X-ray bursting neutron star atmosphere models using an exact relativistic kinetic equation for Compton scattering

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\textbf{ABSTRACT}

\textbf{Context.} Theoretical spectra of X-ray bursting neutron star (NS) model atmospheres are widely used to determine the basic NS parameters such as their masses and radii. Compton scattering, which plays an important role in spectra formation at high luminosities, is often accounted for using the differential Kompaneets operator, while in other models a more general, integral operator for the Compton scattering kernel is used.

\textbf{Aims.} We construct accurate NS atmosphere models using for the first time an exact treatment of Compton scattering via the integral relativistic kinetic equation. We also test various approximations to the Compton scattering redistribution function and compare the results with the previous calculations based on the Kompaneets operator.

\textbf{Methods.} We solve the radiation transfer equation together with the hydrostatic equilibrium equation accounting exactly for the radiation pressure by electron scattering. We use the exact relativistic angle-dependent redistribution function as well as its simple approximate representations.

\textbf{Results.} We thus construct a new set of plane-parallel atmosphere models in local thermodynamic equilibrium (LTE) for hot NSs. The models were computed for six chemical compositions (pure H, pure He, solar H/He mix with various heavy elements abundances $Z = 1, 0.3, 0.1,$ and $0.01 Z_{\odot}$, and three surface gravities $\log g = 14.0, 14.3,$ and $14.6$. For each chemical composition and surface gravity, we compute more than 26 model atmospheres with various luminosities relative to the Eddington luminosity $L_{\text{Edd}}$ computed for the Thomson cross-section. The maximum relative luminosities $L/L_{\text{Edd}}$ reach values of up to 1.1 for high gravity models. The emergent spectra of all models are redshifted and fitted by diluted blackbody spectra in the $3−20$ keV energy range appropriate for the RXTE/PCA. We also compute the color correction factors $f_c$.

\textbf{Conclusions.} The radiative acceleration $g_{\text{rad}}$ in our luminous, hot-atmosphere models is significantly smaller than in corresponding models based on the Kompaneets operator, because of the Klein-Nishina reduction of the electron scattering cross-section, and therefore formally “super-Eddington” model atmospheres do exist. The differences between the new and old model atmospheres are small for $L/L_{\text{Edd}} < 0.8$. For the same $g_{\text{rad}}/g$, the new $f_c$ are slightly larger (by approximately 1%) than the old values. We also find that the model atmospheres, the emergent spectra, and the color correction factor computed using angle-averaged and approximate Compton scattering kernels differ from the exact solutions by less than 2%.

\textbf{Key words.} radiative transfer – scattering – methods: numerical – stars: atmospheres – stars: neutron – X-rays: stars

1. Introduction

X-ray bursting neutron stars (NSs) are members of low-mass X-ray binaries with quasi-periodical thermonuclear flashes on their surfaces (see reviews by Lewin et al. 1993; Strohmayer & Bildsten 2006). Thermonuclear burning occurs at the bottom of the freshly accreted matter and can be so powerful that the luminosity reaches the Eddington limit. These bursts lead to photospheric radius expansion (PRE) and are a potentially powerful tool for determining the NS masses and radii (EbisuZaki 1987; Damen et al. 1990; van Paradijs et al. 1990). The knowledge of NS basic parameters is extremely important for establishing the physical properties (equation of state) of supra-nuclear dense matter in the NS inner cores (see Lattimer & Prakash 2007, for a review).

The precise radius determination of the NSs from X-ray bursts is impossible without accurate spectral models. The observed spectra of X-ray bursts are often well-fitted by a blackbody (Galloway et al. 2008). Theoretical models of hot NS atmospheres show (London et al. 1986; Lapidus et al. 1986; Pavlov et al. 1991) that the emergent spectra are close to diluted blackbody spectra $F_\text{E} \approx f_c^{-2}B_{\lambda}(f_c T_{\text{eff}})$ owing to strong energy exchange caused by Compton scattering. The color correction factor $f_c \equiv T_{\text{eff}}/T_{\text{c}}$, which relates the color temperature of the spectrum $T_{\text{c}}$ to the effective temperature of the atmosphere $T_{\text{eff}}$, takes values of about 1.3−1.9. Theoretical dependences of the color correction factor on luminosity for various chemical compositions and gravities were computed by Suleimanov et al. (2011b, hereafter SPW11). The atmosphere the physical properties (equation of state) of supra-nuclear dense matter in the NS inner cores (see Lattimer & Prakash 2007, for a review).
and the relative NS luminosity $l = L/L_{\text{Edd}}$, where $L_{\text{Edd}}$ is the Eddington luminosity measured at the NS surface
\begin{equation}
L_{\text{Edd}} = \frac{4\pi G M c}{\kappa_e} (1 + z),
\end{equation}
for the Thomson scattering opacity
\begin{equation}
\kappa_e = \sigma_T N_e / \rho = 0.2 (1 + X) \text{ cm}^2 \text{ g}^{-1}.
\end{equation}
Here $\sigma_T = 6.65 \times 10^{-25} \text{ cm}^2$ is the Thomson cross-section, $\rho$ is the gas density, and $N_e$ is the electron number density. The gravitational redshift is related to the NS parameters as
\begin{equation}
1 + z = (1 - 2GM/c^2R)^{-1/2}.
\end{equation}
We assume that the flux is constant throughout the NS surface. Our calculations are valid for a patch on the NS surface if instead of the relative luminosity we consider the relative flux, $l = F/F_{\text{Edd}}^*$ as a parameter, where
\begin{equation}
F_{\text{Edd}}^* = \frac{L_{\text{Edd}}}{4\pi R^2} = \frac{G M c}{R^2\kappa_e} (1 + z).
\end{equation}
The effective temperature $T_{\text{eff}}$ can be expressed via $l$ as
\begin{equation}
T_{\text{eff}} = l^{1/4} T_{\text{Edd}},
\end{equation}
where the Eddington temperature $T_{\text{Edd}}$ is the maximum possible effective temperature on the NS surface, which is evaluated using the Thomson scattering opacity
\begin{equation}
\sigma_{SB} T_{\text{Edd}}^4 = F_{\text{Edd}}^* = \frac{g c}{\kappa_e}.
\end{equation}
The structure of the atmosphere for an X-ray bursting NS is described by a set of differential equations. The first one is the hydrostatic equilibrium equation
\begin{equation}
\frac{dP_g}{dm} = g - g_{\text{rad}},
\end{equation}
where $g_{\text{rad}}$ is the radiative acceleration and $P_g$ is the gas pressure and the column density $m$ is defined as
\begin{equation}
dm = -\rho \, ds,
\end{equation}
where $s$ is the vertical distance.

The second equation is the radiation transfer equation for the specific intensity $I(x, \mu)$ accounting for Compton scattering (see Appendix A for derivation). In the plane-parallel approximation, it has the form
\begin{equation}
\frac{dI(x, \mu)}{d\tau(x, \mu)} = I(x, \mu) - S(x, \mu),
\end{equation}
where
\begin{equation}
d\tau(x, \mu) = [\sigma(x, \mu) + k(x)] \, dm,
\end{equation}
$\mu = \cos \theta$ is the cosine of the angle between the surface normal and the direction of radiation propagation, $x = h\nu/m_e c^2$ is the photon energy in units of electron rest mass, and $k(x)$ is the “true” absorption opacity. The electron scattering opacity accounting for the induced scattering is
\begin{equation}
\sigma(x, \mu) = \kappa_e \frac{1}{X} \int_x^\infty \partial_1 R(x_1, \mu_1; x, \mu) \left(1 + \frac{C I(x_1, \mu_1)}{x_1^3}\right),
\end{equation}
and the relative NS luminosity $l = L/L_{\text{Edd}}$, where $L_{\text{Edd}}$ is the Eddington luminosity measured at the NS surface
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\begin{equation}
\mu \frac{dI(x, \mu)}{d\tau(x, \mu)} = I(x, \mu) - S(x, \mu),
\end{equation}
where
\begin{equation}
d\tau(x, \mu) = [\sigma(x, \mu) + k(x)] \, dm,
\end{equation}
$\mu = \cos \theta$ is the cosine of the angle between the surface normal and the direction of radiation propagation, $x = h\nu/m_e c^2$ is the photon energy in units of electron rest mass, and $k(x)$ is the “true” absorption opacity. The electron scattering opacity accounting for the induced scattering is
\begin{equation}
\sigma(x, \mu) = \kappa_e \frac{1}{X} \int_x^\infty \partial_1 R(x_1, \mu_1; x, \mu) \left(1 + \frac{C I(x_1, \mu_1)}{x_1^3}\right),
\end{equation}
and
\[ C = \frac{1}{2m_e} \left( \frac{\hbar}{m_e c^2} \right)^3. \]

The source function is a sum of the thermal part and the scattering part
\[ S(x, \mu) = \frac{k(x)}{\sigma(x, \mu) + k(x)} B_x + \frac{\kappa_e}{\sigma(x, \mu) + k(x)} \times \left( 1 + \frac{C(x, \mu)}{x} \right) x^2 \int_0^{\infty} dx_1 x_1 \int_{-1}^{1} d\mu_1 R(x, \mu; x_1, \mu_1) I(x_1, \mu_1), \]
with the dimensionless energy cosine of the angle between the directions of the photon propagating in the direction corresponding to \( \mu_1 \) scattered to energy \( x \) and in a direction corresponding to \( \mu \). This function is found by integrating over the azimuthal angle \( \varphi \) of the RF \( R(x, x_1, \eta) \), which depends on the cosine of the angle between the directions of the photon propagation before and after scattering \( \eta \)
\[ R(x, \mu; x_1, \mu_1) = \int_0^{2\pi} R(x, x_1, \eta) d\varphi, \]
\[ \eta = \mu_1 + \sqrt{1 - \mu^2} \sqrt{1 - \mu_1^2} \cos \varphi. \]

The RF depends on the depth \( s \) through the electron temperature and satisfies the relation (see Eq. (A.7))
\[ R(x_1, \mu_1; x, \mu) = R(x, \mu; x_1, \mu_1) \exp \left( \frac{x - x_1}{\Theta} \right). \]

which is the consequence of the detailed balance relation (Pomraning 1973; Nagirner & Poutanen 1994, see Appendix A). This implies that the source function given by Eq. (14) equals the Planck function for the photon field described by the Bose-Einstein distribution of any chemical potential.

In this paper, we use two RFs for Compton scattering. The first one is the fully relativistic exact RF valid for any photon energy and electron temperature (Aharonian & Atoyan 1981; Nagirner & Poutanen 1993, 1994; Poutanen & Svensson 1996, see Eqs. (A.18) and (A.22) in Appendix A.2). The second one is an approximate RF corresponding to the isotropic scattering in the electron rest frame (Eq. (A.26) in Appendix A.2), which is accurate at temperatures below about 100 keV and non-relativistic photon energies (Arutyunyan & Nikogosyan 1980; Poutanen 1994; Poutanen & Svensson 1996). In both cases, we also consider the angle-averaged RFs
\[ R(x, x_1) = \frac{1}{2} \int_{-1}^{1} d\eta R(x, x_1, \eta). \]

The formal solution of the radiation transfer Eq. (10) is obtained using the short-characteristic method (Olson & Künzner 1987) in three angles in each hemisphere, and the full solution is found with an accelerated \( \Lambda \)-iteration method (see details in Appendix B).

The radiation pressure acceleration \( g_{\text{rad}} \) is computed using the RF as
\[ g_{\text{rad}} = \frac{dP_{\text{rad}}}{dm} = \frac{2\pi}{c} \int_0^{\infty} dx \int_{-1}^{1} \mu^2 I(x, \mu) d\mu. \]

where the derivative with respect to \( m \) is replaced by the first moment of the radiation transfer Eq. (10). When the source functions and the opacities are isotropic, this expression is reduced to the standard definition
\[ g_{\text{rad}} = \frac{4\pi}{c} \int_0^{\infty} [\sigma(x) + k(x)] H_\ell(m) dx, \]
where
\[ H_\ell = \frac{1}{2} \int_{-1}^{1} \mu I(x, \mu) d\mu \]
is the first moment of specific intensity. These equations are completed by the energy balance equation
\[ \int_0^{\infty} dx \int_{-1}^{1} [\sigma(x) + k(x)] [I(x, \mu) - S(x, \mu)] d\mu = 0, \]
the ideal gas law
\[ P_g = N_{\text{tot}} kT, \]
where \( N_{\text{tot}} \) is the number density of all particles, and the particle and charge conservation equations. In our calculations, we assumed local thermodynamic equilibrium (LTE), therefore the number densities of all ionization and excitation states of all elements were calculated using the Boltzmann and Saha equations. We accounted for the pressure ionization effects on hydrogen and helium populations using the occupation probability formalism (Hummer & Mihalas 1988) as described by Hubeny et al. (1994). In addition to electron scattering, we took into account the free-free opacity as well as the bound-free transitions for all ions of the 15 most abundant chemical elements (H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe, Ni) (see Ibragimov et al. 2003) using opacities from Verner & Yakovlev (1995).

2.2. Method of solution

To solve the above equations, we used our version of the computer code ATLAS (Kurucz 1970, 1993), modified to deal with high temperatures (Suleimanov & Poutanen 2006; Suleimanov & Werner 2007). The code was further developed to account for Compton scattering using the RF approach.

In our computations, we used 300–360 logarithmically equidistant frequency points in the range \( 10^{14} - 10^{19} \) Hz (\( \approx 4 \times 10^{-4} - 400 \) keV) for the luminous model atmospheres \( f \geq 0.1 \), and \( 10^{14} - 10^{19} \) Hz for \( f < 0.1 \). The calculations were performed at a set of 98 depth points \( m_i \) distributed equidistantly on the logarithmic scale from \( 10^{-6} \) to \( m_{\text{max}} = 10^5 \) g cm\(^{-2}\). The appropriate value of \( m_{\text{max}} \) was chosen to satisfy the condition \( \sqrt{\tau_{\text{sh}, f-t-f}(m_{\text{max}})} \tau_{\text{sh}}(m_{\text{max}}) > 1 \) at all frequencies, where \( \tau_{\text{sh}, f-t-f} \) is the optical depth computed with the true opacity only (bound-free and free-free transitions, without scattering). This requirement was necessary for satisfying the inner boundary condition of the radiation transfer problem.
The course of the calculations was the same as for the method that adopts the Kompaneets operator (SPW11). First, a starting grey atmosphere model was calculated and opacities at all depth points and all frequencies were obtained. The solution of the radiative transfer Eq. (10) was checked for the energy balance Eq. (23), together with the surface flux condition and the energy balance error

\[ \varepsilon_{\text{ff}} = 1 - \frac{H_0}{\int_0^\infty H_x(m)\,dx}, \]

and the energy balance error

\[ \varepsilon_A(m) = \frac{1}{2} \left[ \int_0^\infty \left( \int_{-1}^1 \left( \sigma(x,\mu) + \sigma_{\text{CS}}(x,\mu) \right) \left[ I(x,\mu) - S(x,\mu) \right] \,d\mu \right) \,dx \right] \]

were calculated as functions of depth. Temperature corrections were then evaluated using three different procedures. In the upper atmospheric layers, we used the integral A-iteration method, modified for Compton scattering, based on the energy balance Eq. (23). The temperature correction for a particular depth was found as

\[ \Delta T_A = -\varepsilon_A(m) \left( \int_0^\infty \left[ \frac{\Lambda_d(x) - 1}{1 - \alpha(x)\Lambda_d(x)} \right] k(x) \frac{dB_x}{dT} \,dx \right)^{-1}, \]

where \( \alpha(x) = \sigma_{\text{CS}}(x)/k(x) + \sigma_{\text{CS}}(x) \), and \( \Lambda_d(x) \) is the diagonal matrix element of the \( \Lambda \)-operator. Here \( \sigma_{\text{CS}}(x) \) is the Compton scattering opacity averaged over the relativistic Maxwellian electron distribution (see Eq. (A16) in Poutanen & Svensson 1996, which is equivalent to Eq. (12) if one ignores the induced scattering). In the deep layers, we used the Avrett-Krook flux correction based on the relative flux error \( \varepsilon_{\text{ff}}(m) \). Finally, the third procedure was the surface correction based on the emergent flux error (see Kurucz 1970, for a detailed description of the methods).

The iteration procedure is repeated until the relative flux error is smaller than 0.1%, and the relative flux derivative error is smaller than 0.01%. As a result, we obtain a self-consistent NS model atmosphere, together with the emergent spectrum of radiation. We note that this accuracy is unachievable for luminous models with \( g_{\text{rad}} \approx g \), and that these models can have larger relative flux errors, up to 2–3%.

### 2.3. Accuracy of computation

To compute a new extended set of hot NS model atmospheres, we accelerated the convergence of the iterations of the radiation transfer equation by using the source function from the previous temperature iteration as the first approximation (see Appendix B). However, in every fifth temperature iteration the radiation transfer equation was solved using the pure thermal source function as a first approximation. We compared a pure hydrogen model atmosphere computed for \( T_{\text{eff}} = 1.8 \times 10^7 \) K and \( \log g = 14.0 \) (the fiducial model) using this accelerated approach with the model computed without acceleration. The temperature structures differ by less than 0.3%, and the differences between the emergent spectra are about 1% in the 3–20 keV energy range (typical of RXTE/PCA) and larger in the Wien tail (Fig. 1).

Fig. 1. Emergent spectrum (top panel) and temperature structure (bottom panel) of the fiducial model (pure hydrogen, \( T_{\text{eff}} = 1.8 \times 10^7 \) K, \( \log g = 14.0 \)) computed using three different methods. In accurate method 1 every \( \Lambda \)-iteration starts from the thermal part of the source function (solid curves give the results for the relative accuracy of \( 10^{-4} \)). In accelerated method 2, the \( \Lambda \)-iterations start from the source function taken from previous temperature iteration, but at every fifth temperature correction they start from the thermal part of the source function (dashed curves show results for the relative accuracy of \( 10^{-5} \)). Method 3 is the same as method 2, but for the relative accuracy of \( 10^{-3} \) (dotted-dashed curve). In the top lower panel, the ratios of the spectra for methods 2 and 3 to the spectrum computed with method 1 are shown. The ratio of the temperature structures computed using methods 2 and 1 is shown in the bottom lower panel.

2.4. Various RFs and the Kompaneets operator

A comparison of model atmospheres, which were computed using our new code with four different RFs (exact angle-dependent, exact angle-averaged, approximate angle-dependent, and approximate angle-averaged) is shown in the left panels of Fig. 2. The model computed using the approximate angle-dependent RF is almost indistinguishable from the reference model calculated using the exact angle-dependent RF. This is unsurprising, because the approximate function matches the accurate one very well up to the temperatures of about 100 keV. Similar

\[ 4\pi \int_0^\infty H_x(m = 0)\,dx = 4\pi H_0 = \sigma_{SB}T_{\text{eff}}. \]

in the mean intensity at all depths and energies. To determine the uncertainty in the final spectrum caused by this criterion, we compared the emergent spectra computed for the same model atmosphere with the accuracies of \( 10^{-4} \) and \( 10^{-5} \) (see top panel of Fig. 1). We see that the relative error is smaller than 1% at all energies, which is then the intrinsic accuracy of our model spectra. We note that a similar error is introduced into the angular dependence of the specific intensities by ignoring polarization (see e.g. Chandrasekhar 1960, compare his Tables XV and XXIV).
results were obtained by Poutanen & Svensson (1996) for the Comptonization spectra in the optically thin slabs. The differences are smaller than 1% for the emergent spectra and below 0.3% for the temperature structure. Deviations of model atmospheres computed using the angle-averaged RF of the reference model are more significant, at about 2% for both the temperature structure and spectra.

The model atmosphere calculated employing the Kompaneets operator has more significant differences from the reference model (see right panels in Fig. 2), of up to 10% in the temperature structure and about 3−4% in the emergent flux at 1 keV. The deviations are much smaller (<1%) near the spectral maximum and larger in the Wien tail. A rather good agreement between model atmospheres computed with the relativistic exact angle-dependent RF and the non-relativistic angle-independent Kompaneets operator again is unsurprising, because temperatures of the upper atmosphere layers where the emergent spectra form are sufficiently low (∼2−4 keV) and relativistic corrections are small.

3. New grid of models
3.1. General properties

We computed a new set of hot NS model atmospheres using the exact relativistic angle-dependent RF. The models were calculated for six chemical compositions (pure hydrogen, pure helium, and solar hydrogen/helium mix with various heavy element abundances: of solar and 0.3, 0.1 and 0.01 of solar). For every chemical composition, 26−28 models with relative luminosities spanning the interval from $l = 0.001$ to $1.06−1.10$ for three values of the surface gravity ($\log g = 14.0, 14.3$ and $14.6$) were calculated. Because the radiative acceleration in our models is smaller than in the models based on the Thomson opacity owing to the Klein-Nishina reduction in the cross-section (see below), there exist formally “super-Eddington” (relative to $L_{\text{Edd}}$) models. The Klein-Nishina reduction depends on the electron temperature, which is higher for larger surface gravities, therefore the limiting luminosity is higher for larger log $g$.

Examples of emergent spectra and temperature structures for the models with log $g = 14.0$ and various chemical compositions (pure hydrogen and solar mix) are shown in Fig. 3. The corresponding emergent spectra and temperature structures computed with the old code employing the Kompaneets operator are also shown. At low luminosities, the models are very close to each other, which is expected as at low temperatures the diffusion (Kompaneets) approximation is an accurate representation of Compton scattering. For models close to the Eddington limit, the treatment of the radiative acceleration becomes important. Contribution of the radiation force to the hydrostatic equilibrium $g_{\text{rad}}/g$ is smaller in the new models despite $l$ being the same for both model sets. It is well-known that the model spectra with large contributions of radiative acceleration are harder, and their surface temperatures are higher (London et al. 1986; Lapidus et al. 1986; Ebisuzaki 1987; Pavlov et al. 1991). In

1 The spectral energy distributions of fluxes and specific intensities for all models are described in Appendix D.
complete agreement with this, the old models with large $l$ are harder and hotter than new models. However, for the same $g_{rad}/g$ the new model spectra are hotter. Normalizing the spectra to the maximum flux and plotting them against the scaled photon energies $E/kT_{eff}$, one also sees that the new spectra are harder (see Fig. 4).

### 3.2. Limb-darkening

Knowledge of the angular distribution of the emergent radiation is important when only part of the star is visible (for example, is partially blocked by the accretion disk), or when there are inhomogeneities at the NS surface related, for example, to the varying gravitational acceleration due to the rapid rotation. Computation of the amplitude of reflection from the accretion disk also requires that information. The limb-darkening law (i.e. angular dependence of the intensity) for the radiation emerging from the optically thick electron-scattering-dominated atmosphere is described by the $H(0)(\mu)$ function (Chandrasekhar & Breen 1947; Chandrasekhar 1960; Sobolev 1949, 1963). A simple approximation to this function is $I(\mu) = 1 + 2.06\mu$. Our simulations show that the intensity closely (within a couple of percents) follows the $H(0)(\mu)$ function around the peak of the spectrum, in the observed energy range (see Fig. 5). At photon energies below 1 keV, the computed angular distribution becomes more isotropic, because there free-free absorption dominates over electron scattering and the upper atmosphere layers are almost isothermal. The low-inclination intensity is above and the high-inclination intensity is below the electron-scattering limb-darkening law at energies above the peak, because the temperature of the layer where the photons originate drops with the inclination. The iron absorption edge at $\sim 9$ keV significantly affects the angular distribution for the solar abundance models (Fig. 5, bottom panel). Above the edge, radiation becomes more directed along the surface normal.

The angular distribution of the intensity also depends on the specific form of the RF used in the calculations. The approximate angle-dependent gives results very close to the reference intensity spectra, within 2% for the largest angle $\theta$ (see Fig. 6, bottom panel).
top panel). The exact, but angle-averaged, RF, does not give such accurate results (see Fig. 6, bottom panel).

### 3.3. Color correction factors

All computed emergent spectra of the new atmosphere models were fitted by a diluted blackbody spectrum

\[ F_E \approx w B_E (f_c T_{\text{eff}}) \]  

(29)

using five different fitting procedures described in SPW11. We calculated the color correction \( f_c \) and dilution \( w \) factors in the energy band \((3-20) \times (1+z) \) keV corresponding to the observed range of the RXTE/PCA detector. We calculated redshifts from \( \log g \) by adopting a NS mass equal to 1.4 \( M_\odot \) (see Eqs. (1) and (4)): for \( \log g = 14.0, 14.3, \) and 14.6, we get \( R = 14.80, 10.88, 8.16 \) km and \( z = 0.18, 0.27, 0.42, \) respectively. Varying the mass in the interval \( 1-2 M_\odot \) has a smaller than 0.1% effect on the color corrections (SPW11). The results of the fitting procedures are presented in Table 1 (see also Appendix D).

Deviations of the new model spectra from the best-fit diluted blackbodies are similar to those for the old spectra based on the Kompaneets operator (Fig. 7). Comparison of the new and old color correction factors is shown in Figs. 8 and 9. Although the old \( f_c-l \) dependences for different gravities were almost identical at high luminosities, we see that now these dependences deviate, because of the dependence of the limiting relative luminosity on \( \log g \). However, the old and new color-correction factors have very similar dependences on \( g_{\text{rad}}/g \) for all \( \log g \) and chemical compositions (see Figs. 8 and 9), with the new \( f_c \) being about 1% larger. The difference grows at \( g_{\text{rad}}/g \) close to unity.

Pavlov et al. (1991) derived an approximate analytical formula for the ratio of the surface model atmosphere temperature to the effective one

\[ \frac{T_{\text{surf}}}{T_{\text{eff}}} \approx \left( 0.14 \ln \frac{3 + 5X}{1-l} + 0.59 \right)^{-4/5} \left( \frac{3 + 5X}{1-l} \right)^{2/15} l^{3/20}, \]  

(30)

which is correct for the highly luminous \((l > 0.9) \) model atmospheres. The numerical constants 0.14 and 0.59 were found from the fitting of their model atmospheres based on the Kompaneets operator description of Compton scattering. If the models were instead computed using an exact RF for Compton scattering, it is obvious that \( l \) should be substituted by the relative radiation acceleration \( g_{\text{rad}}/g \). We fit our color correction factors computed using the first fitting procedure (see SPW11) with a formula similar to Eq. (30) and found numerical constants that also depend
3.4. Radiative acceleration

Notes. Results for other chemical compositions and gravities are given in Table D.1 available in electronic form at the CDS.

This approximation is based on calculations by Buchler & Yueh (1976), who underestimated the opacity at low temperatures, but the dependence on the surface gravity is stronger.

where certain approximations were made because of severe numerical problems. A better approximation in the range 2–50 keV that is of interest here is (J. Poutanen et al., in prep.)

\[ \kappa_{R}(T) \approx \kappa_{e} \left[ 1 + \left( \frac{kt}{39.4 \text{ keV}} \right)^{0.976} \right]^{-1} \]  

(35)

It is clear that the radiative acceleration decreases in the deep, hotter atmosphere layers and the ratio of radiation pressure force to the surface gravity decreases inwards (see Fig. 11). The radiative acceleration is smaller than that corresponding to the Thomson opacity, even in the upper atmosphere layers. The actual radiative acceleration in the surface layers (see top panel in Fig. 11) computed from the models using Eq. (20) is perfectly described by Eqs. (35) and (33) throughout the whole atmosphere (compare dotted and solid curves at the top panel in Fig. 11), while Paczynski’s approximation underestimates it.

Radiative acceleration computed using the angle-averaged RFs is larger than that computed using angle-dependent RFs (see bottom panel in Fig. 11), because the high-energy photons scatter on the relatively cold electrons in a predominantly forward direction, reducing the magnitude of the momentum transfer in comparison with the isotropic case.

Radiative acceleration in the surface layers that we obtain from the models can be expressed through \( T_{\text{eff}} \) and \( f_{e} \) as

\[ \kappa_{R}(T) \approx \kappa_{e} \left[ 1 + \left( \frac{kt}{38.8 \text{ keV}} \right)^{0.86} \right]^{-1} \]  

(36)

where \( \alpha_{e} = 1.01 + 0.067 (\log g - 14.0) \) (see Fig. 12). The relation \( g_{\text{rad}}/g - l \) also slightly depends on the chemical composition, but the dependence on the surface gravity is stronger.

on the chemical composition

\[ f_{c} \approx \left( \frac{0.102 + 0.008X}{100} \right) \left[ \frac{3 + 5X}{1 - g_{\text{rad}}/g} + 0.63 - 0.06X \right]^{-4/5} \]

\[ \times \left( \frac{3 + 5X}{1 - g_{\text{rad}}/g} \right)^{2/15} \left( g_{\text{rad}}/g \right)^{3/20}. \]  

(31)

This approximation works well for \( g_{\text{rad}}/g > 0.8 \) (see Fig. 10).

The radiative acceleration can formally be represented as a product of the flux and the temperature-dependent effective opacity

\[ g_{\text{rad}} = \kappa(T) \frac{\sigma_{SB} T_{\text{eff}}^{4}}{c}. \]  

(32)

This expression can alternatively be written as

\[ g_{\text{rad}} = l \frac{\kappa(T)}{\kappa_{e}}. \]  

(33)

In diffusion approximation, \( \kappa(T) \) is given by the Rosseland mean opacity. When electron scattering dominates, it is often approximated (neglecting the electron degeneracy) as (Paczynski 1983)

\[ \kappa(T) = \kappa_{R}(T) \approx \kappa_{e} \left[ 1 + \left( \frac{kt}{38.8 \text{ keV}} \right)^{0.86} \right]^{-1}. \]  

(34)

This approximation is based on calculations by Buchler & Yueh (1976), who underestimated the opacity at low temperatures,
The relation of the effective temperature to the effective opacity given by Eq. (36) allows us to estimate $\sigma_{\text{grad}}/g$ for the given model parameters $(l, T_{\text{eff}})$ without actually computing the atmosphere models. We can make a first guess of $f_c$, substitute $T = f_c T_{\text{eff}}$ to Eq. (36), then use this $\kappa$ in Eq. (33), find a new $f_c$ through Eq. (31), and iterate.

4. Application to observations

In our previous works (S11 and SPW11), we suggested a new method for the determination of NS radii and masses. It is based on the spectral (blackbody) normalization $K$ at late phases of PRE X-ray bursts depending on the color correction factor only

$$K \equiv \left( \frac{R_{\text{bb}}(\text{km})}{D_{10}} \right)^2 = \frac{1}{f_c^2} \left( \frac{R(\text{km})(1+z)}{D_{10}} \right)^2 = (A f_c)^{-4},$$  \hspace{1cm} (37)

where $D_{10} = D/10$ kpc is the distance. The observed relation $K^{-1/4} - F_{\text{bb}}$ between the blackbody flux $F_{\text{bb}}$ and normalization $K$ can be fitted by the theoretical dependence $f_c - l$ obtained from the atmosphere models. The fit gives two parameters: the value of $A = [R(\text{km})(1+z)/D_{10}]^{-1/2}$ and the observed Eddington flux $F_{\text{Edd}} = L_{\text{Edd}} (1+z)^{-2}/(4\pi D^2)$. The distance-dependent quantities $A$ and $F_{\text{Edd}}$ can be combined to the distance-independent Eddington temperature which is the apparent effective temperature corresponding to $L_{\text{Edd}}$:

$$T_{\text{Edd,lo}} = \left( \frac{g c}{\sigma_T K_c} \right)^{1/4} \frac{1}{1+z} = 6.4 \times 10^9 A F_{\text{Edd,lo}}^{1/4} K_c.$$  \hspace{1cm} (38)

If the distance to the source is known (for example, for sources in globular clusters), we can plot three curves on the $M - R$ plane corresponding to the values of $A$, $F_{\text{Edd}}$, and $T_{\text{Edd,lo}}$. Two crossing points give two pairs of NS mass and radius values that satisfy the observed data.

It is now important to understand how the new models affect results based on formulae that use the Thomson cross-section for electron scattering. We have seen that owing to the Klein-Nishina reduction in the cross-section, the actual Eddington limit is reached at luminosities of 6–10% higher than $L_{\text{Edd}}$ and the shape of the $f_c - l$ relation differs somewhat from the Kompaneets-based results. As an illustration, we consider a long PRE X-ray burst of 4U 1724–307 in the globular cluster Terzan 2 studied by S11, who obtained a rather large NS radius for this source ($R \geq 14$ km). We now use new sets of theoretical relations $f_c - l$ that we fit to the observed relation $K^{-1/4} - F_{\text{bb}}$, taking pure hydrogen models as an example. We note that the new relations significantly depend on the surface gravity (see Fig. 8, top panel), therefore, in principle, it would be possible also to find the surface gravity that provides the best fit to the observed relation. This is, however, difficult in practice, because a change in log $g$ can be compensated for by varying $F_{\text{Edd}}$. 

Fig. 7. Relative deviations of the new, exact RF-based (solid curves) and old Kompaneets-based (dashed curves) spectra from the best-fit diluted blackbodies versus photon energy for hydrogen (top panel) and solar H/He mixture with $Z = 0.3 Z_e$ (bottom panel) low gravity ($\log g = 14.0$) models. Corresponding relative luminosities and the effective temperatures are given at the curves. The vertical dotted line shows the lower boundary of the energy band, where the fitting procedures were performed. For clarity, models with $l = 0.1$ and 0.5 are shifted up by 0.2 and 0.1, respectively.

Fig. 8. Color correction factors $f_{c,1}$ (computed using method 1 from SPW11) for model atmospheres of two chemical compositions (pure hydrogen and solar hydrogen/helium mix with 30% of solar heavy-element abundance) and different $\log g$ as functions of the relative luminosity $l$ (top panel) or $\sigma_{\text{grad}}/g$ (bottom panel). The new models based on the exact RF are shown by the solid curves, and the old models, based on the Kompaneets operator, by dashed curves.
Fig. 9. Same as Fig. 8, but for different chemical compositions and log $g = 14.0$.

Fig. 10. Color correction factor $f_c$ versus $g_{\text{rad}}/g$ for models of various chemical compositions. Solid curves are the results of calculations based on the exact Compton RF, the dotted curves give the approximation (31). For clarity, the curves for pure H models (shown for three log $g$) are shifted up by +0.2.

The theoretical $f_c - l$ curve for log $g = 14.0$ gives the best fit to the data (Fig. 13) for $A = 0.168$ and $F_{\text{Edd}} = 4.93 \times 10^{-8}$ erg s$^{-1}$ cm$^{-2}$. The corresponding old, Kompaneets-based values are 0.170 and $5.25 \times 10^{-8}$, respectively. This small change in the best-fit parameters leads to a small decrease of $T_{\text{Edd},\infty}$ from 1.64 $\times 10^7$ K to 1.60 $\times 10^7$ K and a corresponding increase in the NS radii (see Fig. 13, bottom panel). Interestingly, the new $T_{\text{Edd},\infty}$ curve crosses with the curve log $g = 14.0$ at the NS mass close to 1.5 $M_\odot$, and the curve $A = 0.168$ also passes through the same crossing point when $D_{\odot} = 0.53$ (i.e., 5.3 kpc, the distance to Terzan 2, Ortolani et al. 1997). The uncertainties in the obtained values arising owing to uncertainties in the data are very close to the differences between the old and the new values of the best-fit parameters (see Table 1 in S11).

A few attempts to find NS mass and radius from the direct fitting of the observed X-ray burst spectrum by NS atmosphere model spectra were performed (Majczyna & Madej 2005; Miller et al. 2011; Kuśmierek et al. 2011). They have proposed finding the best fit for a fixed log $g$ by varying the relative luminosity $l$ (or effective temperature $T_{\text{eff}}$) and the gravitational redshift $z$. The best-fit between all trial log $g$ values then gives the desired log $g$ and $z$. Thereafter, the NS mass and radius can be found using Eqs. (1) and (4). Unfortunately, the curves on the $M-R$ plane corresponding to the fixed values of log $g$ and $z$ cross at very small angles (see Fig. 1 in SPW11). Therefore, the uncertainties are expected to be large. More importantly, the model spectra are very close to the blackbody in the observed
RXTE/PCA energy band. This means that for an arbitrary product $f_c T_{\text{eff}}$ (i.e. color temperature of the theoretical spectrum) we can find the redshift $z$ that makes the combination $f_c T_{\text{eff}}/(1+z)$ equal to the observed color temperature $T_{\text{bb}}$, and in turn this method extremely unreliable.

5. Summary

We have considered hot NS model atmospheres taking into account Compton scattering using the relativistic kinetic equation with the exact angle-dependent RF and cross-section (Nagirner & Poutanen 1994; Poutanen & Svensson 1996), accounting also for the induced scattering. We have developed a method to solve the obtained radiation transfer equation using a short characteristic method with the accelerated $\Lambda$-iteration. We have implemented this solution in our computer code for the model atmosphere calculations (SPW11).

We have examined the properties of the new model atmospheres. The main difference in comparison with the old models computed with the Kompaneets operator concerns radiative acceleration. In the new approach, the Klein-Nishina reduction in the electron scattering cross-section leads to a decrease in the radiative acceleration relative to that for the Thomson scattering cross-section. The role of the radiation pressure reduces in the deeper, hot, optically thick layers due to the same effect.

We computed a new set of 484 hot NS model atmospheres. Following SPW11, we computed the models for six different chemical compositions (pure hydrogen, pure helium, solar hydrogen/helium mix with various abundances of heavy elements $Z = 1, 0.3, 0.1$, and $0.01 Z_\odot$) and three surface gravities $(\log g = 14.0, 14.3, \text{and} 14.6)$. The relative luminosities range from $l = 0.001$ to $1.06 \text{ to } 1.1$ (depending on $\log g$). The new models with $l < 0.8$ are almost identical to the old models based on the Kompaneets operator approach. At higher $l$, the deviations are more significant due to a different treatment of the radiative acceleration. The difference between the new and old models is small if instead of $l$ one uses the relative radiative acceleration $g_{\text{rad}}/g$ as a parameter.

The spectra of the new and old models deviate by less than 5% in the region around the spectral peak, and the deviation grows at higher energies. We have also tested various approximate and angle-averaged RFs for Compton scattering and found that they produce spectra that deviate from the exact solution typically by less than 2%. The comparison of our spectra to the models computed using Madej’s code (Madej 1991; Madej et al. 2004; Majczyna et al. 2005) revealed dramatic differences in the spectral shape. We attribute these differences to their usage of the incorrect RF from Guilbert (1981) and/or to the non-convergence of their radiation transfer calculations.

The spectra of all our models were fitted by the diluted backlight spectra in the RXTE/PCA energy band (3–20 keV) using the same five fitting procedures as in SPW11. The new $f_c - l$ relations are similar in shape to the old relations, but depend significantly on the surface gravity. However, the dependencies of the color correction on $g_{\text{rad}}/g$ are almost indistinguishable, with the new $f_c$ being larger by approximately 1%. The color corrections with the corresponding dilution factors, the theoretical emergent spectral energy distributions, and specific intensities at various angles for all models are available at CDS.

In the present paper, we have also tested how the new $f_c - l$ relations affect the determination of the NS masses and radii derived from the spectral evolution observed during the cooling stages of PRE bursts. We found that the best-fit NS radius increases by about 10% from the value obtained using the old model based on the Kompaneets equation (S11). We note that bursting NSs are rapidly rotating and accounting for the latitudinal variation in gravity and the Doppler effect will affect the estimated NS radius. This will be a subject of a separate publication.

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Appendix A: Relativistic kinetic equation for Compton scattering and the RFs

For completeness let us rederive here the exact relativistic expressions for the Compton scattering RFs. For the detailed derivation, see Nagirner & Poutanen (1993) and Poutanen & Vurm (2010), where more general problems have been solved. In the first paper, the redistribution matrices describing Compton scattering of polarized radiation in terms of Stokes parameters were derived, while in the second the RFs for anisotropic electron distribution have been obtained. We start from the relativistic kinetic equation (RKE) for photons that describes Compton scattering.

A.1. Radiative transfer equation

A description of interactions between photons and electrons via Compton scattering accounting for the induced scattering and electron degeneracy can be provided by the explicitly covariant RKE for photons (Buchler & Yueh 1976; de Groot et al. 1980; Nagirner & Poutanen 1993, 1994)

\[
\xi \cdot \nabla n(x) = \frac{\kappa}{2c} \int \frac{dp}{\gamma} \frac{d\Omega}{\gamma} \frac{d\Omega'}{\gamma'} x F \delta^4(p_1 + \xi_1 - p - \xi) \times \{ n(x_1)(1 + n(x))\bar{n}(p_1)(1 - \bar{n}(p_1)) \} - n(x)(1 + n(x_1))\bar{n}(p)(1 - \bar{n}(\bar{p}(p_1))),
\]  

(A.1)

where \(\nabla = (\partial / \partial t, \vec{V})\) is the four-gradient, \(c_0\) is the classical electron radius, \(\lambda_c = h/m_e c\) is the Compton wavelength, \(F\) is the Klein-Nishina reaction rate (Berestetskii et al. 1982)

\[
F = \left( \frac{1}{\xi} - \frac{1}{\xi_1} \right)^2 + 2 \left( \frac{1}{\xi} - \frac{1}{\xi_1} \right) + \frac{\xi}{\xi_1} + \frac{\xi_1}{\xi},
\]  

(A.2)

and

\[
\xi = p_1 \cdot \xi = p \cdot \xi, \quad \xi_1 = p_1 \cdot \xi = p \cdot \xi_1
\]  

(A.3)

are the four-products of the corresponding momenta (second equalities in Eq. (A.3) arising from the four-momentum conservation law represented by the delta-function in Eq. (A.1)). Here we define the dimensionless photon four-momentum as \(\hat{x} = (x, x) = x(1, \omega)\), where \(\omega\) is the unit vector in the photon propagation direction and \(x \equiv h\nu/m_e c^2\). The photon distribution is described by either the occupation number \(n\) or the specific intensity (per dimensionless energy interval) \(I(x) = x^2 n(x)/C\), where the constant \(C\) is given by Eq. (13). The dimensionless electron four-momentum is \(p = (\gamma, p) = (\gamma, p\Omega) = \gamma(1, \beta\Omega)\), where \(\Omega = p / \sqrt{p^2 - 1}\) is the electron Lorentz factor and its momentum in units of \(m_e c\), and \(\beta = v / c\) is the velocity in units of \(c\). The electron distribution is described by the occupation number \(n_e\). For the isotropic electron distribution, we use the electron distribution function \(f_e(p) = 2n_e(p)/\lambda_e^2 N_c\), normalized to unity

\[
4\pi \int_0^\infty f_e(p) p^2 dp = 1.
\]  

(A.4)

In the following, we consider a steady state and ignore electron degeneracy, because in the upper atmosphere layers, where the radiation spectrum is formed, electrons are non-degenerate. We define the RF as

\[
R(x_1 \to x) = \frac{3}{16\pi} \int \frac{dp}{\gamma} \frac{d\Omega}{\gamma} f_e(p_1) F \delta^4(p_1 + \xi_1 - p - \xi).
\]  

(A.5)

For the relativistic Maxwellian distribution of temperature \(T = kT_e/m_e c^2\) (Jüttner 1911; Synge 1957),

\[
f_e(p) = \frac{1}{4\pi T^2 K_2(1/T)} \exp(-\gamma/T)
\]  

(A.6)

where \(K_2\) is the modified Bessel function, the RF satisfies the symmetry property

\[
R(x \to x_1) e^{-\gamma/x} = R(x_1 \to x) e^{-\gamma/x},
\]  

(A.7)

which follows from its definition in Eq. (A.5) and the energy conservation \(\gamma_1 = \gamma + x_1\), or from the detailed balance condition (see Eq. (8.2) in Pomraning 1973). Using this result it is easy to show that the Bose-Einstein distribution \(n(x) = 1/(\exp[|x - \mu|/T] - 1)\) with any chemical potential is a solution of the RKE (A.1).

In the absence of strong magnetic field, the medium is isotropic, therefore the RF depends only on the photon energies and the scattering angle (where \(\eta\) is its cosine), i.e. we can write \(R(x_1 \to x) = R(x, x_1, \eta)\). The kinetic Eq. (A.1) can then be recast in a standard form of the radiative transfer equation

\[
\frac{\omega \cdot \nabla n(x)}{\sigma_T N_e} = -n(x) \frac{1}{x} \int_0^\infty \int_0^\infty \int_0^\infty d\Omega \omega_1 R(x_1, x, \eta)([1 + n(x_1)]) + [1 + n(x)] \int_0^\infty \int_0^\infty \int_0^\infty d\Omega \omega_1 R(x, x_1, \eta)n(x_1).
\]  

(A.8)

For the plane-parallel atmosphere, this reduces to

\[
\frac{\mu}{d\tau_T} \frac{dn(x, \mu)}{d\tau_T} = n(x, \mu) \int \int \int d\Omega d\mu R(x_1, x_1, x_1, \mu)([1 + n(x_1)]) + [1 + n(x)] \int \int \int d\Omega d\mu R(x, x_1, x_1, x_1)([1 + n(x_1)])
\]  

(A.9)

where \(d\tau_T = -\sigma_T N d\Omega = \kappa_e d\nu, \mu\) and \(\mu_1\) are the cosines of the angle relative to the normal, \(\eta = \mu_1 + \sqrt{1 - \mu^2} \cos \varphi\) and

\[
R(x, x_1, \eta) = \int_0^{2\pi} R(x, x_1, \eta, \varphi) d\varphi.
\]  

(A.10)

is the azimuth-integrated RF. Rewriting Eq. (A.9) in terms of the intensity \(I(x, \mu, \eta)\), we get the radiative transfer Eq. (10) that accounts for electron scattering with the scattering opacity and the source function given by Eqs. (12) and (14), respectively.

A.2. Redistribution functions

The expression (A.5) for the RF can be simplified by taking the integral over \(p\) with the help of the three-dimensional delta-function and using the identity \(\delta(\gamma_1 + x_1 - \gamma - x) = \gamma \delta(\gamma_1 + x_1 - \gamma - x) = \gamma_\delta(\xi_1 + p - \xi = \xi_1 + p - \xi)

\[
R(x, x_1, \eta) = \frac{3}{16\pi} \int \frac{dp}{\gamma} f_e(p) F \delta(\Gamma),
\]  

(A.11)

where we have dropped the subscript 1 from the electron quantities and

\[
\Gamma = \gamma(x_1 - x) - p(x_1 \omega_1 - x \omega) \cdot \Omega = q,
\]  

(A.12)

\[
q = x \cdot x_1 = xx_1(1 - \eta).
\]  

(A.13)

To integrate over angles in Eq. (A.11), we follow the recipe proposed by Aharonian & Atoyan (1981) (see also
A very simple approximate expression for the RF can be obtained by assuming that the scattering in the electron rest frame proceeds in the Thomson regime (i.e. coherent) and is isotropic. This is equivalent to substituting $F$ by $4/3$ in Eq. (A.19). We then get (Arutyunyan & Nikogosyan 1980; Poutanen 1994; Poutanen & Svensson 1996)

$$R(x, x_1, \eta, \gamma) = \frac{4}{3Q}$$

(A.25)

Integrating it over the Maxwellian distribution (A.6) gives

$$R(x, x_1, \eta) = \frac{1}{8\pi Q K_2(1/\Theta)}.$$  

(A.26)

This approximate RF is also used in the calculations. We note that this RF also satisfies the detailed balance condition (A.7).

### Appendix B: Method for solving the radiation transfer equation

The formal solution of the radiative transfer equation gives a relation between the outward $I^+(x, \mu)$ and the inward $I^-(x, \mu)$ intensities at some depth point $i$ (on the optical depth grid $\tau_i^\pm$, $i = 1, ..., N$) with the adjacent intensities

$$I^+(x, \mu) = I^+(x, \mu) \exp[-(\tau_i^+ - \tau_i^-)/\mu]$$

(B.1)

$$+ \int_{\tau_i^-}^{\tau_i^+} S^+(t, x, \mu) \exp[-(t - \tau_i^-)/\mu] \, dt/\mu,$$

(B.2)

$$I^-(x, \mu) = I^-(x, \mu) \exp[-(\tau_i^+ - \tau_i^-)/\mu]$$

$$+ \int_{\tau_i^-}^{\tau_i^+} S^-(t, x, \mu) \exp[-(t - \tau_i^-)/\mu] \, dt/\mu.$$

The integrals can be replaced by the sums using the parabolic approximation

$$I^+(x, \mu) = I^+(x, \mu) \exp[-\Delta \tau_i^+/(\Delta \tau_i^+ + 2\Delta \tau_i^-)]$$

(B.3)

$$+ \alpha_i^+ S_{i+1}^+(x, \mu) + \beta_i^+ S_i^+(x, \mu) + \gamma_i^+ S_{i+1}^+(x, \mu),$$

(B.4)

$$I^-(x, \mu) = I^-(x, \mu) \exp[-\Delta \tau_i^-/(\Delta \tau_i^+ + 2\Delta \tau_i^-)]$$

$$+ \alpha_i^- S_{i-1}^-(x, \mu) + \beta_i^- S_i^-(x, \mu) + \gamma_i^- S_{i-1}^+(x, \mu),$$

where

$$\Delta \tau_i^+ = (\tau_i^+ - \tau_{i-1}^-)/|\mu|,$$

(B.5)

$$\alpha_i^+ = e_{0,i}^+ + \frac{e_{2,i}^- - (\Delta \tau_i^+ + 2\Delta \tau_i^-) e_{4,i}^+}{\Delta \tau_i^+ (\Delta \tau_i^+ + 2\Delta \tau_i^-)},$$

and

$$e_{0,i}^+ = 1 - \exp(-\Delta \tau_i^-),$$

$$e_{2,i}^+ = \Delta \tau_i^+ - e_{0,i}^+,$$

$$e_{4,i}^+ = (\Delta \tau_i^+)^2 - 2e_{2,i}^+.$$

At the first depth point, the coefficients are

$$a_i^+ = 0, \quad \beta_i^+ = e_{1,i}^+ / \Delta \tau_i^+, \quad \gamma_i^+ = e_{0,i}^+ / \Delta \tau_i^+.$$  

(B.7)
and at the last point they are
\[ \alpha_N = e_0^N - \beta_N, \quad \beta_N = e_1^N / \Delta T_N, \quad \gamma_N = 0. \] (B.8)

We note that the inward and the outward opacities along the same ray are different (see Eq. (12)).

The formal solution for a given source function starts for the inward intensities from the outer boundary condition (the lack of incoming radiation at the surface)
\[ I^\text{i}_1(x, \mu) = \beta_1 \bar{S}^\text{i}_1(x, \mu) + \gamma_1 \bar{S}^\text{f}_1(x, \mu) \] (B.9)

up to the last depth point \( N \). The intensities at the innermost depth point are found using the inner boundary condition, which is taken from the diffusion approximation
\[ I^\text{i}_N(x, \mu) = I^\text{f}_N(x, \mu) + 2 \frac{B^\text{i}_N - B^\text{f}_N}{\Delta T_N}. \] (B.10)

The full solution is found iteratively using an accelerated \( \Lambda \)-iteration. At the first iteration, the thermal part of the source function starts for the subsequent iteration \( n \), the intensities obtained from the previous iteration \( n-1 \) are used to compute the current source functions \( S_{n,1} \). Iterations are continued until the relative change becomes smaller than the predetermined accuracy
\[ \max \left[ \frac{J^\text{f}_n(x)}{J^\text{f}_{n-1}(x)} - 1 \right] < 10^{-4}, \] (B.11)

where \( J_n(x) \) are the mean intensities. This solution method of the radiation transfer equation was tested for a rather optically thin (Thomson optical depth \( \tau_\text{T} = 2 \)) and hot \( (kT_e = 60 \text{ keV}) \) electron slab back-illuminated by soft blackbody photons of \( kT_{\text{BB}} = 1 \text{ keV} \). The solution for the emergent intensities obtained at five angles using our method were compared with the solution obtained with the Comptonization code \textsc{compps} (Poutanen \\& Svensson 1996, see Fig. B.1).

In the optically thick case \( (\tau_\text{T} \gg 1) \), which is typical of NS atmospheres, the convergence of the solution can be accelerated using the following procedure. The difference between the formal solution obtained in the current iteration \( I_{n,1}^{\text{f},n} \) and the solution at iteration \( n-1 \) is increased by some factor
\[ I^{\text{f},n}(x, \mu) - I_{n-1}^{\text{f},n-1}(x, \mu) = \frac{I^{\text{f},n}(x, \mu) - I_{n-1}^{\text{f},n-1}(x, \mu)}{1 - \epsilon^{\text{f},n}(x, \mu) \Lambda^{\text{f}}_1(x, \mu)}, \] (B.12)

where
\[ \epsilon^{\pm,n}(x, \mu) = \frac{\sigma^{\pm,n}_1(x, \mu)}{\sigma^{\pm,n}_1(x, \mu) + \kappa(x)}, \] (B.13)

and \( \Lambda^{\text{f}}_1(x, \mu) \) is the diagonal term of the approximate \( \Lambda \)-operator
\[ \Lambda^{\text{f}}_1(x, \mu) = \frac{1}{4} \left[ \beta_1^2(x, \mu) + \beta_1^1(x, \mu) \right] \times x^2 \int_0^{\infty} \frac{d\chi}{\chi^2} \int_{-1}^1 \hat{\varepsilon}_1 R(x, \mu, \chi, \mu). \] (B.14)

The acceleration is not high (about 30–40%) and the number of necessary iterations is still large (see Fig. B.2). However, in the process of the model atmosphere computation it is possible to use the source function from the previous temperature iteration as the starting approximation for the current source function (see details in Sect. 2). In this case, the acceleration depends on the value of the temperature corrections \( \Delta T_i \). At the first few temperature iterations, when \( \Delta T_i \) are large, the acceleration is insignificant, but at later iterations, when \( \Delta T_i \) are relatively small, the accelerated \( \Lambda \)-iterations converge very quickly (Fig. B.2).

Appendix C: Comparison with Madej’s code

The only other attempt to compute NS atmospheres using an integral approach to Compton scattering going beyond the Kompaneets approximation was that of J. Madej et al. (Madej 1991; Madej et al. 2004; Majczyna et al. 2005). They used an angle-averaged RF for Compton scattering derived by Guilbert (1981). It is important to compare our results with those obtained by Madej’s code for the same input parameters. We selected our fiducial model as a testbed and computed two models. In the first, we approximated electron scattering by coherent Thomson scattering. In the second, the exact fully relativistic RF for Compton scattering was used. Calculations for identical parameters were performed with Madej’s code (J. Madej \\& A. Różańska, priv. comm.). A comparison between the results is shown in Fig. C.1.

We see that the Thomson scattering models are very close to each other, in terms of both the spectra and the temperature structures (Fig. C.1, left panels). However, the models with Compton scattering differ substantially (Fig. C.1, right panels). Temperatures in the upper layers with column densities less than \( 10^3 \text{ g cm}^{-2} \) are lower in our model by up to 5–15\%, and our spectrum (solid curve) is much more peaked and softer than
Left panels: comparison of emergent spectra and temperature structures of the models computed by our code (solid curves) and Madej’s code (dashed curves), when electron scattering is approximated by coherent Thomson scattering. Right panels: same as left, but when the exact RF was used to compute Compton scattering. The spectrum computed by us using the Madej’s temperature structure is shown by the dotted curve and the spectrum computed with a relative accuracy of $10^{-2}$ is presented by dash-dots.

that computed by Madej’s code (dashed curve). We also note that our spectrum is very close to the diluted blackbody spectra, which cannot be said about Madej’s spectrum.

We can suggest two hypotheses to explain the discrepancies. First, there is a difference in the RF used by the two codes. We employed the exact relativistic RF (see Appendix A.2), which had been extensively studied and tested against Monte-Carlo simulations (Stern et al. 1995; Zdziarski et al. 2000). Madej and collaborators (Madej 1991; Madej et al. 2004; Majczyna et al. 2005) used the (angle-averaged) RF derived by Guilbert (1981) (see his Eqs. (8) and (10)), which differs from the correct expression (A.19) by an additional factor $(1 - \beta \cdot \mathbf{n} \cdot \mathbf{\omega})/(1 - \beta \cdot \mathbf{\omega})$, which appeared from an error in the Jacobian. Guilbert’s RF also does not satisfy the detailed balance condition (A.24) and therefore the RF integrated over the electron distribution does not satisfy the condition (A.7) either. Because the energy transfer by Compton scattering scales as $\beta^2$, the error on the order of $\beta$ obviously invalidates all the results obtained with this RF.

Second, some of the discrepancies could be connected to a difference in the computation of the radiation transfer and the atmosphere modeling. We illustrate this in Fig. C.1 (top right panel). Using our radiation transfer code, we computed the spectrum using the temperature structure from Madej’s calculations. When calculations proceeded until the accuracy of $10^{-4}$ was reached (dotted curve), the spectrum was much above our benchmark spectrum, i.e. it had a much higher effective (and color) temperature. If calculations were stopped at a lower accuracy of $10^{-2}$ (dash-dotted curve), the spectrum was found to be similar to Madej’s spectrum. This suggests that the radiation transfer iterations with Madej’s code did not sufficiently converge.

Madej et al. use the partial linearization method described in Mihalas (1978, p. 179) and modified to include Compton scattering. Their radiation transfer equation is rewritten to include the linearized part of the radiative equilibrium equation. The solution of this generalized radiation transfer equation satisfies simultaneously the radiative equilibrium to the first order. Using the computed radiation field, the temperature correction for the current temperature structure of the atmosphere is found. This procedure is iterated until some convergence criterion is satisfied, for example, the emergent bolometric flux is accurate to within 0.1%. In this method, the accuracy of the current solution of the radiation transfer equation is on the order of $\Delta T / T$, which is about $10^{-2} - 10^{-3}$ at the last iteration. We have shown above that this internal accuracy is insufficient to obtain the exact solution of the radiation transfer equation when Compton scattering is taken into account. We note that using this method is not possible to solve the radiation transfer equation for a given atmosphere model or, for example, for a homogeneous isothermal slab. This means that it cannot be checked independently of the atmosphere modeling.

Appendix D: Atmosphere model spectra and color-corrections

Table D.1 gives the color-correction and dilution factors from the blackbody fits to 484 atmosphere model spectra (fluxes), which in their turn are given in Table D.2. Table D.3 contains the emergent specific intensities at three angles. Tables D.1–D.3 are only available in electronic form at the CDS. The Xspec code utilizing the models is available from the authors on request.