Implementation of Ionic processes in SKIRT

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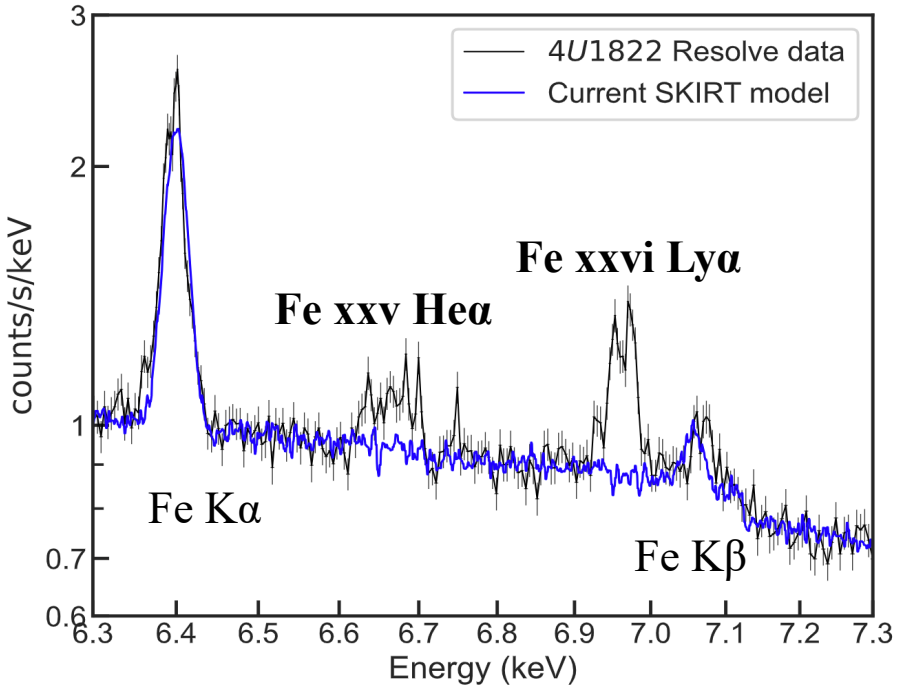
1. Introduction

- **Processes involving ions** have not yet been implemented in SKIRT.
- X-ray spectra of compact objects are rich in numerous features arising from **highly ionized ions.**



Resolve spectrum of a LMXB (4U1822-371) and a SKIRT model.

2-a. Scope

■ **Current status of ionic processes in SKIRT**

- Photo-absorption of all ions with Z=1-30 (Lauwers et al. in prep.).
- Fluorescence Kα_1 and Kα_2 lines of ions with the number of electrons $N \geq 5$ and Z=5-30 (Lauwers et al. in prep.).
- **Lyman-series lines of H-like ions (Sameshima et al. submitted).**

※Available only on the PR branch.

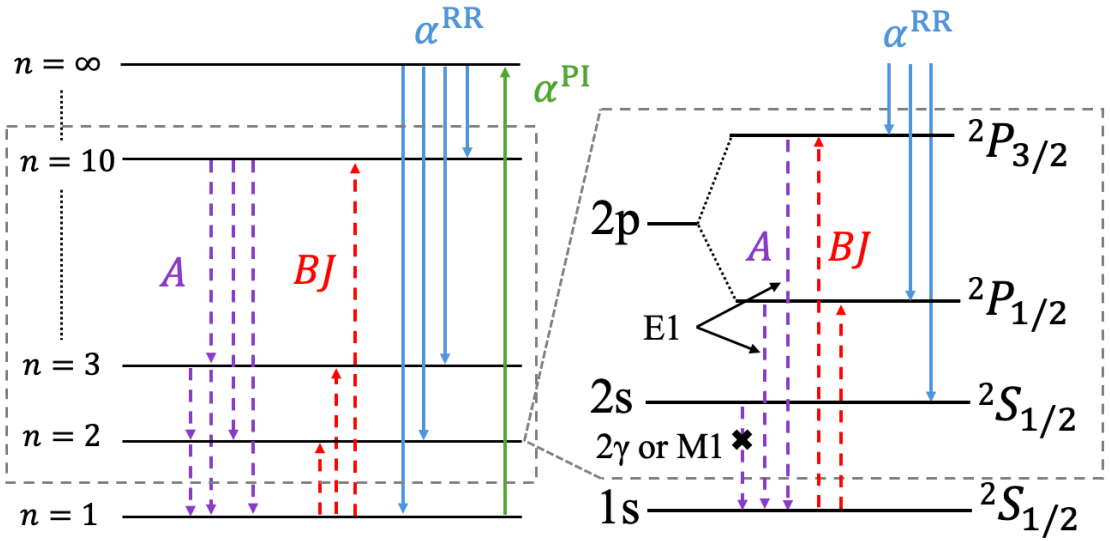
- He-like line complexes in progress (Sameshima et al. in prep.) .

■ **We focus on the Lyman-series lines of H-like ions.**

- Resonance scattering for Lyα line of H has been implemented in SKIRT (Camps et al. 2021).
- We make the following extensions:

1. Other elements up to $Z = 30$.
2. Higher Lyman series with $1 < n \leq 10$ levels.
3. Distinguish the fine-structure levels of Lyα_1 and Lyα_2.
4. Linear polarization.

2-b. Atomic processes

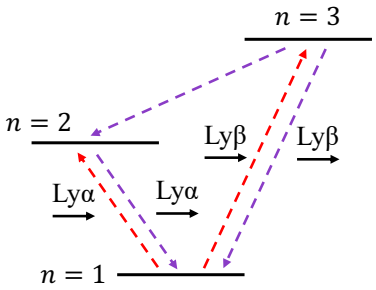


Levels and atomic processes considered in this implementation.

■ **Population processes:**

- Radiative recombination directly and in cascade through intermediate levels.
- Radiative excitation from the ground level.

※A fraction of Lyβ degrades to Lyα.



■ **De-population processes:**

- Radiative E1 transition for the excited levels.
- Two-photon decay (2γ) or M1 transition for the meta-stable levels.
- Photo-ionization from the ground level.

2-c. Formalism

- The rate equation for the density n_i of the the exicited level $i \in \{1,2,\dots,N\}$ at a steady-state condition is given by

$$\dot{\boldsymbol{n}} = \boldsymbol{\Gamma n} + \boldsymbol{S} = 0$$

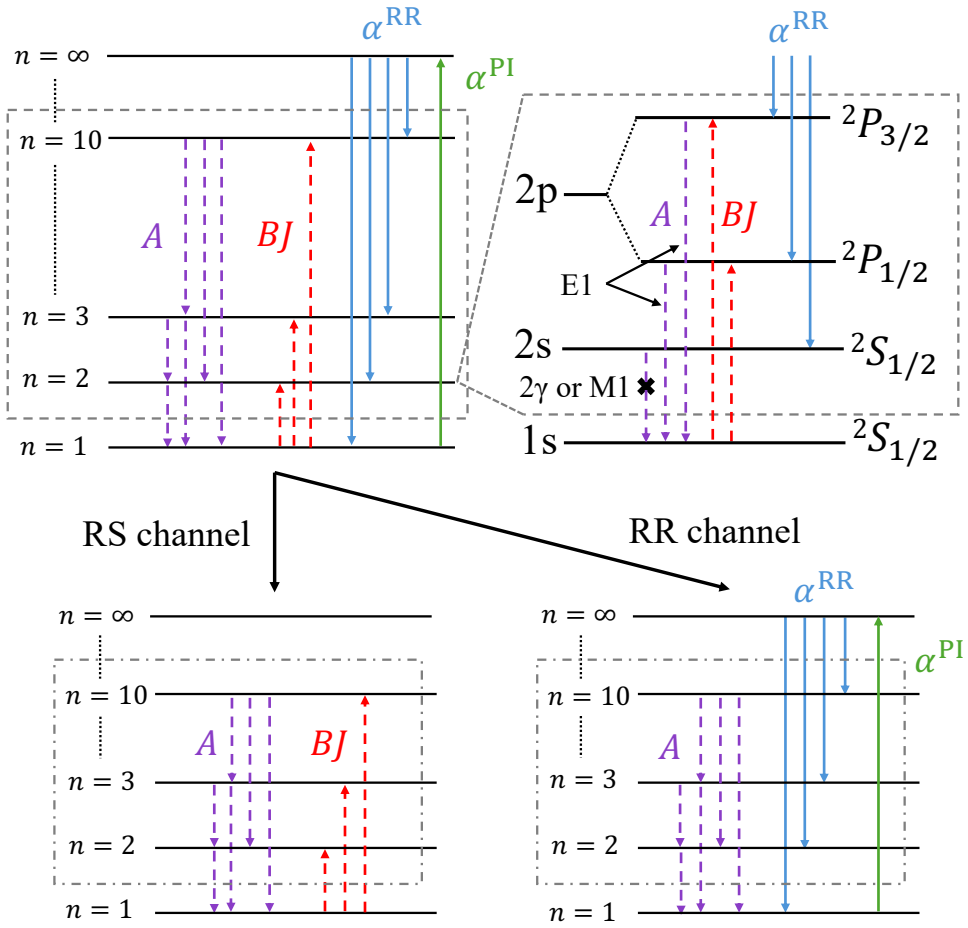
  - Cascade matrix $\boldsymbol{\Gamma}$ with Γ_{ij} represents the spontaneous radiative decay (A) from the level j to i.
  - Source term $\boldsymbol{S}$ with S_i represents the populating rates of the level i from n_0 and n_∞.

$$S_i = n_e n_\infty \alpha_i^{RR}(T) + n_0 B_{0i} J(\nu = \nu_{i0})$$

- We treat two channels separately:

RS channel $\quad \boldsymbol{\Gamma n}_{\mathrm{RS}} + \boldsymbol{S}_{\mathrm{RS}} = \boldsymbol{0}$

RR channel $\quad \boldsymbol{\Gamma n}_{\mathrm{RR}} + \boldsymbol{S}_{\mathrm{RR}} = \boldsymbol{0}$

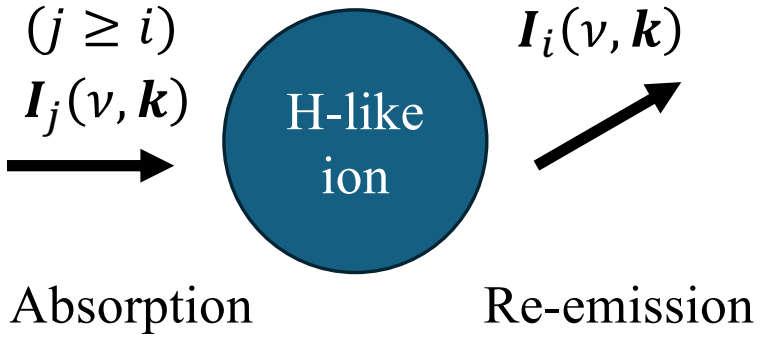


3-a. Resonance scattering

$$\frac{d\boldsymbol{I}_i(\nu', \boldsymbol{k}')}{ds} = \sum_{j \geq i} \boldsymbol{R}_{ij}(\nu, \boldsymbol{k}, \nu', \boldsymbol{k}') P_{ij} \alpha^{RS}{}_j(\nu) \boldsymbol{I}_j(\nu, \boldsymbol{k})$$

- $\boldsymbol{I}_j(\nu, \boldsymbol{k})$: Stokes vector (I_j, Q_j, U_j) of photons between the ground level and the excited level j.
- α_j^{RS}: Amplitude of resonance scattering.
- P_{ij} : Branching ratio to represent the degradation probability from j to i.
- $\boldsymbol{R}_{ij}$: Matrix to represent the redistribution of frequency and direction.

※We retrieve the atomic data from SPEX v.3.08.01 (Kaastra et al. 2024).



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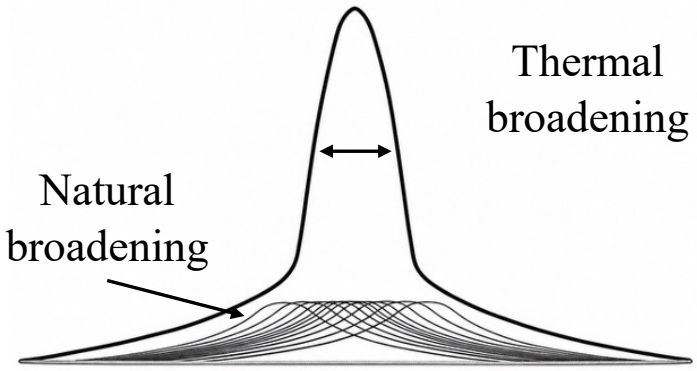
Amplitude

We consider both the natural and thermal broadening.
→ **Voigt profile.**



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Branching ratio

- When a $0 \rightarrow j$ radiative excitation occurs, subsequent radiative cascades determine the equilibrium level population.
- To obtain the level population, we solve the rate equation in which the source term only includes the $0 \rightarrow j$ radiative excitation rate.

$$\boldsymbol{\Gamma n}_{\mathrm{RS}} + \boldsymbol{S}_{\mathrm{RS}} = \boldsymbol{0}$$

$$S_k{}^{\mathrm{RS}} = \begin{cases} n_0 B_{0j} J_j(\nu = \nu_{0j}), & k = j \\ 0, & k \neq j \end{cases}$$

- The branching ratio is given as the fraction of the $i \rightarrow 0$ transition rate over the $0 \rightarrow j$ radiative excitation rate by

$$P_{ij} = \frac{n_i A_{i0}}{n_0 B_{0j} J_j(\nu = \nu_{0j})}$$

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$$\frac{d\boldsymbol{I}_i(\nu', \boldsymbol{k}')}{ds} = \sum_{j \geq i} \boldsymbol{R}_{ij}(\nu, \boldsymbol{k}, \nu', \boldsymbol{k}') P_{ij} \alpha^{RS}{}_j(\nu) \boldsymbol{I}_j(\nu, \boldsymbol{k})$$

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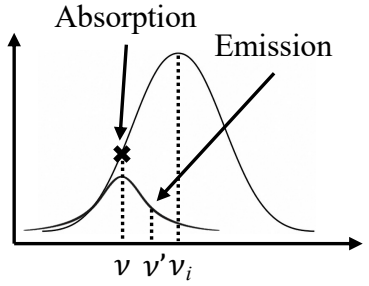
Redistribution

■ **Frequency**

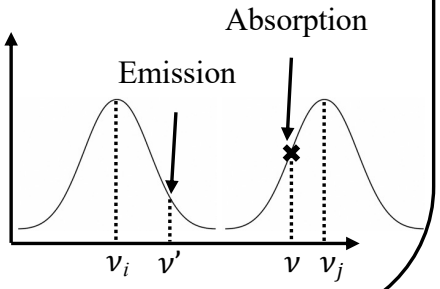
- For RS without photon degradation ($i = j$), the absorbed and re-emitted photons are coherent.

→ **Partial redistribution.**



- For RS with photon degradation ($j > i$), the coherency does not hold.

→ **Complete redistribution.**



3-a. Resonance scattering

$$\frac{d\boldsymbol{I}_i(\nu', \boldsymbol{k}')}{ds} = \sum_{j \geq i} \boldsymbol{R}_{ij}(\nu, \boldsymbol{k}, \nu', \boldsymbol{k}') P_{ij} \alpha^{RS}{}_j(\nu) \boldsymbol{I}_j(\nu, \boldsymbol{k})$$

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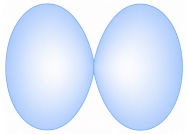
Redistribution

■ **Direction**

- Redistribution function is different for the three Stokes parameters. → 3 × 3 **Müller matrix**.
- Linear combination of monopole and dipole distribution, depending on the quantum number J and ΔJ (Hamilton 1947).

$$\begin{aligned} \boldsymbol{M}(\theta) &= E_1 \boldsymbol{M}^{(m)}(\theta) + E_2 \boldsymbol{M}^{(d)}(\theta) \\ &= E_1 \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &+ E_2 \frac{3}{8} \begin{pmatrix} 1+\cos\theta^2 & -\sin\theta^2 & 0 \\ -\sin\theta^2 & 1+\cos\theta^2 & 0 \\ 0 & 0 & 2\cos\theta \end{pmatrix} \end{aligned}$$

- Lyα$_1$ $(J = 1/2,\ \Delta J = 1) \rightarrow E_1 = E_2 = 1/2$.
- Lyα$_2$ $(J = 1/2,\ \Delta J = 0) \rightarrow E_1 = 1, E_2 = 0$.
- RS with photon degradation $\rightarrow E_1 = 1, E_2 = 0$.

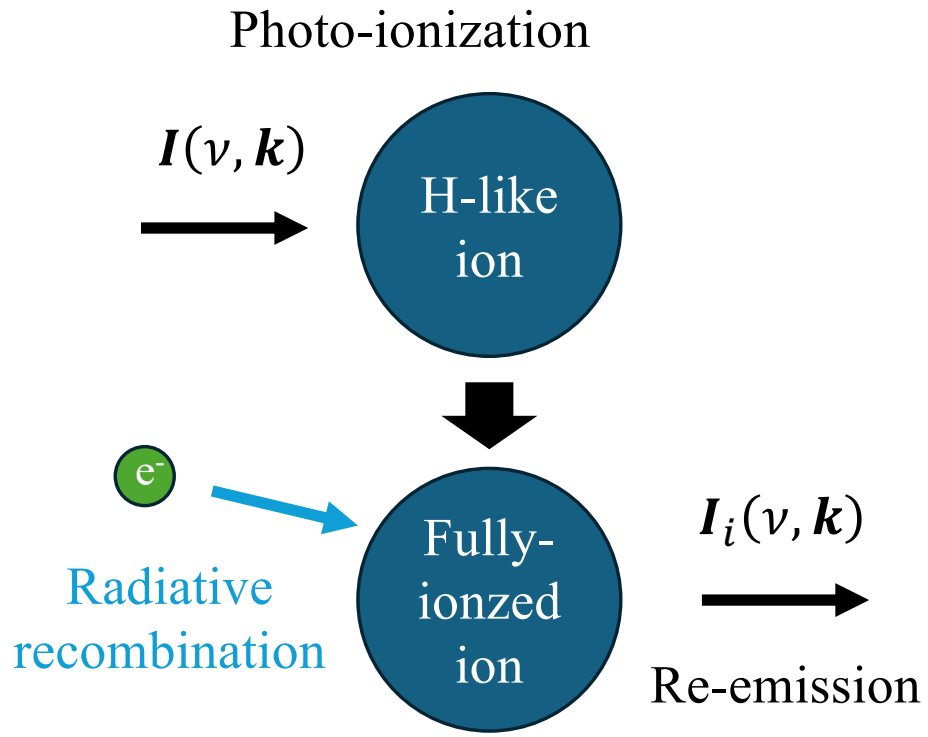
monopole  dipole 

3-b. Radiative recombination

$$\frac{d\boldsymbol{I}_i(\nu', \boldsymbol{k}')}{ds} = \boldsymbol{R}_i(\nu, \boldsymbol{k}, \nu', \boldsymbol{k}')P_i\alpha^{\mathrm{PI}}(\nu)\boldsymbol{I}(\nu, \boldsymbol{k})$$

- $\boldsymbol{I}(\nu, \boldsymbol{k})$: Stokes vector (I, Q, U) of ionizing photons.
- α^{PI}: Amplitude of photo-ionization.
- P_i: Branching ratio that a single photo-ionization event yields a Lyman $i \rightarrow 0$ photon.
- $\boldsymbol{R}_i$: Matrix to represent the redistribution of frequency and direction.

※We retrieve the atomic data from SPEX v.3.08.01 (Kaastra et al. 2024).



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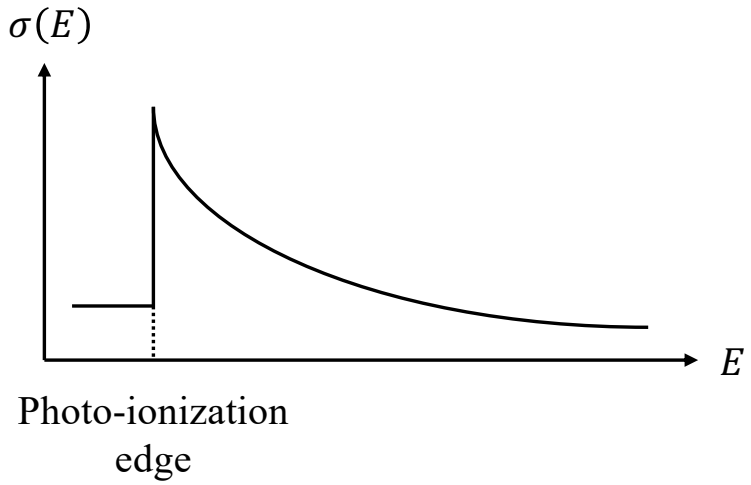
Amplitude

Verner & Yakovlev (1995) provided a parametrized description of **the photo-ionization cross-section for the ground state of H-like ions.**



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Branching ratio

- When a fully-ionized ion recombines with an electron, subsequent radiative cascades determine the equilibrium level population.
- To obtain the level population, we solve the rate equation in which the source term is the level-resolved radiative recombination rate $\alpha_i^{RR}(T)$ from Mao & Kaastra (2016).

$$\boldsymbol{\Gamma n}_{\mathrm{RR}} + \boldsymbol{S}_{\mathrm{RR}} = \boldsymbol{0}$$

$$S_i^{RR} = n_e n_\infty \alpha_i^{RR}(T)$$

- The branching ratio is given as the fraction of the $i \rightarrow 0$ transition rate over the total recombination rate by

$$P_i = \frac{n_i A_{i0}}{n_e n_\infty \sum_k \alpha_k{}^{RR}(T)}$$

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- $\boldsymbol{R}_i$: **Matrix to represent the redistribution of frequency and direction.**

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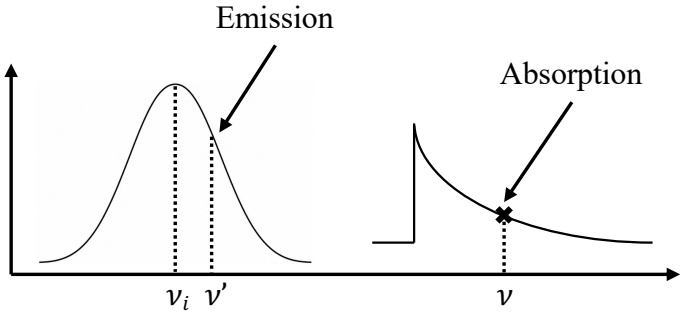
Redistribution

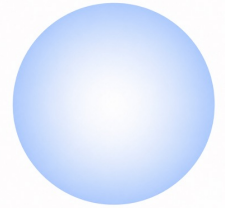
■ **Frequency**

Incoherent emission for RR



■ **Direction**

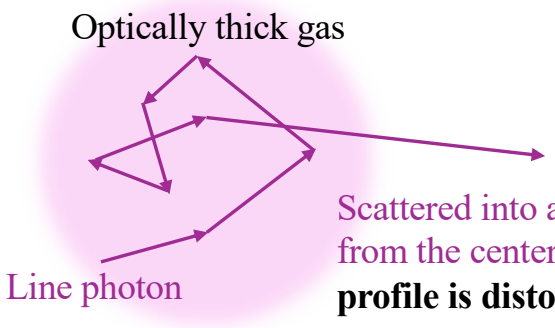
Monopole emission for RR



4-b. Radiative transfer effects (1/3)

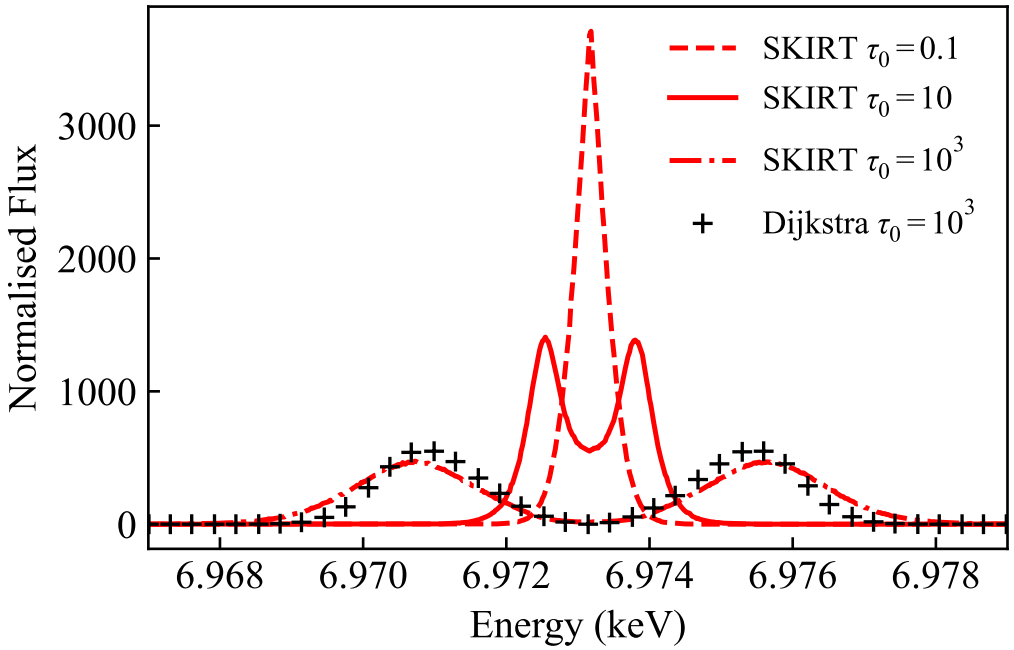
■ **Distortion of line profile**

- The emergent line profile can be distorted by frequency redistribution, **which is not captured by 1D- RT models that use the escape-probability approximation.**



Scattered into a frequency far from the center → **Emergent line profile is distorted.**

- We obtained the Fe Lyα_1 line profile with $\tau_0 = 0.1, 10, 10^3$ with SKIRT.
- The SKIRT result for $\tau_0 = 10^3$ is close to an asymptotic expression by Dijkstra et al. (2006).



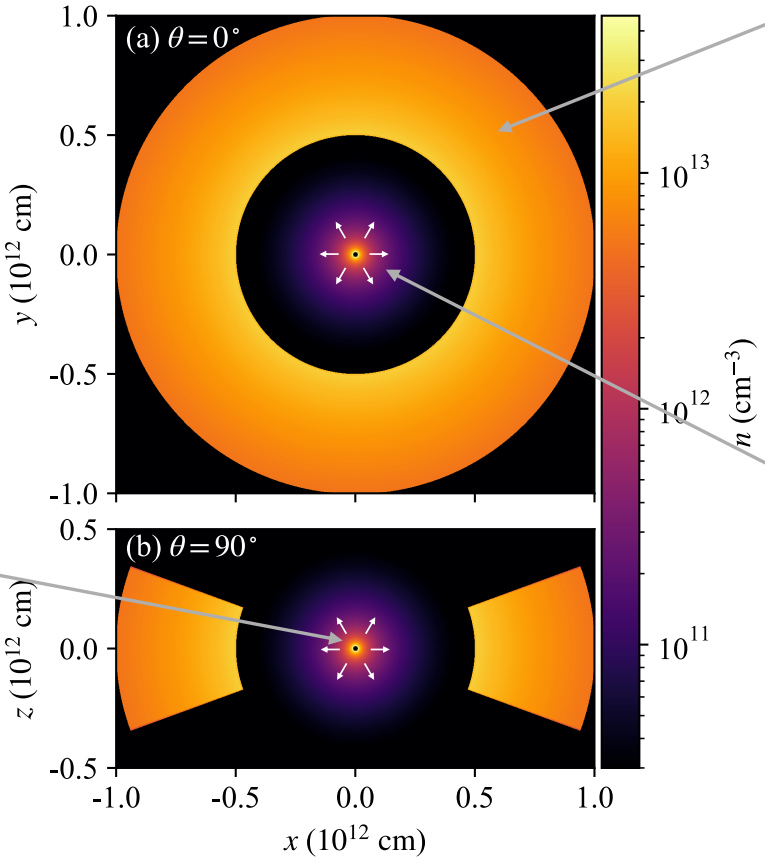
Lyα_1 line profile calculated using SKIRT for $\tau_0 = 0.1, 10, 10^3$.

5-a. Setup

- We make a demonstration for a more realistic setup.

→ LMXB consisting of a cold outer disk and a hot outflowing wind.

Density distribution.



Source

- Point-like.
- Multi-temperature blackbody.
- Anisotropic emission from an inner accretion disk (Netzer 1987).

$$L(\theta) \propto \begin{cases} \cos\theta\,(2\cos\theta + 1), & 0 \le \theta \le \frac{\pi}{2}, \\ \cos\theta\,(2\cos\theta - 1), & \frac{\pi}{2} \le \theta \le \pi. \end{cases}$$

Outer disk

- Neutral atoms with a solar abundance.
- Opening angel 20° .
- **Block the emission from the wind at the edge-on.**

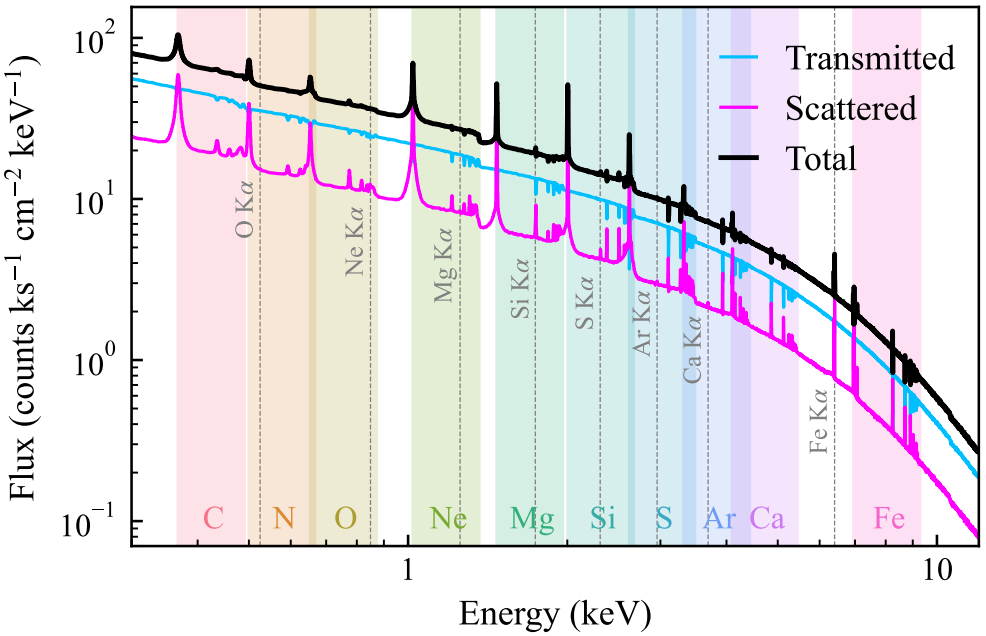
Outflowing wind

- Ion density calculated with Cloudy.
- Radial velocity of 100 km/s.
- **Production site of Lyman-series lines.**

5-b. Spectra

■ **Overall spectra**
- Transmitted: Continuum attenuation by electron scattering, together with absorption lines and edges by H-like ions.
- Scattered: Lyman-series lines as well as fluorescence lines by neutral atoms.

■ **Close-up view of the Fe Lyα doublet**
- P Cygni profiles at $\theta = 30°$ and $60°$.
- The transmitted component is completely lost and only the emission line is observed at $\theta = 90°$.



Overall spectra synthesized with SKIRT at $\theta = 60°$.

5-b. Spectra

- **Overall spectra**
  - Transmitted: Continuum attenuation by electron scattering, together with absorption lines and edges by H-like ions.
  - Scattered: Lyman-series lines as well as fluorescence lines by neutral atoms.

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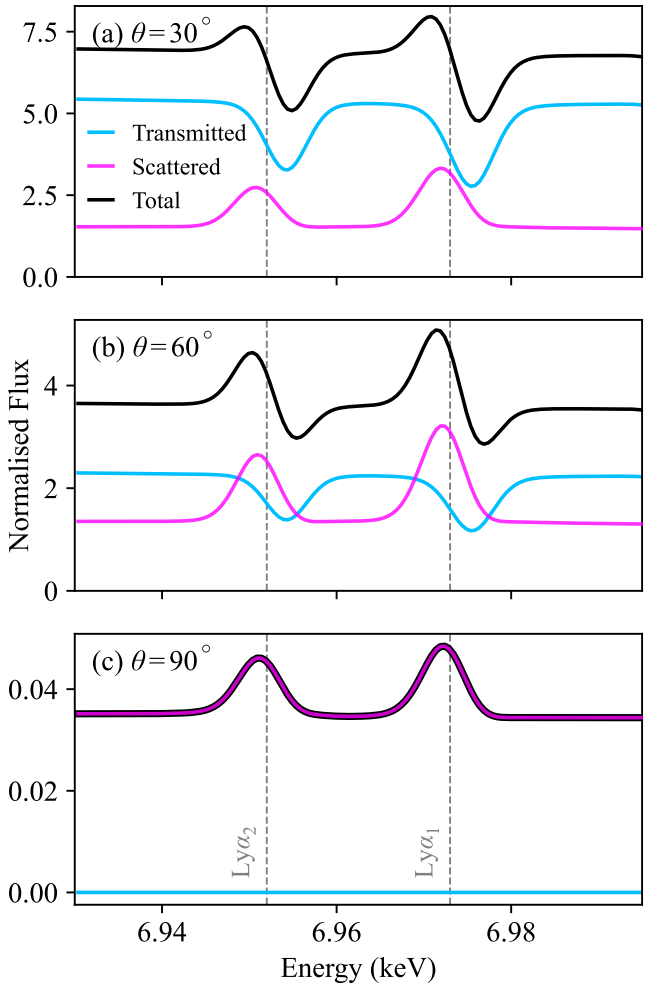
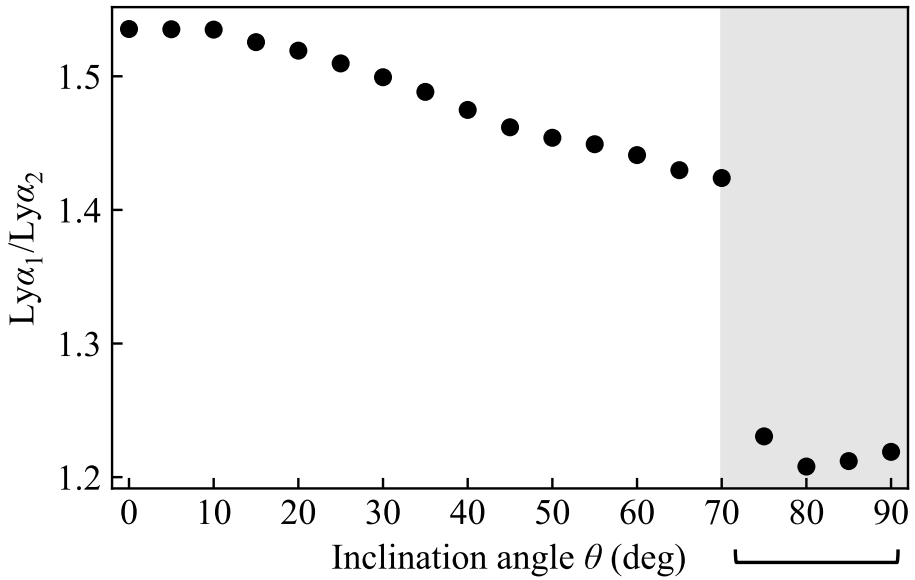


Close-up view of the Fe Lyα doublet at different viewing angles.

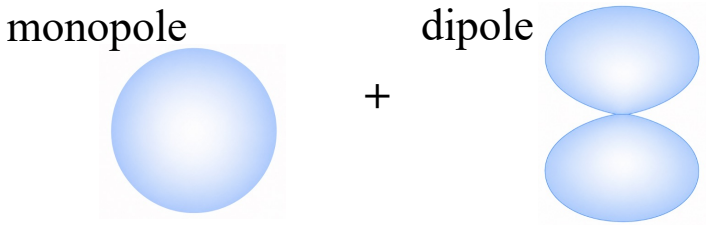
5-c. Lyα$_1$/Lyα$_2$ ratio

■ **The doublet ratio decreases as θ increases** because of scattering phase function effects.

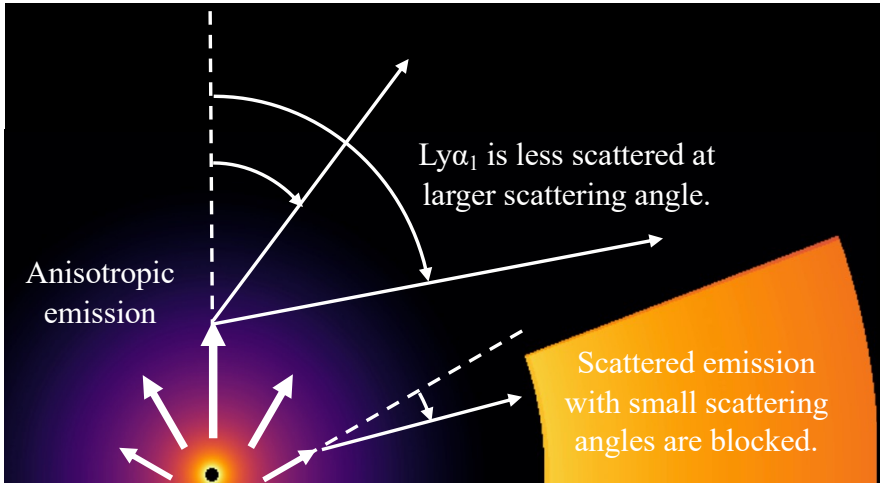


The outer disk is in the line of sight.

■ **Lyα$_1$ scattering phase function**:



→ Scattering becomes less likely at larger θ.
→ **Anisotropic emission and shielding by the outer disk enhance this effect.**



6. Summary

1. **Motivation**: To interpret reprocessed X-ray emission from photo-ionized plasmas around compact objects, observed by XRISM and IXPE.

2. **Method**: We have implemented the Lyman-series lines H-like ions in the MC-RT code SKIRT.

3. **Implementation**:
   a. Atomic processes: Resonant scattering (RS) and Radiative recombination (RR)
   b. Microphysics: Cross-section, Branching ratio and Redistribution

4. **Verification:**
   a. The implemented microphysics show good agreement with Cloudy.
   b. The code successfully reproduces RT effects (line-profile distortion, Lyman decrement, and P Cygni profiles).

5. **Demonstration**: Anisotropy of the radiation field, geometry, and velocity structure significantly affect observable features in the spectra (P Cygni profile and the Lyα fine-structure doublet ratio).