (`lin`), and ranging (`ry`) from 0 to 25 Counts s^{-1} $Å^{-1}$:

```
SPEX> plot uy fa
SPEX> plot y lin
SPEX> plot ry 0:25
```

Use `ignore`[10] command to ignore the data set below 2 keV and above 12 keV for instrument 1 (EPIC-pn here), and ignore the data set above 2 keV for instrument 2 (RGS here):

```
SPEX> ignore instrument 1 0:2 unit kev
SPEX> ignore instrument 1 12:100 unit kev
SPEX> ignore instrument 2 2:100 unit kev
```

Optically bins (`obin`[11] command) the data channels 1:10000 for instrument 1 (EPIC-pn here), and bins (`bin`[12] command) the data channels 1:10000 by a factor of 4 for instrument 2 (RGS here):

```
SPEX> obin instrument 1 1:10000
SPEX> bin instrument 2 1:10000 4
```

Set the plot with data line weight (`lw`) of 3 and without displaying subtracted background (`back`), the plot identification (`cap id`), the upper title text (`cap ut`), and the lower title text (`cap lt`):

[10] https://spex-xray.github.io/spex-help/reference/commands/ignore.html
[11] https://spex-xray.github.io/spex-help/reference/commands/obin.html
[12] https://spex-xray.github.io/spex-help/reference/commands/bin.html

```
SPEX> plot set all
SPEX> plot data lw 3
SPEX> plot back disp f
SPEX> plot cap id disp f
SPEX> plot cap ut disp f
SPEX> plot cap lt disp f
```

Set the data colour (`data col`) of instrument 1 (EPIC-pn here) to blue:

```
SPEX> plot set 1
SPEX> plot data col 4
```

Finally, refresh the plot (see Figure 1.1):

```
SPEX> plot
```

The user can open a colour postscript graphics device and save the output file to data.ps:

```
SPEX> plot dev cps data.ps
SPEX> plot
SPEX> plot close 2
```

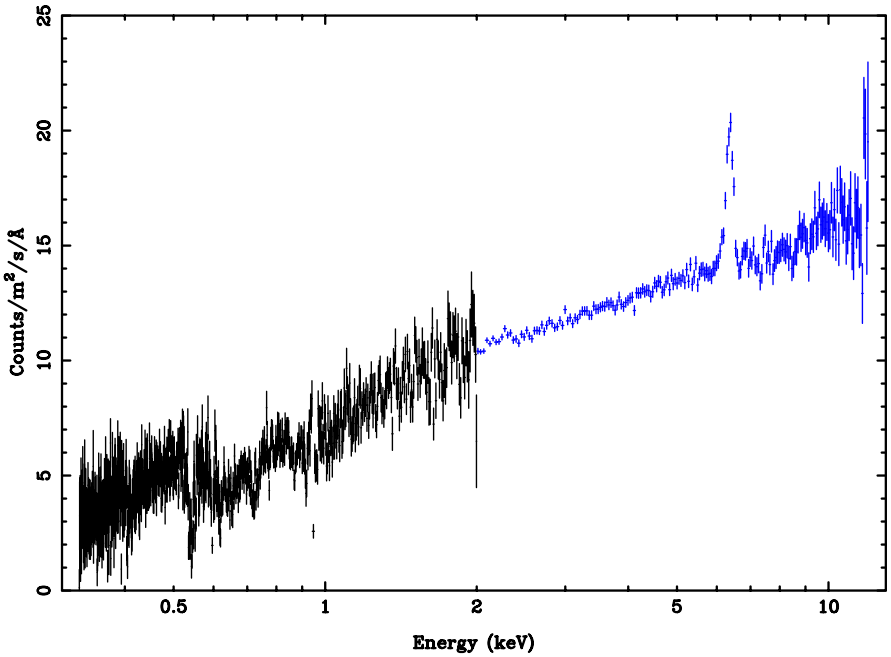

Fig. 1.1: The data spectra. *Black points:* XMM-Newton/RGS. *Blue points:* XMM-Newton/EPIC-pn.

1.6 Define model components and component relations (step-by-step)

Here we are looking at the components in this Seyfert 1 galaxy. For a typical Seyfert 1 galaxy, the spectral-energy-distribution (SED) of the intrinsic continuum above the Lyman limit along our line-of-sight has three components [15, 20] (see Figure 1.2):

- A Comptonised disk component (`comt`: comptonisation model) for optical to soft X-ray data, which is produced by the accretion disk radiation,
- A power-law component (`pow`: power law model) for X-ray data, which is produced by Comptonisation of optical/UV disk photons by a corona of hot electrons,
- A neutral reflection component (`refl`: reflection model) for hard X-rays data, which is produced by the reprocessing of the X-ray photons from the corona by the molecular torus, the BLR, and the disk.

This intrinsic continuum represents the central radiation of this galaxy. However, we cannot directly observe this intrinsic continuum. Because before arriving at the observer, the intrinsic continuum will pass through various types of gases in itself (such as WAs), be redshifted, and then pass through the interstellar medium in our

Milky Way (see Figure 1.2; in some cases, it will experience more complex physical processes). This long journey will be represented as the multiple absorption features on the continuum. Next we will define the model components to describe the spectra in order to trace these physical processes.

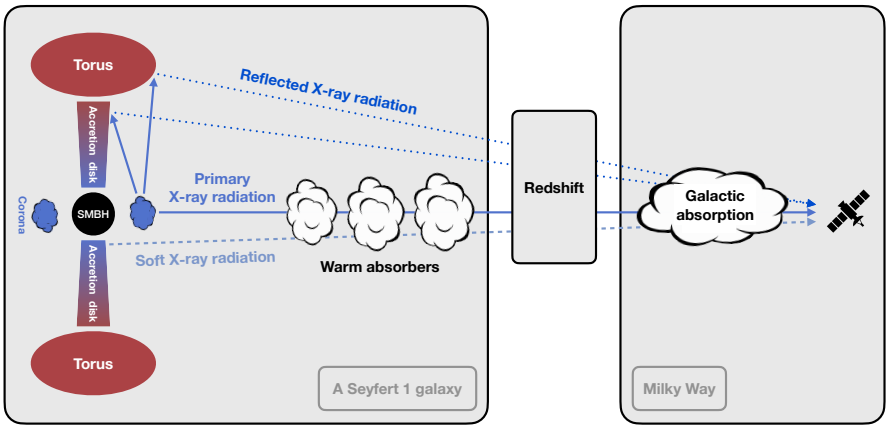

Fig. 1.2: Cartoon of the X-ray radiation from the central region of a typical Seyfert 1 galaxy to the observer (not to scale). Here three WA components are shown and numbers of them will vary in different cases.

1.6.1 Set the distance of the source

The distance of the source must be set in order to calculate the flux received at Earth. The user can specify the distance in a number of different units (please see details here[13]). Here we use redshift (parameter `z` in the following):

```
SPEX> distance 0.00386 z

Distances assuming H0 = 70.0 km/s/Mpc, Omega_m = 0.300 Omega_Lambda = 0.700 Omega_r = 0.000
Sector        m       A.U.         ly         pc        kpc       Mpc  redshift      cz    age(yr)
-------------------------------------------------------------------------------------------------
1     5.116E+23  3.420E+12  5.408E+07  1.658E+07  1.658E+04  16.5808    0.0039  1157.2  5.377E+07
-------------------------------------------------------------------------------------------------
```

[13] https://spex-xray.github.io/spex-help/reference/commands/distance.html

1.6.2 Set the redshift component

The user can use `com`[14] command to add `reds`[15] model in order to apply a redshift effect. Next we use `par`[16] command to set its redshift (`z`) value (`val`) to be 0.00386.

```
SPEX> com reds
You have defined    1 component.
SPEX> par 1 1 z val 0.00386
```

1.6.3 Set the galactic absorption

The radiation from the source will pass through the neutral gas in our Milky Way, which will produce absorption features in the X-ray spectra. In SPEX, these absorption features can be described by the `hot`[17] model. This model calculates the transmission of a plasma in the collisional ionisation equilibrium with cosmic abundances.

We set the hydrogen column density (`nh`) value of the plasma to be 2.07×10^{-4} (in the unit of 10^{28} m^{-2}) and set its electron temperature (`t`) value to be 5×10^{-4} (in the unit of keV). We make the state (`stat`) of `nh` and `t` being frozen (`f`) in the fit, which means that they will not be fitted in the fit:

```
SPEX> com hot
You have defined 2 components.
SPEX> par 1 2 nh val 2.07e-4
SPEX> par 1 2 t val 5e-4
SPEX> par 1 2 t stat f
SPEX> par 1 2 nh stat f
```

[14] https://spex-xray.github.io/spex-help/reference/commands/component.html
[15] https://spex-xray.github.io/spex-help/models/reds.html
[16] https://spex-xray.github.io/spex-help/reference/commands/par.html
[17] https://spex-xray.github.io/spex-help/models/hot.html

1.6.4 Set the SED

As we mentioned in Section 1.6, the SED of this source has three components: a Comptonised disk component (`comt`[18] model), a power-law component (`pow`[19] model), and a neutral reflection component (`refl`[20] model)

We set the normalisation (`norm`) value of the power-law component to be 4.5×10^6 (in the unit of 10^{44} photon s^{-1} keV^{-1}) and set the photon index (`gamm`) value to be 1.88. We make the state of `norm` and `gamm` being free (`t`) in the fit:

```
SPEX> com pow
You have defined 3 components.
SPEX> par 1 3 norm val 4.5e6
SPEX> par 1 3 gamm val 1.88
SPEX> par 1 3 norm stat t
SPEX> par 1 3 gamm stat t
```

We set the cut-off energy (`ecut`) value of the ionising spectrum to be 300 (in the unit of keV), set the value of parameters from the incoming power law (`pow`) to Full general relativity used (`fgr`) to be 0 (make these components not working), and set the scale for reflection (`scal`) value to be 0.68. We make the `ecut` state being frozen and make the `scal` state being free in the fit. We couple (`couple`) the `norm` and `gamm` of the `refl` component to those of the `pow` component, which means that these two parameters of these two components will be simultaneously fitted:

```
SPEX> com refl
You have defined 4 components.
SPEX> par 1 4 ecut val 300
SPEX> par 1 4 pow:fgr val 0
SPEX> par 1 4 scal val 0.68
SPEX> par 1 4 ecut stat f
SPEX> par 1 4 scal stat t
SPEX> par 1 4 norm couple 1 3 norm
SPEX> par 1 4 gamm couple 1 3 gamm
```

We set the normalisation (`norm`) value of the `comt` component to be 10^{10} (in the unit of 10^{44} photon s^{-1} keV^{-1}), set the seed photons temperature (`t0`) value to be 0.01 (in the unit of keV), set the plasma temperature (`t1`) value to be 0.06 (in the unit of keV), and set the optical depth (`tau`) value to be 30. We make the state of these parameters being free in the fit:

[18] https://spex-xray.github.io/spex-help/models/comt.html
[19] https://spex-xray.github.io/spex-help/models/pow.html
[20] https://spex-xray.github.io/spex-help/models/refl.html

```
SPEX> com comt
You have defined 5 components.
SPEX> par 1 5 norm val 1.0e10
SPEX> par 1 5 t0 val 0.01
SPEX> par 1 5 t1 val 0.06
SPEX> par 1 5 tau val 30
SPEX> par 1 5 norm stat t
SPEX> par 1 5 t0 stat t
SPEX> par 1 5 t1 stat t
SPEX> par 1 5 tau stat t
```

1.6.5 Apply an exponential cut-off to the power-law

Use `etau`[21] model to apply exponential cut-offs to the power-law component of the SED both below the low-energy cut-off and above the high-energy cut-off. The low-energy cut-off is related to the Lyman limit, while the high-energy cut-off is related to the temperature and optical depth of the plasma of hot electrons in corona. For `etau` model, the spectrum has a high-energy cut-off with $a > 0$, while it has a low-energy cut-off with $a < 0$, and for $a = 0$ the transmission is flat. The larger the value of a, the sharper the cut-off is.

We set the index (`a`) value of the first `etau` component to be 1 in order to make this component becoming a high-energy cut-off. We set the optical depth (`tau0`) value to be 3.2361×10^{-3} in order to make the high-energy cut-off energy being around 300 keV. We make the state of `a` and `tau0` being frozen:

```
SPEX> com etau
You have defined 6 components.
SPEX> par 1 6 a val 1
SPEX> par 1 6 tau0 val 3.2362e-3
SPEX> par 1 6 a stat f
SPEX> par 1 6 tau0 stat f
```

We set the index (`a`) value of the second `etau` component to be -1 in order to make this component becoming a low-energy cut-off. We set the `tau0` value to be 1.3605×10^{-2} in order to make the low-energy cut-off energy being 0.0136 keV (Lyman limit). We make the state of `a` and `tau0` being frozen:

[21] https://spex-xray.github.io/spex-help/models/etau.html

```
SPEX> com etau
You have defined 7 components.
SPEX> par 1 7 a val -1
SPEX> par 1 7 tau0 val 1.3605e-2
SPEX> par 1 7 a stat f
SPEX> par 1 7 tau0 stat f
```

1.6.6 Set the `pion` (absorption) components

We think that there are three WA components in this system, therefore we introduce three `pion`[22] components (`pion`: `SPEX` photoionised plasma model) to model the warm absorber outflows. The `pion` model calculates the transmission and emission of a slab of photo-ionised plasma, where all ionic column densities are linked through a photo-ionisation model. **The `pion` model can self-consistently calculate the photo-ionisation equilibrium using the available plasma routines of `SPEX`.** The relevant parameter is the ionisation parameter $\xi = L/nr^2$ [18], where L is the source luminosity, n is the hydrogen density of the plasma and r is the distance of the plasma from the ionising source.

For the first WA component, we set the hydrogen column density (`nh`) value to be 2×10^{-2} (in the unit of 10^{28} m^{-2}), set the ionisation parameter (`xil`) value to be 3.3 (in the log scale; in the unit of W m), set the average systematic velocity (`zv`) value to be -1300 (in the unit of km s^{-1}), and set the root mean square velocity (`v`) value to be 20 (in the unit of km s^{-1}):

```
SPEX> com pion
You have defined 8 components.
** Pion model: take care about proper COM REL use!
** Check the manual in case of errors at:
https://spex-xray.github.io/spex-help/models/pion.html
SPEX> par 1 8 nh val 2.0e-2
SPEX> par 1 8 xil val 3.3
SPEX> par 1 8 zv val -1300
SPEX> par 1 8 v val 20
```

For the second WA component, we set the `nh` value to be 2.5×10^{-3} (in the unit of 10^{28} m^{-2}), set the `xil` value to be 2.5 (in the log scale; in the unit of W m), set the `zv` value to be -500 (in the unit of km s^{-1}), and set the `v` value to be 100 (in the unit of km s^{-1}):

[22] https://spex-xray.github.io/spex-help/models/pion.html

```
SPEX> com pion
You have defined 9 components.
** Pion model: take care about proper COM REL use!
** Check the manual in case of errors at:
https://spex-xray.github.io/spex-help/models/pion.html
SPEX> par 1 9 nh val 2.5e-3
SPEX> par 1 9 xil val 2.5
SPEX> par 1 9 zv val -500
SPEX> par 1 9 v val 100
```

For the third WA component, we set the `nh` value to be 2×10^{-3} (in the unit of 10^{28} m^{-2}), set the `xil` value to be -1.0 (in the log scale; in the unit of W m), set the `zv` value to be -100 (in the unit of km s^{-1}), and set the `v` value to be 200 (in the unit of km s^{-1}):

```
SPEX> com pion
You have defined 10 components.
** Pion model: take care about proper COM REL use!
** Check the manual in case of errors at:
https://spex-xray.github.io/spex-help/models/pion.html
SPEX> par 1 10 nh val 2.0e-3
SPEX> par 1 10 xil val -1.0
SPEX> par 1 10 zv val -100
SPEX> par 1 10 v val 200
```

We make the state of these four parameters of all the WA components (`8:10`) being free in the fit:

```
SPEX> par 1 8:10 nh stat t
SPEX> par 1 8:10 xil stat t
SPEX> par 1 8:10 zv stat t
SPEX> par 1 8:10 v stat t
```

1.6.7 Set the component relations for radiation along line-of-sight

As Figure 1.2 shows, photons from both the Comptonised disk and power-law components are screened by the warm absorber components at the redshift of the target, as well as the galactic absorption before reaching the detector. Photons from the neutral reflection component is assumed not to be screened by the warm absorber for simplicity. It is still redshifted and requires the galactic absorption.

We define the component relations (`com rel`[23]) according to the order from the source to the observer. For example, from the source to the observer, the power-law continuum will experience the following journey (see Figure 1.2): power-law continuum (component 3 defined before) → high-energy cut-off (component 6) → low-energy cut-off (component 7) → high-ionisation WA in this source (component 8) → mid-ionisation WA in this source (component 9) → low-ionisation WA in this source (component 10) → being redshifted (component 1) → interstellar medium in our Milky Way (component 2):

```
SPEX> com rel 3 6,7,8,9,10,1,2
SPEX> com rel 4 1,2
SPEX> com rel 5 8,9,10,1,2
```

Assuming that the WA components closer to the central engine are defined first (with a smaller component index), photons transmitted from the inner `pion` components are screened by all the outer `pion` components at the redshift of the target, as well as the galactic absorption before reaching the detector. The ionisation parameter of the WA component from the inner to the outer region usually decreases, which is the basis of defining the relations between different WA components:

```
SPEX> com rel 8 9,10,1,2
SPEX> com rel 9 10,1,2
SPEX> com rel 10 1,2
```

1.6.8 Check the model settings and calculate

We check the setting of the component relations. The following `model show`[24] command prints the currently-used spectral models to the screen that include all additive and multiplicative components.

[23] https://spex-xray.github.io/spex-help/reference/commands/component.html
[24] https://spex-xray.github.io/spex-help/reference/commands/model.html

```
SPEX> model show
-----------------------------------------------------
Number of sectors : 1
Sector: 1 Number of model components: 10
Nr. 1: reds
Nr. 2: hot
Nr. 3: pow [6,7,8,9,10,1,2 ]
Nr. 4: refl[1,2 ]
Nr. 5: comt[8,9,10,1,2 ]
Nr. 6: etau
Nr. 7: etau
Nr. 8: pion[9,10,1,2 ]
Nr. 9: pion[10,1,2 ]
Nr. 10: pion[1,2 ]
```

We check the setting of the free parameters and calculate the 1–1000 Ryd ionising luminosity which is usually used to calculate the ionisation state of plasma. For this, we need to set the energy band using `elim`[25]:

[25] https://spex-xray.github.io/spex-help/reference/commands/elim.html

```
SPEX> elim 1:1000 Ryd
Fluxes and luminosities will be calculated between
1.360570E-02 and 13.6057 keV
SPEX> calculate
SPEX> par show free

-----------------------------------------------------------------------------------------------------
sect comp mod  acro parameter with unit    value          status  minimum   maximum  lsec lcom lpar

   1    3 pow  norm Norm (1E44 ph/s/keV)   4500000.       thawn   0.0       1.00E+20
   1    3 pow  gamm Photon index           1.880000       thawn  -10.       10.

   1    4 refl scal Scale for reflection   0.6800000      thawn   0.0       1.00E+10

   1    5 comt norm Norm (1E44 ph/s/keV)   1.0000000E+10  thawn   0.0       1.00E+20
   1    5 comt t0   Wien temp (keV)        9.9999998E-03  thawn   1.00E-05  1.00E+10
   1    5 comt t1   Plasma temp (keV)      5.9999999E-02  thawn   1.00E-05  1.00E+10
   1    5 comt tau  Optical depth          30.00000       thawn   1.00E-03  1.00E+03

   1    8 pion nh   X-Column (1E28/m**2)   2.0000000E-02  thawn   1.00E-14  1.00E+20
   1    8 pion xil  Log xi (1E-9 Wm)       3.300000       thawn  -7.0       10.
   1    8 pion v    RMS Velocity (km/s)    20.00000       thawn   0.0       3.00E+05
   1    8 pion zv   Average vel. (km/s)   -1300.000       thawn  -1.00E+05  1.00E+05

   1    9 pion nh   X-Column (1E28/m**2)   2.4999999E-03  thawn   1.00E-14  1.00E+20
   1    9 pion xil  Log xi (1E-9 Wm)       2.500000       thawn  -7.0       10.
   1    9 pion v    RMS Velocity (km/s)    100.0000       thawn   0.0       3.00E+05
   1    9 pion zv   Average vel. (km/s)   -500.0000       thawn  -1.00E+05  1.00E+05

   1   10 pion nh   X-Column (1E28/m**2)   2.0000001E-03  thawn   1.00E-14  1.00E+20
   1   10 pion xil  Log xi (1E-9 Wm)      -1.000000       thawn  -7.0       10.
   1   10 pion v    RMS Velocity (km/s)    200.0000       thawn   0.0       3.00E+05
   1   10 pion zv   Average vel. (km/s)   -100.0000       thawn  -1.00E+05  1.00E+05

Instrument     1 region    1 has norm    1.00000E+00 and is frozen
Instrument     2 region    1 has norm    1.00000E+00 and is frozen
-----------------------------------------------------------------------------
Fluxes and rest frame luminosities between  1.36057E-02 and    13.606     keV

sect comp mod    photon flux  energy flux   nr of photons luminosity
                (phot/m**2/s)   (W/m**2)    (photons/s)         (W)
   1    3 pow    250.552      7.133011E-14  2.239087E+52  4.630977E+35
   1    4 refl   4.11401      4.715256E-15  1.381814E+49  1.542371E+34
   1    5 comt   24.2510      1.208219E-15  4.796796E+52  3.859213E+35
   1    8 pion   0.00000      0.00000       0.00000       0.00000
   1    9 pion   0.00000      0.00000       0.00000       0.00000
   1   10 pion   0.00000      0.00000       0.00000       0.00000

-----------------------------------------------------------------------------
Fit method        : Classical Levenberg-Marquardt
Fit statistic     : C-statistic
C-statistic       :       972.73
Expected C-stat   :       996.07 +/-        44.71
Chi-squared value :      1047.12
Degrees of freedom:         0
W-statistic       :       914.11
Contributions of instruments and regions:
  Ins   Reg    Bins      C-stat  Exp C-stat  Rms C-stat      chi**2      W-stat
    1     1     205      187.43      205.05       20.25      188.68      186.71
    2     1     788      785.30      791.02       39.86      858.44      727.40
```

After defining model components, it is quite important to use `calculate`[26] command to evaluate the current model spectrum. In addition, here we only show the

[26] https://spex-xray.github.io/spex-help/reference/commands/calculate.html

free parameters (`par`[27]) in the fit using `par show free` command and the user can use `par show` command to show all the parameters.

1.7 Show the plotting of data and model

According to the plot setting in Section 1.5 and models defined in Section 1.6, we can refresh the plot to simultaneously show data and model:

```
SPEX> plot
```

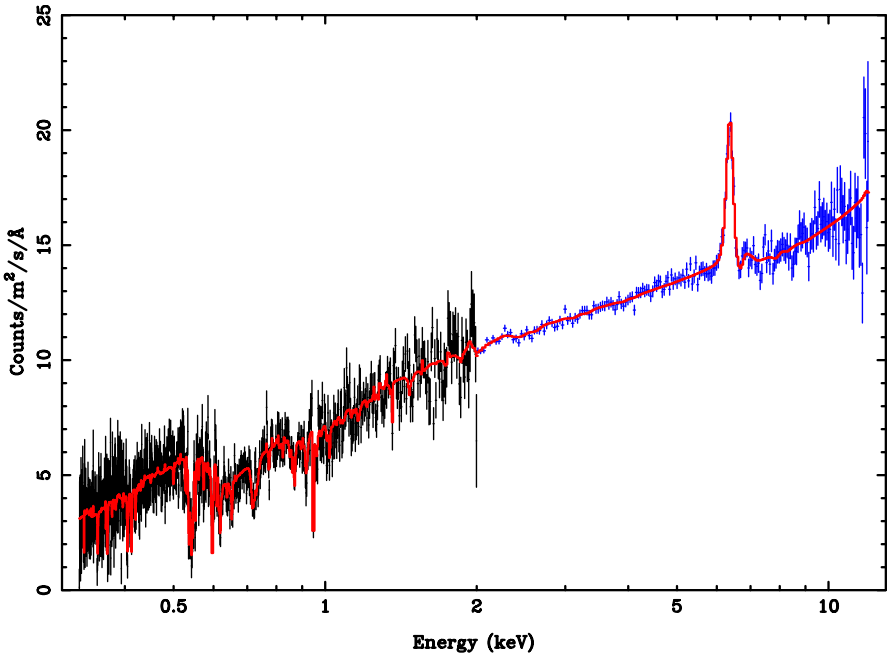

Fig. 1.3: The full data spectra with the best-fit model. *Black points*: XMM-Newton/RGS. *Blue points*: XMM-Newton/EPIC-pn. *Red solid curve*: the best-fit model.

Next we aim to check the absorption features in the soft X-ray band which are usually shown in the unit of Å:

[27] https://spex-xray.github.io/spex-help/reference/commands/par.html

```
SPEX> plot ux a
SPEX> plot x lin
SPEX> plot rx 5:39
SPEX> plot
```

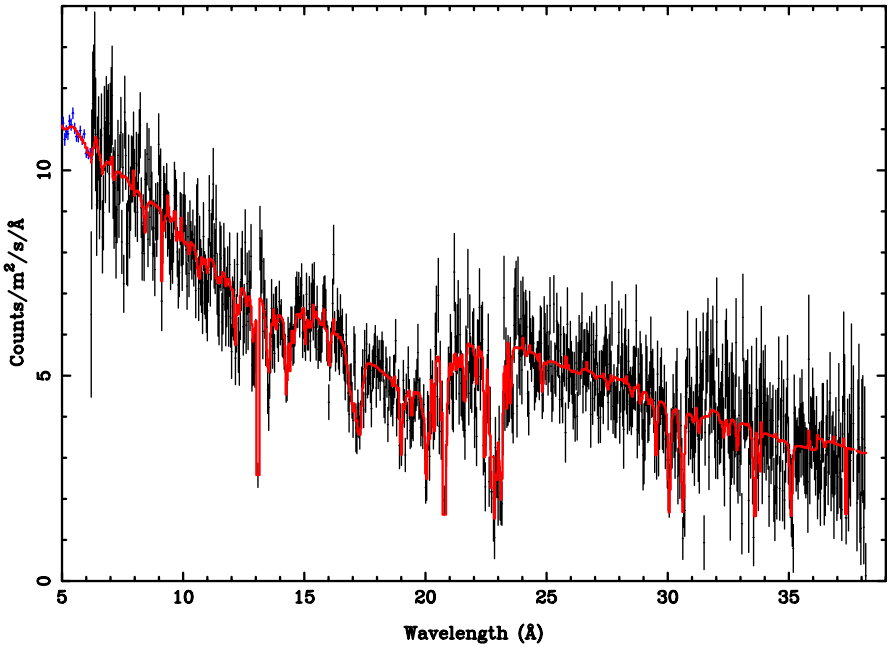

Fig. 1.4: The RGS spectra with the best-fit model. *Black points*: XMM-Newton/RGS. *Blue points*: XMM-Newton/EPIC-pn. *Red solid curve*: the best-fit model.

1.8 Check the properties of absorption lines and absorption edges

The properties (e.g., elements, stages, energies, equivalent widths, optical depths) of the absorption lines (shown in Figure 1.4) for the component 8 (the high-ionisation WA component) can be listed in the terminal screen using `ascdump`[28] command:

[28] https://spex-xray.github.io/spex-help/reference/commands/ascdump.html

```
SPEX> ascdump terminal 1 8 tral

line elem stage  Energy     Wavelength    Tau_0          EW            EW            Voigt a
                   (keV)          (Ang)                 (keV)         (Ang)
 759   Fe XXII   0.10712    115.75        4.2051         3.85446E-05   4.16502E-02   8.94509E-04
 760   Fe XXII   0.12475    99.389        0.88081        1.95927E-05   1.56101E-02   1.26834E-04
 550   Fe XX     0.13096    94.675        4.35724E-03    1.35269E-07   9.77926E-05   2.88913E-05
 551   Fe XX     0.13295    93.258        4.89333E-05    1.54372E-09   1.08287E-06   2.23606E-07
 277   Si XII    0.30276    40.951        2.79305E-03    2.45433E-07   3.31967E-05   2.96351E-03
 278   Si XII    0.30306    40.911        5.53082E-03    4.86056E-07   6.56145E-05   2.93412E-03
   9    C V      0.30790    40.268        1.91740E-03    2.35922E-07   3.08544E-05   4.20995E-03
 222   Mg X      0.31255    39.668        1.57774E-05    1.50299E-09   1.90753E-07   3.11122E-04
 221   Mg X      0.31255    39.668        3.16863E-05    3.02110E-09   3.83424E-07   3.12345E-04
 223   Mg X      0.32936    37.644        1.57210E-05    1.57768E-09   1.80320E-07   1.72276E-04
 252   Al XI     0.33800    36.682        1.33400E-05    1.32498E-09   1.43799E-07   8.43703E-04
 253   Al XI     0.33809    36.672        2.66722E-05    2.65278E-09   2.87734E-07   8.43457E-04
  10    C V      0.35452    34.973        3.62351E-04    5.13706E-08   5.06768E-06   1.05290E-03
  16    C VI     0.36747    33.740        0.43801        5.55453E-05   5.09989E-03   3.22985E-03
......
```

The properties (e.g., elements, shells, energies, equivalent widths, optical depths) of the absorption edges can be listed in the terminal screen:

```
SPEX> ascdump terminal 1 8 trac

ion and shell     Energy          Wavelength      Tau             EW              EW
                    (keV)           (Ang)                         (keV)           (Ang)
C  VI     1s     0.49000         25.303          7.38102E-04     2.13157E-07     1.10071E-05
N  VII    1s     0.66700         18.588          4.42054E-04     1.63087E-04     4.54501E-03
O  VII    1s     0.73930         16.770          3.87275E-05     1.71190E-05     3.88333E-04
O  VIII   1s     0.87140         14.228          5.90685E-03     2.86425E-03     4.67674E-02
Ne IX     1s      1.1958         10.368          4.96937E-05     1.78049E-06     1.54380E-05
Ne X      1s      1.3622         9.1018          3.20888E-03     2.43262E-03     1.62539E-02
Na XI     1s      1.6487         7.5201          8.32970E-05     2.43262E-03     1.10958E-02
Mg XI     1s      1.7618         7.0374          8.53158E-05     1.14050E-03     4.55564E-03
Mg XII    1s      1.9626         6.3173          2.09907E-03     1.69477E-04     5.45523E-04
Al XII    1s      2.0860         5.9436          1.54262E-05     1.71190E-05     4.87772E-05
Al XIII   1s      2.3041         5.3810          2.33232E-04     6.12695E-11     1.43090E-10
Si XIII   1s      2.4377         5.0861          3.76672E-04     3.22897E-08     6.73705E-08
Si XIV    1s      2.6731         4.6382          3.55321E-03     4.06117E-08     7.04672E-08
......
```

The user can save these outputs into a self-defined ascii-file or fits-file:

```
SPEX> ascdump file mydump 1 8 tral
SPEX> ascdump fits mydump.fits 1 8 tral
```

Note:

Except the properties of absorption lines and edges, the user can use command `ascdump` to check various spectral properties for any spectral component that uses the basic plasma code of SPEX, such as ionic concentrations, recombination rates, individual line fluxes, ionic column densities etc.

1.9 Check the fit residuals

The user can plot the fit residuals to check whether the model matches the data at different energies or whether extra absorption/emission features exist. Set the plot type to the fit residuals (`chi`) and plot the y-axis in the unit of "(Observed - Model) / Model" (`plot uy rel`):

```
SPEX> plot type chi
SPEX> plot ux kev
SPEX> plot uy rel
SPEX> plot x log
SPEX> plot y lin
SPEX> plot rx 0.3:12
SPEX> plot ry -0.5:0.5
SPEX> plot
```

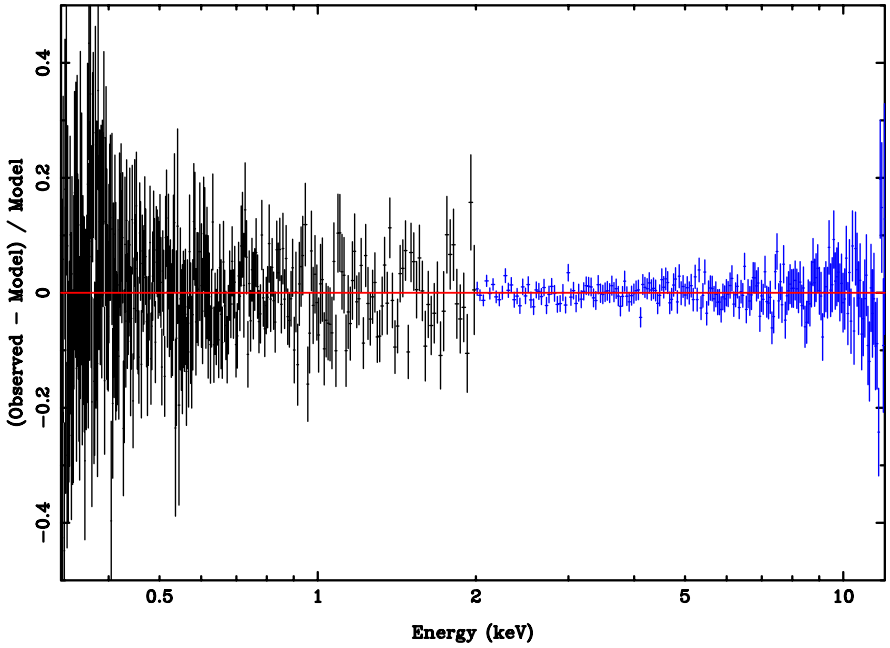

Fig. 1.5: The fit residuals. *Black points:* XMM-Newton/RGS. *Blue points:* XMM-Newton/EPIC-pn.

1.10 Check the model

When we set the plot type to data, the observed spectrum and the model can be shown simultaneously (see Section 1.7 and Figure 1.4). However, the model that is shown in this plot type is folded through the response matrix. Therefore, in order to show the model spectrum that is not convolved by any instrumental profile, the user can set the plot type to model (`plot type model` command).

1.10.1 Check the best-fit model

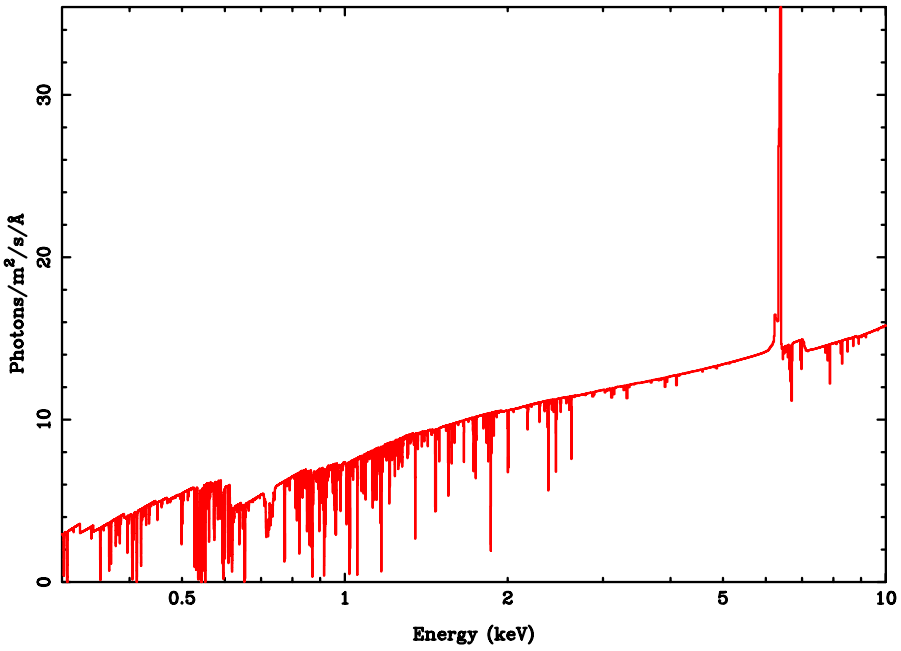

Fig. 1.6: The best-fit model in the plot type of model.

This best-fit model can be shown using the following commands:

```
SPEX> plot type model
SPEX> plot ux kev
SPEX> plot uy a
SPEX> plot x log
SPEX> plot y lin
SPEX> plot rx 0.3:10
SPEX> plot ry 0:40
SPEX> plot fill disp f
SPEX> plot
```

1.10.2 Check the intrinsic continuum model

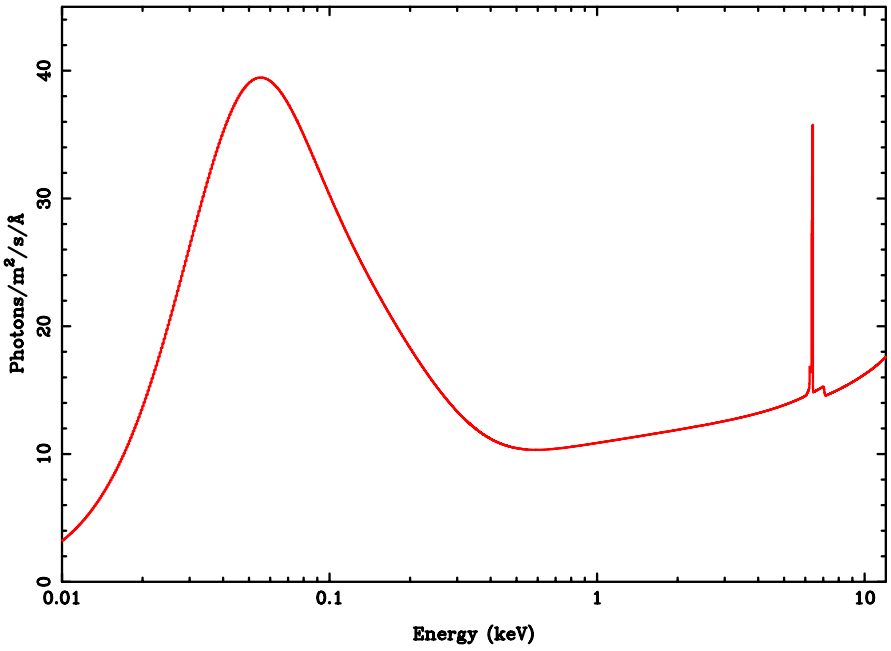

Fig. 1.7: The intrinsic continuum model.

In order to show this intrinsic continuum model, it is necessary to remove the effect from the warm absorbers and neutral gas in our Milky Way. Therefore, the user can set the "`fcov`" parameter to 0.0 (`fcov val 0.0`), which means that the plasma gas does not the cover the central radiation region (`fcov=1` means a full covering). It is more convenient than changing the normalisation of spectral models:

```
SPEX> par 1 2 fcov val 0.0
SPEX> par 1 8:10 fcov val 0.0
SPEX> calculate
SPEX> plot rx 0.01:12
SPEX> plot ry 0:45
SPEX> plot
```

1.11 Check the warm absorber components with different outflowing velocities

Sometimes the user needs to the check how much potential components with different outflowing velocities at a reference energy. It can be achieved in SPEX through plotting the x-axis in velocity units (km s^{-1}) with a reference energy provided (here is 20.062 Å that corresponds to the O IV absorption edge):

```
SPEX> plot type data
SPEX> plot ux vel 20.062 ang
SPEX> plot uy fa
SPEX> plot x lin
SPEX> plot y lin
SPEX> plot rx -3000:3000
SPEX> plot ry -1:9
```

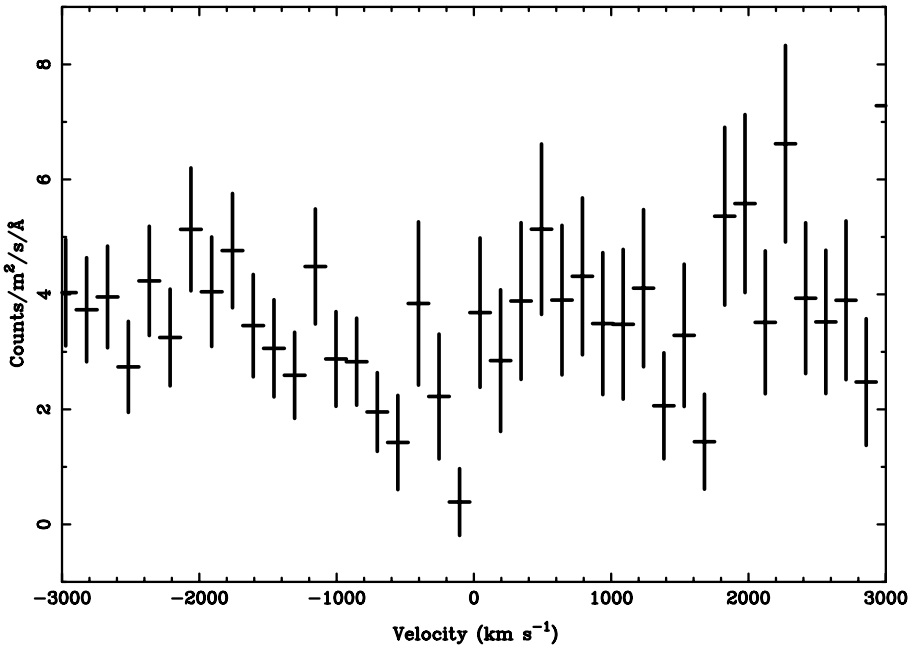

Fig. 1.8: The velocity spectrum at 20.062 Å.

1.12 Final remarks

This is the end of this analysis thread. If you want, you can quit SPEX now:

```
SPEX> quit
Thank you for using SPEX!
```

Below, we provide a useful command file.

1.12.1 running scripts

The user can save all the above commands of this thread to a self-defined file named **myrunning.com**. Then use log[29] to load the above command file into SPEX:

```
SPEX> log exe myrunning
```

[29] https://spex-xray.github.io/spex-help/reference/commands/log.html

1.13 Summary

In this chapter, we provide some commands and threads to analyse the high-resolution X-ray spectra of a typical Seyfert 1 galaxy with SPEX. Using SPEX, we could simultaneously fit the continuum radiation and the absorption features caused by warm absorber outflows to obtain relevant physical parameters. SPEX also provides some methods to check the physical properties of absorption lines and edges, and obtain the physical model, and to present the different outflowing components, etc. We cannot introduce all the commands and threads of SPEX in this chapter, so the reader could refer to SPEX GitHub page (https://spex-xray.github.io/spex-help/getstarted/install.html) to know more details about SPEX.

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