Electron–Positron Pair Creation Close to a Black Hole Horizon: Redshifted Annihilation Line in the Emergent X-Ray Spectra of a Black Hole. I.

Philippe Laurent1,2 and Lev Titarchuk3

1 CEA/DRF/IRFU/DAp, CEA Saclay, F-91191 Gif sur Yvette, France; philippe.laurent@cea.fr
2 Laboratoire APC, 10, rue Alice Domon et Léonie Duquet, F-75205 Paris Cedex 13, France
3 Dipartimento di Fisica, Università di Ferrara, Via Saragat 1, I-44100 Ferrara, Italy; titarchuk@fe.infn.it

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Abstract

We consider a Compton cloud (CC) surrounding a black hole (BH) in an accreting BH system, where electrons propagate with thermal and bulk velocities. In that cloud, soft (disk) photons may be upscattered off these energetic electrons and attain energies of several MeV. They could then create pairs due to photon–photon interactions. In this paper, we study the formation of the 511 keV annihilation line due to this photon–photon interaction, which results in the creation of electron–positron pairs, followed by the annihilation of the created positrons with the CC electrons. The appropriate conditions for annihilation-line generation take place very close to a BH horizon within $(10^3$–$10^5)\,m$ cm from it, where $m$ is the BH hole mass in solar units. As a result, the created annihilation line should be seen by the Earth observer as a blackbody bump, or the so-called reflection bump at energies around $(511/20)$ ($20/\,z$) keV, where $z \sim 20$ is a typical gravitational redshift experienced by the created annihilation-line photons when they emerge. This transient feature should occur in any accreting BH system, either galactic or extragalactic. Observational evidences for this feature in several galactic BH systems is detailed in an accompanying paper. An extended hard tail of the spectrum up to 1 MeV may also be formed due to X-ray photons upscattering off created pairs.

Key words: black hole physics – radiation mechanisms: non-thermal – relativistic processes – X-rays: general

1. Introduction

Accreting stellar-mass black holes (BHs) in Galactic binaries exhibit high-soft and low-hard spectral states and transition between them (the intermediate state; see details in Shaposhnikov & Titarchuk 2009, hereafter ST09). Usually, an increase in the soft blackbody (BB) luminosity component leads to the appearance of an extended power law. However, the extension of the power law is not a monotonic function of the power-law index. Using data from the Rossi X-ray Time Explorer (RXTE) for the black hole candidate (BHC) XTE J1550–564, Titarchuk & Shaposhnikov (2010) demonstrate that the efold energy $E_{\text{fold}}$ of the spectra decreases when the photon index $\Gamma$ increases starting from $\Gamma \sim 1.4$, and then, at some value of $\Gamma \sim 2.2$, it starts increasing toward energies of 200 keV. An important observational fact is that this effect is seen as a persistent phenomenon only in BH candidates, and thus it is apparently a unique BH signature. In neutron star (NS) sources, $E_{\text{fold}}$ gradually decreases toward the soft state (see, e.g., Seifina & Titarchuk 2011 and Titarchuk et al. 2013, hereafter TSF13). Although similar power-law components are detected in the hard and intermediate states (hereafter the LHS and the IS, respectively) in NSs, their extension (or $E_{\text{fold}}$) becomes smaller with increasing luminosity (see Di Salvo et al. 2000 and Farinelli & Titarchuk 2011, hereafter FT11).

Moreover, ST09 find that the photon index $\Gamma$ saturates with the dimensionless mass accretion rate $\dot{m} = \dot{M}/M_{\text{crit}}$, where $M_{\text{crit}} = L_{\text{Edd}}/c^2$, with $L_{\text{Edd}} = 4\pi G M m_p c/\sigma_T$ the Eddington luminosity, $m_p$ the proton mass, $\sigma_T$ the Thomson cross-section, and $c$ the speed of light. Naturally, the photon index $\Gamma$ saturates with a quasi-periodic oscillation frequency (QPO; and the mass accretion rate) in BH sources while FT11 and TSF13 demonstrate that $\Gamma$ stays almost the same, around 2, in NSs. Thus, it seems a reasonable assumption that we deal here with a unique spectral signature of BH binaries, which is directly tied to the BH event horizon.

In Laurent & Titarchuk (1999, hereafter LT99), we suggested that the BH X-ray spectrum in the high-soft state (HSS) is formed in a relatively cold accretion flow with a relativistic bulk velocity $v_{\text{bulk}} \sim c$ and with the plasma (electron) temperature of a few keV or less, for which the thermal electron velocity $v_{\text{th}} \ll c$. It is worth pointing out that in such a flow, the effect of bulk Comptonization is much stronger than the effect of thermal Comptonization, which is second order with respect to $v_{\text{th}}/c$ (LT99). Very close to the horizon, X-ray photons can be upscattered by bulk electrons to very high energies, of order 1 MeV, and higher, but the observer on Earth will see these upscattered photons at lower energies, on the order of 300–400 keV, because of gravitational redshift.

Using Monte Carlo simulations, LT99 compute the X-ray spectra of such BH sources. They take into account the upscattering of the soft (disk) photons illuminating the Compton cloud (CC), and they implement a full relativistic treatment to reproduce these spectra. The resulting spectra obtained using this treatment can be described as the sum of a thermal (disk) component and the convolution of some fraction of this component with the CC upscattering spread (Green’s) function. The upscattered part of the spectrum is seen as an extended power law over energies much higher than the characteristic energy of the soft photons. LT99 show that the photon index $\Gamma$ increases with an increase of the mass accretion rate and then it stabilizes at $\Gamma = 2.8 \pm 0.1$, similarly to what was observed by ST09. This index stability occurs over a wide
range of the plasma temperature, 0–10 keV, and dimensionless mass accretion rates \( \dot{m} \) (higher than 2 in Eddington units).

LT99 also demonstrate that the sharp high-energy cutoff occurs at energies of 200–400 keV, which are related to the average energy of the electrons, \( m_e c^2 \), impinging on the event horizon. The spectrum, however, is practically identical to the standard thermal Comptonization spectrum (see, e.g., Hua & Titarchuk 1995) when the Compton cloud (CC) plasma temperature is reaching of order of 50 keV (the typical values for the hard state of the BH). In this case, one can only see the effect of the bulk motion at high energies, where there is an excess in the spectrum with respect to the pure thermal one. Furthermore, LT99 demonstrate that the change of spectral shape from the soft X-ray state to the hard X-ray state is clearly related to the CC temperature. Indeed, the effect of the bulk Comptonization compared with the thermal one gets stronger when the plasma temperature drops below 10 keV.

Furthermore, Laurent & Titarchuk (2001, hereafter LT01) have shown that the high-energy photon production (source function) is distributed with the characteristic maximum at about the photon-bending radius \( 1.5r_S \), where \( r_S = 2GM/c^2 \) is the Schwarzschild radius and \( M \) is a BH mass, independently of the seed (soft) photon distribution. Most of these photons fall down into the BH, but some of them have time to interact with another X-ray photon via a photon–photon process to make electron–positron pairs (Svensson 1982). In this paper, we explore in detail the consequences of this pair-creation process that occurs very close to a BH horizon, \((10^3–10^4)m\) cm from it (\( m \) is the BH hole mass in solar units), and we elaborate the observational consequences of this effect.

In the next section, we proceed with the details of the Monte Carlo simulations of the upscattering of the soft (disk) photons in the converging flow (CF) and of the pair creation due to the interaction of these upscattered photons with unscattered X-ray photons in the close vicinity of a BH horizon. Then, we explore in detail the observational consequences of this effect. In the Appendix, we give an analytical derivation of some key results obtained through simulations.

2. The Monte Carlo Simulations

The geometry used in these simulations is similar to the one used in LT99, consisting of a thin disk with an inner radius of \( 3r_S \), merged with a spherical CC harboring a BH in its center. The CC outer radius is \( r_{out} \). The disk is assumed always to be optically thick. In addition to the free fall into the central BH,
with the bulk velocity of the infalling plasma given by \( v(r) = c(r_S/r)^{1/2} \), where \( r_S \) is the Schwarzschild radius (Titarchuk et al. 1997), we have also taken into account the thermal motion of the CC electrons, simulated in most of the results shown here at an electron temperature of 5 keV, which is typical of the CC in the HSS of galactic BHs (see Figure 1). The CC temperature is less than the temperature of the sub-Keplerian inflow (presumably located above the disk), but it is higher than the temperature of the disk flow, which is of order of a few keV or less (e.g., Shakura & Sunyaev 1973).

The seed X-ray photons were generated uniformly and isotropically at the surface of the border of the accretion disk, from \( r_{in} = 3r_S \) to \( r_{out} = 10r_S \). These photons were generated according to a thermal spectrum with a single temperature of 0.9 keV, similar to the ones measured in BH binary systems (see, for example, Borozdin et al. 1999). To reach a satisfactory statistic level for our computations, we performed simulations using \( 10^6 \) seed (disk) photons.

In Figure 1, we present the geometry of X-ray spectral formation in a BH source. Soft X-ray photons coming from the disk illuminate the CC and its innermost part, where the bulk velocity is dominating in the CF region). These photons upscatter off electrons in these configurations, and some part of these photons arrive at the observer, which are then seen as a specific Comptonization spectrum.

In our simulations (see also the kinetic formalism in Titarchuk & Zannias 1998, hereafter TZ98), we use the number density \( n_{th} \) of the flow measured in the laboratory frame of the flow \( n_{th} = \dot{m}(r_S/r)^{1/2}/(2\pi R_T) \). Here, \( \dot{m} = \dot{M}/\dot{M}_{Edd}, \dot{M} \) is the mass accretion rate, \( \sigma_T \) is the Thomson cross-section, and \( \dot{M}_{Edd} \equiv L_{Edd}/c^2 = 4\pi GMm_p/\sigma_T c \) is the Eddington accretion rate. The parameters of our simulations are thus the BH mass \( m \) in solar units, the CC electron temperature \( T_e \), the mass accretion rate \( \dot{m} \), and the CC outer radius \( r_{out} = 10r_S \). The cloud’s Thomson optical thickness is expressed using the mass accretion rate \( \dot{m} \) according to the following formulae (see e.g., TZ98):

\[
\tau_T = \frac{\dot{m}}{2} \int_{x_{in}}^{x_{out}} \frac{dx}{x^{3/2}(1-x^{-1})} = \dot{m} \left( \frac{\pi}{2} - \arcsin \frac{r_S}{r_{out}} \right),
\]

where \( x_{out} = r_{out}/r_S \).

In Figure 2, we show the average photon energy of the upscattered photons (black histogram) and the blueshifted energy of injected soft photons (blue line) as a function of radius. As one can see, the injected (disk) photons illuminating the innermost region of the CF are strongly blueshifted; at 30 m from a BH horizon (for a 10 solar mass BH), their energy is of order of a few MeV. One should keep in mind, however, that only a few of these photons can directly reach a BH horizon when the accretion rate is high (in the HSS) as the CF optical depth \( \tau_T \gtrsim 1 \) for \( \dot{m} \gtrsim 1 \) (see Equation (1)). In addition to the Compton effect, we compute the probability of making a pair, using the pair-creation cross-section given by Svensson (1982). The kinetic properties of the pair are computed in the local rest frame using standard formulae, derived from energy and momentum conservation, and the results stored in a file for subsequent treatment. The properties of the created pair are described below. Afterward, using another Monte Carlo simulation, we propagate the pairs in the Schwarzschild metric, slowing them down by Coulomb scattering, and checking
whether the positrons annihilate or not. The resulting annihilation photons were also tracked by a third Monte Carlo in the CC, to see whether they escape or are scattered off due to the CC optical depth.

3. Properties of Created Pairs

As one can see from Figure 3, the pairs are produced in the Monte Carlo simulations very close to a BH horizon. For a 10 solar mass BH, this creation occurs even at a few hundred meters away from the horizon. This result is confirmed by computations given in the Appendix.

The pair-creation process depends on the properties of the background X-ray photons, and, in particular, of the source X-ray luminosity. We then simulated the pair-creation process for different values of the source X-ray luminosity and computed for each of them the number of positrons created close to the BH. These numbers are presented in Figures 4 and 5 for the LHS and the HSS, respectively. We choose these two BH spectral states in order to demonstrate a trend in the creation of positron number as a function of the luminosity for two cases of the model parameters, the plasma temperature, \( kT_e \), and \( \dot{m} \), even if these states do not span on their own the whole luminosity range. We should point out that although the two curves are similar to each other, the LHS plot is situated a factor of 5 below the HSS one. This is mainly due to the difference in the mass accretion rate \( \dot{m} \) between these two cases. This linear dependence of the number of created pairs on \( \dot{m} \) occurs when the luminosity reaches \( 10^{36} \) erg s\(^{-1} \), when the number of created positrons is equal to around \( 5 \times 10^5 \) for the LHS and \( 5 \times 10^6 \) for the HSS, respectively (see Figures 4 and 5). Simulations also show that, independently of the source X-ray luminosity, the positron kinetic energy spectrum remains nearly the same.

4. The Emergent Photon Spectrum of an Accreting BH

4.1. A Redshifted 511 keV Annihilation-line Feature

As we have already discussed, the pair creation occurs very close to the horizon, of the order of 100 m from the horizon of a 10 solar mass BH. In Figure 6, we show the trajectories of the created positrons in the Schwarzschild background. It can be seen that only a few of the \( 5 \times 10^5 \) positrons simulated to produce this figure can reach 3\( r_S \). This number is even lower if we take into account Coulomb losses and the pair-annihilation process.

Using the results of our first Monte Carlo, we have built another Monte Carlo software with which we simulate the propagation of the created positrons in the cloud, taking into account energy losses due to Coulomb scattering with protons. This process is the dominant cooling one, considering the physical condition of the cloud (see discussion in Moskalenko & Jourdain 1997). We compute also the annihilation probability for positrons, and check whether each positron annihilates or not. If the annihilation occurs, then we store the kinetic energy and location of this positron at the moment of the annihilation. If not, these positrons can either fall into the BH, Compton scatter off background photons, escape from the system, or annihilate farther away, outside the CC, depending on the density of the surrounding material at several Schwarzschild radii. If we suppose that all positrons escaping from the CC annihilate afterward, the maximum expected 511 keV...
photon flux is around $10^{36}$ photons s$^{-1}$ (i.e., $10^{30}$ erg s$^{-1}$) for a luminosity of $10^{38}$ erg s$^{-1}$. In a further step, we derive, using a third Monte Carlo code and the saved annihilated positrons locations, the emergent annihilation radiation. As the 511 keV annihilation emission is produced at a different radius from the BH, the line endures different redshifts, depending on the location of the annihilation, and thus, this annihilation process appears to the external observer as a specific continuum. In Figure 7, we show the resulting spectra for a CC electron temperature of 5 keV.

In this set of simulations, $m_\dot{m}$ was set equal to 1 (blue line), 4 (red line), and 10 (green line). The spectrum becomes harder as $m_\dot{m}$ increases. Also, due to the coinciding effects of the pair-creation efficiency, which increases with $m_\dot{m}$, and the CC opacity to the 511 keV radiation, decreasing with $m_\dot{m}$, we could see in Figure 7 that the spectrum is maximum for intermediate values of $m_\dot{m} = 4$.

We then explored what happens if we keep the mass accretion rate constant ($m_\dot{m} = 4$) while varying the CC electron temperature. The result can be seen in Figure 8, where we present the emergent annihilation spectrum with a CC electron temperature of 5 keV (blue line) and 50 keV (red line). One can notice that the overall spectrum shape does not change much except for the spectrum shift toward higher energies when we increase the cloud temperature, $kT_e$.

In Figure 9, we show also the emergent Comptonized spectrum of the CC, with an electron temperature of $kT_e = 5$ keV, including the gravitationally redshifted annihilation line. In the encapsulated upper-right-hand panel, we include the redshifted annihilation line as a ratio of the resulting spectral values to the Comptonized continuum. These simulations show that the emergent annihilation spectrum is quasi-universal whatever the CC physical conditions.

In Figures 7 and 8, we demonstrate also that these redshifted annihilation lines can be represented by a blackbody-like shape, as shown by the dashed lines, which give the best blackbody fit for the $m_\dot{m} = 1$ and $m_\dot{m} = 4$ case respectively.

However, observationally, this feature should be transient and will not be observed in all BH spectral states. Indeed, if the resulting X-ray luminosities $L_\gamma \gg 10^{37}(M_{BH}/10 M_\odot)$ erg s$^{-1}$, the dimensionless mass accretion rate (see Titarchuk & Zannias 1998) will be much greater than 1, and the produced pairs and annihilation photons generated near a BH horizon cannot escape, as they are effectively scattered off converging electrons. In the LHS, we cannot see the high-temperature blackbody (HBB) either, and consequently, the redshifted annihilation line, because $\tau_\gamma \approx 1$ and pairs are not effectively generated. Moreover, in the LHS, the CF is surrounded by a hot, relatively thick CC with plasma temperature of order of 50–80 keV. Thus, the escaping HBB photons are scattered off hot electrons of the CC, and the bump is smeared out. So, we expect this feature to be seen only during the intermediate state when the mass accretion rate is sufficient to trigger the effect but not strong enough to hide it afterward.

4.2. Emergent Spectrum Taking into Account the Pair Creation

In the previous section, we demonstrated that the pairs are created very close to the BH horizon due to photon–photon interactions. In fact, these photons reach the necessary conditions for pair creation when the product of their energies $E_1E_2 > (m_e c^2)^2$. In Figure 10, we show the redshifted annihilation line and the classical bulk motion Comptonization
spectrum, plus the result of the photon upscattering off these energetic pairs, which leads to an extension of the emergent spectrum up to 10 MeV. In that case, the CC temperature is $5 \text{ keV}$ ($\dot{m} = 4$). In Figure 11, we illustrate the light propagation in the Schwarzschild metric, while in Figures 12 and 13, we also demonstrate the photon and pair distributions (spectra) for different radii within the CF, respectively.

It is worth noting that similar spectra in the HSS in quite a few BH binaries were observed by the OSSE and COMPTEL instruments (see Grove et al. 1998 and McConnell 1994, respectively). In particular, seven BH transient sources, GRO J0422+32, GX 339–4, GRS 1716–249, GRS 1009–45, 4U 1543–47, GRO J1655–40, and GRS 1915+105, observed by OSSE demonstrated two Gamma spectral states (HSS and LHS) and the transition between these two states. Grove et al. (1998) emphasize that, in the LHS, the emergent spectra are characterized by hard spectra with photon indices $\Gamma < 2$ and exponential cutoff of energies $\sim 100 \text{ keV}$. This form of the spectra is consistent with the thermal Comptonization case (see Sunyaev & Titarchuk 1980). These spectra were observed by Grove et al. (1998) for GRO J0422+32, GX 339–4, GRS 1716–249, and GRS 1009–45, while GRS 1009–45, 4U 1543–47, GRO J1655–40, and GRS 1915+105 show the HSS with a relatively soft photon index, $\Gamma$, in the range from 2.5 to 3. Furthermore, Grove et al. (1998) have found that the HSS emergent spectrum in GRO J1655–40 is extended to 690 keV without any sign of a rollover at low energies. One can compare Grove’s spectrum with our Monte Carlo simulated HSS spectrum demonstrated in Figure 10.

McConnell (1994) provided details of the Cyg X-1 observations in the 0.75–30 MeV energy range using the COMPTEL instrument in CGRO. They found the Cyg X-1 spectrum in the HSS to be extended up to at least 1 MeV without any break. No physical explanation was suggested to explain this observational result besides a suggestion of incorporating a spectral component that represents the reflection of the hard X-rays from an optically thick accretion disk (see Haardt & Maraschi 1993). However, this reflection scenario is inconsistent with the soft-state emergent Cyg X-1 spectrum because spectra with photon index higher than 2 do not demonstrate the reflection effect. Indeed, the spectrum is too steep and there is not enough photons at high energies to transfer them to lower energies to make a reflection (or downscattering) bump (see Laurent & Titarchuk 2007). However, we argue using our simulations that the combined OSSE–COMPTEL spectrum for Cyg X-1 in the HSS demonstrated in McConnell (1994) can result from the Comptonization of the soft (disk) photons by pairs in the CF, as shown in Figure 10.

5. A Redshifted Annihilation Radiation. A High-temperature BB (HBB) Component

Titarchuk et al. (2018, hereafter TSC18, paper II) found observational evidence of an HBB bump around 20 keV, which could be fitted by a $\sim 4.5 \text{ keV}$ blackbody profile, in BH accreting systems. Evolutions of the spectral characteristics of GRS 1915+105, SS 433, and V4641 Sgr are very similar, and all of them show the HBB feature, which is centered around 20 keV. Using RXTE and INTEGRAL data, TSC18 demonstrated that the HBB component is needed in the IS broadband flux.
spectra of SS 433. On the other hand, a comparative analysis of the BeppoSAX and RXTE data shows that the flaring pattern for GRS 1915+105 and V4641 Sgr, respectively, demonstrates a transition from the IS to the LHS. It is interesting that the HBB feature is usually observed in the same X-ray luminosity range ($5 \times 10^{36} - 5 \times 10^{37}$ erg s$^{-1}$) for different sources. Thus, one can naturally raise a question on the origin of this HBB.

TSC18 estimated the optical depth for photon–photon interaction to be very close to a BH horizon. In order to do this, they calculated the photon density $N_{\gamma}$ near a BH horizon, assuming that most photons have energy greater than $m_e c^2 = 511$ keV:

$$N_{\gamma} = \frac{L_\gamma}{4\pi r_s^2 c m_e c^2},$$

where $L_\gamma \approx 10^{37} (m/10)$ erg s$^{-1}$, $r_s = 2GM/c^2$ is the Schwarzschild radius (or $r_s = 3 \times 10^8 (m/10)$ cm), $c$ is the speed of light ($3 \times 10^{10}$ cm/s), and the electron rest energy, $m_e c^2$ is about $5 \times 10^{-7}$ erg. As a result, they obtain that $N_{\gamma} \approx 0.6 \times 10^{19} (M_{\text{BH}}/10M_\odot) \text{ cm}^{-3}$. Then, the optical depth for photon–photon interactions can be estimated as

$$\tau_{\gamma-\gamma} \sim \sigma_{\gamma-\gamma} N_{\gamma} r_s.$$  

The cross-section for $\gamma-\gamma$ interaction, $\sigma_{\gamma-\gamma} \sim 0.2\sigma_T$, where $\sigma_T = 6 \times 10^{-25}$ cm$^2$ is the Thomson cross-section. Thus, they find that $\tau_{\gamma-\gamma} \sim (1-2)$ using Equations (2) and (3). It is important to emphasize that $\tau_{\gamma-\gamma}$ is independent of the BH mass. We demonstrate in our Monte Carlo simulations (see also TSC18) that the IS luminosity of order $10^{37}$ erg s$^{-1}$ is sufficient to get a high-enough optical depth $\tau_{\gamma-\gamma}$ to trigger photon–photon interaction very close to a BH horizon.

So, pairs (electrons and positrons) are effectively generated as a result of $\gamma-\gamma$ interactions near a BH horizon, within a shell of order of $100 (M_{\text{BH}}/10M_\odot)$ m. The generated positrons propagate and may interact with accreting electrons, leading to the formation of the annihilation line at 511 keV. A significant fraction of these line photons can directly escape to the Earth observer if the Klein–Nishina optical depth, $\tau_{\text{KN}}$, at 511 keV is of order of 1. On their way out, these 511 keV line photons undergo gravitational redshift with $z$ around 20, forming the HBB with color temperature around 20 keV. Observationally, this HBB feature has an equivalent width in the interval from 400 to 700 eV (see TSC18, Figure 9).

As noted in Section 4, in the HSS, the dimensionless mass accretion rate is much greater than 1, and the produced pairs and annihilation photons generated near a BH horizon cannot escape, as they are effectively scattered off converging electrons. On the other hand, in the LHS, the CF is surrounded by a hot, relatively thick CC with plasma temperature of order of 50–80 keV, and the escaping HBB photons are scattered off hot electrons of the CC, and the bump is smeared out. So, it is not by chance that we cannot observe the HBB bump in either the HSS when $\dot{m}$ is high.
Figure 7. Emergent photon spectrum of the annihilated positrons. As the 511 keV emission from annihilation is produced at a different radius from the BH, the line endures different redshifts, thus producing a continuum. In this set of simulations, the temperature of the CC was 5 keV, and its density was varied from \( \dot{m} = 1 \) (blue line), 4 (red line), and 10 (green line). The main component of the spectra seems not to change much with \( \dot{m} \), but a hard component rises when \( \dot{m} \) increases. Due to the coinciding effects of the pair-creation efficiency and CC opacity to the 511 keV radiation, the spectrum is maximum for intermediate \( \dot{m} = 4 \). The fit of the \( \dot{m} = 1 \) spectrum with a blackbody spectral shape (\( kT = 6.2 \) keV) is shown by the dashed line.

Figure 8. Emergent photon spectrum of the annihilated positrons. In this set of simulations, \( \dot{m} = 4 \) and the CC electron temperatures are 5 keV (blue line) and 50 keV (red line). The cutoff energy of this annihilation-line spectrum only slightly changes with the cloud temperature. The fit of the \( \dot{m} = 4 \) spectrum with a blackbody spectral shape (\( kT = 6.4 \) keV) is shown by the dashed line.
or in the LHS, but only in the transient IS, where $\dot{m}$ is around 1–2. In Figure 14, we plot the simulated bump equivalent width evolution with $\dot{m}$.

6. Conclusions

We performed extensive Monte Carlo simulations of X-ray spectral formation in the cloud surrounding a BH. We found the emergent spectrum extends to relatively high energies up to 400 keV due to the upscattering of the soft (disk) photons illuminating the CC region. Moreover, one can observe a redshifted annihilation line formed near a BH horizon when the dimensionless mass accretion rate $\dot{m}$ is in the range of 1–2, and the plasma temperature $kT_e$ is of order of or lower than 5 keV. These conditions are met when a BH is observed in the intermediate state. The annihilation line is formed due to the pair production when the upscattered photon energies exceed the 511 keV threshold. The generated positrons on their way out annihilate with incoming electrons, producing the 511 keV line. This line is produced very close to a BH horizon, the photons undergo a significant redshift of order of 20 while

Figure 9. Emergent photon spectrum which includes a gravitationally redshifted annihilated line. In the encapsulated upper-right-hand panel, we include the redshifted annihilation line as a ratio of the resulting spectral values to the Comptonized continuum.

Figure 10. Spectrum at infinity resulting from the redshifted pair-annihilation line (red), the Comptonization of X-ray photons on the CC electrons (blue), and the Comptonization on created pairs (blue). In that case, the CC temperature is 5 keV ($\dot{m} = 4$).
going out to the observer on Earth, and the line is observed as a high-energy bump around 20 keV.

This annihilation line cannot be observed in the LHS characterized by a low mass accretion rate, less than 1, and a hot CC with a plasma temperature of about 50 keV surrounding the CF site (see Figures 1 and 14). Moreover, in the HSS, the annihilation line is effectively generated very close to the horizon but the line photons cannot escape as they are scattered in the optically thick CF (see Figure 14). This line is then observed in the IS, as demonstrated in the accompanying paper (TSC18).

When we take into account the nonlinear effect of the positron–electron (pair) generation very close to a BH horizon, we find that the surrounding photons upscattered off generated pairs form an additional hard tail extending up to a few MeV (see Figure 10). It is worth noting that the observed spectra of a few BHs demonstrated this high-energy extension (see McConnell 1994; Grove et al. 1998) but up to now there has not been any reasonable explanation of this phenomenon in the literature.

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Appendix
Analytical Derivation of Some Key Results of the Simulations

A.1. Elements of General Relativity: Photon Trajectories in Curved Space. Lengths and Optical Paths.

In flat space, the trajectory of unscattered photons is a straight line, the equation for which can be written in terms of the law of sines:

\[ r(1 - \mu^2)^{1/2} = \hat{p} \]  

(4)

where \( r \) is the length of a radius vector \( \mathbf{r} \) at a given point of the line, \( \mu = \cos \beta \) is the cosine of the zenith angle \( \beta \) between the radius vector \( \mathbf{r} \) and the straight line, and \( \hat{p} \) is the impact parameter of this line. The trajectory of unscattered photons in the Schwarzschild background is just a generalization of this law of sines (TZ98):

\[ x(1 - \mu^2)^{1/2} / (1 - 1/x)^{1/2} = p \]  

(5)

where \( x = R/R_S \) and \( R_S = 2GM/c^2 \) is the Schwarzschild radius, \( p = \hat{p}/R_S \), and \( M \) is the BH mass.

Using Equation (5) we can explain all properties of the photon trajectory in the Schwarzschild background. In other words:

(i) The photon can escape from the BH horizon to infinity or vice versa if \( p < p_0 = (6.75)^{1/2} \) (see TZ98).
(ii) The photon, for which \( p = p_0 \), undergoes circular rotation at \( x = 1.5 \) (at \( 3GM/c^2 \)).
(iii) All photons for which \( p > p_0 \) and \( x < 1.5 \) are gravitationally attracted by the BH. In this case, all photon trajectories are finite.
(iv) All photons that start at \( x > 1.5 \) and have \( p > p_0 \) escape to infinity if they are not scattered off electrons on their way out.

The photon trajectory can be presented in polar coordinates \( r \) and \( \varphi \). Using the metric of the Schwarzschild background, we can write (see Figure 11)

\[ rd\varphi = \frac{\tan \beta dr}{(1 - 1/x)^{1/2}}. \]  

(6)

Then, it follows from Equations (5) and (6) that

\[ \varphi = \int_1^x \frac{d\eta}{\eta^2 \sqrt{1/p^2 - (1 - 1/\eta)/\eta^2}}. \]  

(7)

This formula is identical to that derived in Landau & Lifshitz (1971) using the Hamilton–Jacobi (formalism) equation. In fact, the equation of the photon trajectory in polar coordinates readily follows from the law of sines (Equation (5)) and the Schwarzschild metric. Equation (7) is valid for any nonzero \( p \)-photon trajectory except a circular one at \( x_0 = 3/2 \), for which \( p_0 = (6.75)^{1/2} \). Formula (7) should be numerically calculated. From formula (5), it is evident that \( \mu_0 = 1 \) at \( x_0 = 1 \), i.e., the photon always enters a BH horizon along the radial direction.

The length of the radial trajectory \( (p = 0) \) is an integral

\[ l = r_\Sigma \int_1^x dx / \left(1 - 1/x^2\right)^{1/2}. \]  

(8)

For \( \alpha = (x - 1) \ll 1 \), the length from \( r_\Sigma \) to \( r \) is

\[ l \approx 2r_\Sigma \alpha^{1/2}. \]  

(9)

For \( x \gg 1 \), we have

\[ l \approx r_\Sigma x. \]  

(10)

The Thomson optical path on the radial trajectory from \( r_\Sigma \) to \( r \) (or from \( x = 1 \) to \( x = r/r_\Sigma \)) is

\[ T_T(r_\Sigma, r) = r_\Sigma \int_1^x \sigma_T n_e(\eta) d\eta, \]  

(11)

where \( \sigma_T \) is the Thomson cross-section and

\[ n_e(r) = \bar{m}(r_\Sigma/r)^{1/2}/(2r \sigma_T). \]  

(12)
is the electron density (see Turolla et al. 2002 for the derivation of \( n_e \)). The optical path can be found analytically as

\[
T_T(r, r_S) = \tau_T(x, 1) = \frac{m_e}{2} \int_1^x \frac{dx}{x^{3/2} \sqrt{1 - 1/x}} = \tilde{m}[\pi/2 - \arcsin(1/x)].
\]

(13)

Hence, the total radial Thomson optical depth of the CF is

\[
\tau_0 = \tau_T(\infty, 1) = (\pi/2)\tilde{m}.
\]

(14)

For the Thomson optical paths of the finite trajectories entering a BH horizon for which \( x = (x - 1) \ll 1 \), we have

\[
\tau_T(r, r_S) = \sigma_T n(r_S) l \approx m\alpha^{1/2}.
\]

(15)

A.2. Pair-creation Effect Near the BH Horizon.

The Photon Shell.

If the energetic photons have a high number density \( n_{ph} \gg 1/(\sigma_T l) \), where \( l \) is the characteristic scale of the region within which the Comptonization (in our case, the bulk motion Comptonization) takes place, then the process of electron pair production by two photons becomes important. Indeed, when a Compton-upscattered photon of energy \( E_1 \) interacts with another one of energy \( E_2 \), it may produce an electron–positron pair provided their energies satisfy the following relationship:

\[
E_1 E_2 > (m_e c^2)^2.
\]

(16)

The related cross-section for pair production \( \gamma_1 + \gamma_2 \rightarrow e^+ + e^- \) by two photons \( \sigma_{\gamma\gamma} \) (Akhiezer & Berestetsky 1965) depends on the product \( y = [E_1 E_2 / 2(m_e c^2)^2](1 - \Omega_1 \Omega_2) \), where \( (E/c) \Omega \) is the momentum for a given photon of energy \( E \). The cross-section is only nonzero when \( y > 1 \). The maximum of \( \sigma_{\gamma\gamma}(y_{\max}) \approx 0.26\sigma_T \) takes place at \( y^2 \approx 2 \).

The mean energy of the photons upscattered in the CF is (Titarchuk et al. 1997)

\[
\langle E \rangle = E_0[1 + 4/\tilde{m}]^{N_\text{sc}}.
\]

(17)

This formula is obtained without taking into account the gravitational redshift. It presumably works in the part of the CF, where \((1 - 1/x)^{1/2} \) is of order unity (namely, where \( x \gtrsim 1.2 \)). The mean number of scattering \( N_\text{sc} \sim \tilde{m} \). Then, \( \langle E \rangle / E_0 \sim 16 \) and \( \langle E \rangle = 24 \text{ keV} \) for \( \tilde{m} = 4 \) and \( E_0 = 1.5 \text{ keV} \).

These photons of energy \( \langle E \rangle \), when they propagate toward the BH horizon, are blueshifted. Their energy increases by a factor

\[
\langle E \rangle_{\text{ns}} / \langle E \rangle = 1/(1 - 1/x)^{1/2}.
\]

(18)

Photon energies of order \( m_e c^2 = 511 \text{ keV} \) and higher are achieved in the narrow shell around a BH horizon,

\[
0 < \alpha = x - 1 < (\langle E \rangle / m_e c^2)^2.
\]

(19)

For \( \langle E \rangle = 24 \text{ keV} \), we obtain that \( \alpha < 2.5 \times 10^{-3} \). For a 10 solar mass BH, the thickness of the shell where the pairs can be created due to photon–photon interactions is about 70 m. In
Figure 2, we show the average photon energy of Monte Carlo simulated spectrum as a function of radius in CF. We assume in this Monte Carlo simulation that the dimensionless accretion rate of the CF $\dot{m} = 4$ and the electron temperature $kT_e = 5$ keV. The energy of the injected soft photons is 1.5 keV. As seen from Figure 2, the average photon energy is about 25 keV at radius $R \approx 1.2 R_S$, which is very close to our estimate presented above (see Equation (17)). Also, we can see from this figure that the blueshift and Comptonization are equally important below $R = 1.02 R_S$.

The photon density in the converging inflow $n_{\text{ph}}$ near the BH horizon can be estimated using the photon flux injected in the flow, $F_{\text{inj}} = L_{\text{inj}}/E_0$. Thus,

$$n_{\text{ph}} \sim \frac{F_{\text{inj}}}{4\pi r_S^2 e} = 3 \times 10^{21}(L_{\text{inj}}/10^{37} \text{ erg s}^{-1}) \times (m/10)^{-2}(E_0/1.5 \text{ keV})^{-1} \text{ cm}^{-3},$$

and the free path for the pair creation is

$$l_{\gamma\gamma} \sim (n_{\text{ph}}0.25\sigma_T)^{-1} = 2 \times 10^{31}(L_{\text{inj}}/10^{37} \text{ erg s}^{-1})^{-1} \times (m/10)^{2}(E_0/1.5 \text{ keV}) \text{ cm}. \quad (21)$$

The typical length of the photon trajectories $l_{\text{cross}}$ in the shell of width $\alpha$ can be estimated using formula (9),

$$l_{\text{cross}} = 2\alpha^{1/2}R_S > 3 \times 10^2(m/10) \text{ cm}, \quad (22)$$

for $\alpha = 2.5 \times 10^{-3}$. So, the shell photons have enough time to create pairs because

$$t_{\text{cross}}/t_{\gamma\gamma} = l_{\text{cross}}/l_{\gamma\gamma} \gg 1. \quad (23)$$

The optical depth for the pair creation is

$$\tau_{\gamma\gamma} = l_{\text{cross}}/l_{\gamma\gamma} > 150(L_{\text{inj}}/10^{37} \text{ erg s}^{-1}) \times (m/10)^{-1}(E_0/1.5 \text{ keV})^{-1}. \quad (24)$$

A.3. The Pair Spectrum

The spectrum of the created pairs in the photon shell can be calculated using the shell photon spectrum. In Figure 12, we show the Monte Carlo photon spectra computed for three different radius ranges in the flow. The black histogram is the emergent spectrum seen by observers on Earth. The green histogram is the spectrum seen by observers staying at the radial distance $R = (1 - 1.1)R_S$ from the BH. The blue histogram is the spectrum for observers staying at the radial distance $R = (1 - 1.01)R_S$.

As we argue above, the pairs have to be created in the shell very close to the horizon. As seen from the shell photon spectrum presented in Figure 12 (blue histogram there), there are plenty of photons with energy much higher than 511 keV that along with photons with energies between 10 and 100 keV (see the bump in the blue histogram) can create a noticeable number of pairs. The photon spectrum is quite flat, with the index of the high-energy power-law part being about
1.2 (1.2 ± 0.1). It is worth pointing out that the shape of the spectrum is very close to a broken power law.

Because of the gravitational blueshift and upscattering, the peak of the spectrum is located at energies of about 25 keV, which is 17 times more than the energy of the injected soft photons (1.5 keV). The photon index of 1.2 is a typical index for the saturation Comptonization. In fact, the photon index $\Gamma$ can be calculated (see Titarchuk & Lyubarskij 1996, hereafter TL95; Ebisawa et al. 1996) as

$$\Gamma = 1 + \frac{\ln(1/P)}{\ln(1 + \eta)},$$

where $P$ is the probability of photon scattering in a cloud (shell) and $1 + \eta = \langle E' \rangle/E$ is the mean efficiency of the photon energy change at any scattering of photon off electrons. According to TL95 (in their notation, the scattering probability is $\lambda$),

$$1/P = \exp(\beta) = [\tau \ln(1.53/\tau)]^{-1}.\tag{26}$$

This formula is derived for the plane geometry and $\tau \ll 1$.

In the photon horizon shell, the bulk velocity of the flow $v$ is very close to the speed of light, $v = c(r/r_0)^{3/2}$. For $R = 1.01r_0$, the Lorentz factor $\gamma = (1 - (v/c)^2)^{-1/2} = 10$. The mean efficiency (see, e.g., Pozdnyakov et al. 1983) is

$$\langle E' \rangle/E = 1 + \eta = [1 + \frac{4}{3}(\gamma^2 - 1)].\tag{27}$$

For $\dot{m} = 4$, the shell optical depth $\tau \approx 0.4$ (see Equation (15)). We assume for this estimate that $\alpha = (R - R_0)/R_0 = 0.01$. We obtain the photon index $\Gamma \sim 1.13$ using formulae (25)–(27), where we put $\gamma = 10$ and $\tau = 0.4$. This value of $\Gamma = 1.13$ is very close to that obtained in our MC simulations, $\Gamma = 1.2 \pm 0.1$.

The spectrum of the electrons (positrons), the so-called differential yield of the pairs produced by the annihilation of two photons, is proportional to the rate of the number of collisions in a given volume (shell). In general terms, this rate of the number of collisions $\dot{N}_{\text{col}}$ is calculated according to Landau & Lifshitz (1971) as follows

$$\dot{N}_{\text{col}} = n_0(\gamma_+) = C_f c \int_0^{\infty} n_{\text{ph}}(\epsilon_1) d\epsilon_1$$

$$\int_0^{\infty} n_{\text{ph}}(\epsilon_2) \sigma(\gamma_-, \epsilon_1, \epsilon_2) d\epsilon_2,$$

where $\epsilon = E/m_e c^2$ is the dimensionless photon energy, $\gamma_-$ and $\gamma_+$ are the Lorentz factors of the electron/positron, $\sigma(\gamma_-, \epsilon_1, \epsilon_2)$ is the differential cross-section of the pair-production cross-section, and the factor $C_f$ is less than 1.

Formula (28) is valid for an isotropic radiation field where $\sigma(\gamma_-, \epsilon_1, \epsilon_2)$ is the differential cross-section of the pair-production cross-section averaged over a solid angle and $C_f = 1/4$ (see Bottcher & Schlickeiser 1997). In our MC simulation, we implement the exact form of the cross-section where the angular dependence has been included. However, we want to demonstrate that formula (28) (formally derived for
The exact but quite complicated expression for this formula was derived by Bottcher & Schlickeiser (1997). Now, let us consider the simple approximations of formula (28) and compare them with that obtained in the simulations. The first approximation of formula (28) is related to a δ-function approximation of the cross-section suggested by Zdziarski & Lightman (1985, hereafter ZL85),

\[
\sigma' (\gamma, \epsilon_1, \epsilon_2) \approx \frac{1}{3} \sigma_T \epsilon_2 \delta\left(\frac{\epsilon_1}{2} - \gamma_\cdot\right) \delta\left(2 \epsilon_1 - \epsilon_2\right). \tag{29}
\]

To justify this cross-section approximation, ZL85 argue that the photons with \(\epsilon_1 \gg 1\) will produce \(e^+e^-\) pairs mostly with \(\gamma^- \approx \gamma_\cdot \approx \epsilon/2\) (Bonometto & Rees 1971) while colliding with photons of energies of \(\epsilon_2 \approx 2/\epsilon_1\) (Herterich 1974).

The integration in formula (28) using Equation (29) leads to

\[
\Gamma_{\text{pair}} \approx \frac{1}{\gamma_\cdot} c \sigma_T n_{\text{ph}}(1/\gamma_\cdot)n_{\text{ph}}(2 \gamma_\cdot). \tag{30}
\]

\(\Gamma_{\text{pair}}\) should be around 2.5 because the photon index of \(n_{\text{ph}}(1/\gamma_\cdot)\) is about 0.5 for \(1/\gamma_\cdot \ll 1\) and that of \(n_{\text{ph}}(2 \gamma_\cdot)\) is around 1 (see Figure 12). In Figure 13, we present the simulation results for pair energy distribution. As one can see, the simulated pair spectrum is well approximated by a power law of index 2.5.

ORCID iDs
Philippe Laurent @ https://orcid.org/0000-0001-9094-0335
Lev Titarchuk @ https://orcid.org/0000-0002-9998-7591

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