Nonequilibrium Temperature Evolution of Ionization Fronts during the Epoch of Reionization

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Abstract

The epoch of reionization (EoR) marks the end of the Cosmic Dawn and the beginning of large-scale structure formation in the universe. The impulsive ionization fronts (I-fronts) heat and ionize the gas within the reionization bubbles in the intergalactic medium (IGM). The temperature during this process is a key yet uncertain ingredient in current models. Typically, reionization simulations assume that all baryonic species are in instantaneous thermal equilibrium with each other during the passage of an I-front. Here we present a new model of the temperature evolution for the ionization front by studying nonequilibrium effects. In particular, we include the energy transfer between major baryon species (\(e^+\), H I, H II, He I, and He II) and investigate their impacts on the post-ionization front temperature \(T_{\text{post}}\). For a better step-size control when solving the stiff equations, we implement an implicit method and construct an energy transfer rate matrix. We find that the assumption of equilibration is valid for a nonrelativistic ionization front (speed less than \(10^9\) cm s\(^{-1}\)), but deviations from equilibrium occur for faster fronts. The post-front temperature \(T_{\text{post}}\) is lower by up to 19.7\% (at \(3 \times 10^9\) cm s\(^{-1}\)) or 30.8\% (at \(10^{10}\) cm s\(^{-1}\)) relative to the equilibrium case.

Unified Astronomy Thesaurus concepts: Reionization (1383); Intergalactic medium (813); Cosmology (343); Plasma physics (2089)

1. Introduction

The Epoch of Reionization (EoR) is the process when ultraviolet (UV) photons from the first stars ionized almost all of the neutral hydrogen in the intergalactic medium (IGM). This transition is thought to occur around \(z \sim 6 \sim 12\) (Becker et al. 2001; Fan et al. 2006; McGreer et al. 2015; Planck Collaboration et al. 2020).

Temperature evolution of the IGM is one of the key ingredients in any reionization model, constraining the source energy and injection processes into the IGM. This includes both the standard astrophysical sources responsible for hydrogen and helium reionization, as well as potential new physics such as dark matter–baryon interactions (Muñoz & Loeb 2017). Understanding the IGM temperature is also a key element in cosmological constraints with the Ly\(\alpha\) forest (e.g., Viel et al. 2004; McDonald et al. 2005; Viel & Haehnelt 2006; Palanque-Delabrouille et al. 2015; Chabanier et al. 2019), and the thermal evolution shortly after reionization is particularly important for constraints on warm dark matter (e.g., Viel et al. 2008, 2013; Baur et al. 2016, 2017; Iršič et al. 2017a, 2017b; Armengaud et al. 2017; Garzilli et al. 2019). In the standard theory, as ionization fronts (I-fronts) propagate outward from ionization sources, a sharp boundary between ionized particles and neutrals forms (McQuinn 2016; Shin et al. 2008). As I-fronts passing through, the IGM gas is rapidly heated to the order of \(10^4\) K (Miralda-Escudé & Rees 1994; Hui & Gnedin 1997; Hirata 2018; D’Aloisio et al. 2019; Dayal & Ferrara 2018) which is the so-called post-ionization-front temperature \(T_{\text{post}}\). The heated IGM then undergoes a cooling process by the joint effects of adiabatic expansion of the universe and inverse Compton scattering with cosmic microwave background (CMB) photons. It also undergoes a complicated hydrodynamic relaxation process as pre-existing small-scale structures in the IGM are disrupted by the increase in temperature (e.g., Shapiro et al. 2004; Iliev et al. 2005; Hirata 2018; D’Aloisio et al. 2020).

The thermal history of the IGM can also be probed observationally using the Ly\(\alpha\) forest. The temperature of the IGM at the redshift of observation \(z_{\text{obs}}\) contributes to the thermal broadening of the Ly\(\alpha\) forest features, which have been probed using modeling of individual absorption lines (e.g., Schaye et al. 2000; Rudie et al. 2012; Bolton et al. 2014), and also through statistical approaches such as the curvature statistic, wavelets, or cutoff in the 1D Ly\(\alpha\) forest power spectrum (Lidz et al. 2010; Becker et al. 2011; Garzilli et al. 2012; Boera et al. 2014). At a more detailed level, the thermal history of the IGM also affects the Ly\(\alpha\) forest power spectrum through the pressure smoothing in addition to the temperature-density relation at \(z_{\text{obs}}\). With present-day data sets it is possible to simultaneously measure these parameters at higher redshift (Nasir et al. 2016; Walther et al. 2019; Gaikwad et al. 2020). This includes constraints on the timing and energy injection at reionization; Boera et al. (2019) found a \(T_{\text{re}} = 8.5^{+1.1}_{-0.8}\) K, consistent with the Planck determination, and a post-ionization-front temperature consistent with \(\sim 2 \times 10^5\) K.

An example of simulating \(T_{\text{post}}\) is shown in D’Aloisio et al. (2019), where they used high-resolution radiative transfer (RT) simulations. In their work, \(T_{\text{post}}\) mildly depends on incident spectrum and is primarily sensitive to the I-front speeds. One approximation they made is that all baryon species reach equilibrium states instantaneously as I-front passing through. This is assuming the timescale of thermalizing baryon species other than photoelectrons is small compared with the time that gas stays in the I-front. However, it is possible that nonequilibrium effects can influence the thermal evolution in the I-front. This is because if the front speed is large enough, the local gas density is low and the energy-transfer interaction rates become comparable with the timescale that gas stays in the I-front. D’Aloisio et al. (2019, Appendix B) provided order-of-magnitude estimates
arguing that the equilibrium approximation should hold for most of the parameter space of I-front speeds during reionization.

In this paper, we build a nonequilibrium model of $T_{\text{re}}$ by coupling an implicit stiff solver to the one-dimensional grid-based I-front model of Hirata (2018). We solve a set of stiff equations describing the energy transfer between species after photoelectrons are thermalized at each time step. Allowing for nonequilibrium effects, both $T_{\text{re}}$ and equilibrium states in the I-front are affected. We find that at the midpoint of the ionization front (where $x_e \approx 0.5$) the temperatures of the species are in equilibrium in most of the parameter space. However, in the mostly neutral region, there can be significant deviations from equilibrium, and this affects the cooling rate and final temperature if the ionization front is very fast. The source code is placed in a public GitHub repository.\footnote{https://github.com/frankelzeng/reionization}

This paper is structured as follows. In Section 2, we briefly review the one-dimensional grid model. In Section 3, we present our stiff solver algorithm in detail and explain the energy transfer cross sections between species in four categories. In Section 4, we build the dependence of $T_{\text{re}}$ on the incident blackbody spectrum $T_{\text{bb}}$ and I-front speed $v_f$ when nonequilibrium effects are present. We conclude in Section 5.

2. Method: Grid Model

Here we review the grid model for temperature evolution during the epoch of reionization. We only summarize the main results of the model, and detailed derivations are explained in the appendix of Hirata (2018). Following the physical reasoning of Miralda-Escudé & Rees (1994), this model describes density-dependent reionization temperature $T_{\text{re}}$.

The model is a time-dependent ionization front in one-dimension with the depth parameter $N_{\text{H}}$ (units: cm$^{-2}$) the total hydrogen column. The ionization front is built on a grid of $N_{\text{grid}}$ cells of width $\Delta N_{\text{H}}$, and each cell $j \in \{0, \ldots, N_{\text{grid}}\}$ contains a hydrogen neutral fraction $y_{\text{H},j}$, a helium neutral fraction $y_{\text{He},j}$, and an energy per hydrogen nucleus $E_j$. We consider only the first ionization front, i.e., H I/He I → H II/He II; the He II → He III ionization occurs later (see, e.g., the discussion in the review by McQuinn 2016) and is not treated in this paper.

A flux of photons $F$ (units: photons cm$^{-2}$ s$^{-1}$) is incident on the left side of the grid. The ionization front has velocity $v_i = F(1 - v_f/c)/[n_{\text{H}}(1 + f_{\text{He}})]$, where $n_{\text{H}}$ is the three-dimensional hydrogen number density and $f_{\text{He}}$ is the helium-to-hydrogen ratio. The relativistic correction term $v_i/c$ accounts for the finite time that incident photons travel to the I-front. To visualize the temperature in terms of the total hydrogen column $N_{\text{H}}$, we introduce a rescaled time $t' \equiv Ft$ (units: photons cm$^{-2}$).

Breaking the incident flux into a set of wavelength bins $\lambda$ with each bin contains a fraction $f_\lambda$ of the photon flux, the photoionization rates for hydrogen and helium are

$$\frac{d y_{\text{H},j}}{dt'} = \sum_{\lambda} A_{\lambda,j} \frac{\tau_{\text{H},j}}{\tau_{\text{H},j} + \tau_{\text{He},j}},$$

and

$$\frac{d y_{\text{He},j}}{dt'} = \sum_{\lambda} \frac{1}{f_{\text{He}}} A_{\lambda,j} \frac{\tau_{\text{He},j}}{\tau_{\text{H},j} + \tau_{\text{He},j}},$$

Table 1: Energy-temperature Conversion Factors

| $e^{-}$ | H I: $f_1$ | H II: $f_2$ | He I: $f_3$ | He II: $f_5$ |
|--------|----------|-----------|-----------|-----------|
| $x_e$  | $y_{\text{H}}$ | $1 - y_{\text{H}}$ | $f_{\text{He}} y_{\text{He}}$ | $f_{\text{He}} (1 - y_{\text{He}})$ |

Note. For electrons, $x_e = 1 - y_{\text{H}} + f_{\text{He}}(1 - y_{\text{He}})$.

where $\tau_{\text{H},j} = \Delta N_{\text{H}} y_{\text{H},j} \sigma_{\text{H},j}^\text{H} / (1 - v_i/c)$ and $\tau_{\text{He},j} = f_{\text{He}} \Delta N_{\text{H}} y_{\text{He},j} \sigma_{\text{He},j}^\text{He} / (1 - v_i/c)$ are optical depths to photons in frequency bin $\lambda$.

The photoionization and collisional cooling lead to a net heating rate

$$\frac{dE_j}{dt'} = \sum_{\lambda} A_{\lambda,j} \frac{\tau_{\text{H},j}}{\tau_{\text{H},j} + \tau_{\text{He},j}} (h\nu_j - E_j) + \frac{\tau_{\text{He},j}}{\tau_{\text{H},j} + \tau_{\text{He},j}} (h\nu_j - E_{\text{He},j})$$

$$- \frac{y_{\text{H},j} x_{e,j}}{v_i (1 + f_{\text{He}})} \sum_{n=2}^3 q_{n-1} x_e \nu_j (1 - n^{-2}),$$

where $E_j$ is the thermal energy per hydrogen nucleus in grid cell $j$; $x_{e,j}$ is the energy-temperature conversion factor defined in Table 1; $\nu_j \equiv c/\lambda$ is the frequency at each bin; $q_{n-1}$ represents the collisional excitation rate coefficient (units: cm$^3$ s$^{-1}$; we use coefficients from Aggarwal 1983) for exciting a hydrogen atom to the $n$th level; and $I_{\text{H},j}$ and $I_{\text{He},j}$ are the ionization energies.

Here the recombinations and collisional ionizations are neglected; these are potentially most important at low and high ionization front velocities, respectively. We can assess the importance of recombinations by comparing the recombination time $t_{\text{rec}} \sim (\alpha_{\text{H}} N_{\text{H}})^{-1}$ (with $\alpha_{\text{H}} \sim 2.5 \times 10^{-13}$ cm$^3$ s$^{-1}$ at $T = 20,000$ K; Pequignot et al. 1991) to the time spent in the ionization front $t_{\text{front}} \sim \Delta N_{\text{H}} (n_{\text{H}} v_i)$, where $\Delta N_{\text{H}} \sim 10^{10}$ cm$^{-2}$ is the column density of hydrogen nuclei through the front. The ratio is $t_{\text{rec}}/t_{\text{front}} \sim v_i (\alpha_{\text{H}} \Delta N_{\text{H}})$; for the range of front velocities considered here ($v_i \geq 5 \times 10^5$ cm s$^{-1}$) this is $\geq 20$, and recombinations within the front are a small effect. We may also assess the importance of collisional ionization to limiting the electron temperature by comparing the rate of collisional ionization to the rate of energy loss to collisional excitation to H(n = 2, 3) followed by radiative decay. This ratio is $k_{ci,j} \left[ \sum_{n=2}^3 q_{n-1} E_{-n} \nu_j (1 - n^{-2}) \right]$. We use the reaction rates $k_{ci,j}$ (in cm$^3$ s$^{-1}$) for hydrogen collisional ionization (Draine 2011, Section 13.4), and find that the ratio rises from 0.02 at $T_c = 20,000$ K to 0.14 at $T_c = 55,000$ K (the temperature we find in the fast ionization fronts, $v_i = 5 \times 10^9$ cm s$^{-1}$). We thus expect collisional ionization to have only a modest impact on the evolution of the electron temperature. (A subtlety is electrons that cause secondary ionization before thermalizing, as occurs frequently with X-ray ionization; the current code is not appropriate for modeling X-ray driven ionization fronts.)
\( \beta \), ... to denote these components. We write the energy in component \( \alpha \) per hydrogen nucleus as \( E_{\alpha} \), and its temperature as
\[
T_{\alpha} = \frac{2E_{\alpha}}{3k_Bn_{H}},
\]
where \( f_{\alpha} = n_{\alpha}/n_{H} \) is the abundance of that species relative to total hydrogen nuclei. These factors are listed in Table 1. The assumption of equilibrium states that all these temperatures are equal, in which case
\[
T = \frac{2E}{3k_B\sum f_{\alpha}}.
\]
When a neutral atom is ionized, its kinetic energy becomes that of the ion, so we include a kinetic energy transfer from H I to H II and from He I to He II inversely proportional to the neutral fraction.

3. Method: Stiff Solver for Interactions

We extend the equilibrium (electron-only) grid model by investigating the temperature evolution of five species (\( e^{-}, \text{H I}, \text{H II}, \text{He I}, \text{He II} \)) separately. This requires us to study the mutual interactions and energy exchange within different species in the IGM. We only include two-body interactions, which can be represented by \( \binom{5}{2} = 10 \) interaction rates. The system of equations is considered stiff because some of the energy-transfer rates are large compared with the timescale of the overall reionization process, indicating an unacceptably small step size when doing integration. In this work, we construct an implicit stiff solver to reflect the temperature evolution. We make an approximation that the species equilibrate among themselves immediately because this process is much faster than that within different components (e.g., electron—electron or ion—ion is faster than electron—ion).

Under nonequilibrium conditions, the components of the plasma have different temperatures. When time is rescaled to \( t' \) and assuming there is no relative drift, the equilibrium is described by Anders (1990)
\[
\frac{dT_{\alpha}}{dt'} = \frac{dt}{dt} \frac{dT_{\alpha}}{dt} = \frac{1 - \nu_{i}/c}{\nu_{i}n_{H}(1 + f_{\text{He}})} \sum_{\beta=\alpha} \nu_{\alpha\beta}(T_{\beta} - T_{\alpha}),
\]
where \( \nu_{\alpha\beta} \) is the energy-transfer rate between components \( \alpha \) and \( \beta \) in physical time. Conservation of energy in the transfer requires the symmetry relation
\[
f_{\alpha} \nu_{\alpha\beta} = f_{\beta} \nu_{\beta\alpha}.
\]
We express the temperature of each IGM component in an array \( T \) and the energy transferring rate in a matrix \( M \). The stiff equilibration can be converted to a matrix operation
\[
T'(t' + \Delta t') = T(t') + \Delta t' \cdot MT(t' + \Delta t') = (I - \Delta t' \cdot M)^{-1} T(t'),
\]
where \( I \) is the 5 \times 5 identity matrix, \( T \) has components \( T_{\alpha} \), \( M \) has entries of some functions of the interaction rate \( \nu_{\alpha\beta} \), and \( \alpha, \beta \in \{1, 2, ..., 5\} \) denote each IGM species in the order of \( e^{-}, \text{H I}, \text{H II}, \text{He I}, \text{He II} \). We initialize the temperature of all species with \( 10^{-6} \) K, which is 10 orders lower than \( T_{\text{re}} \), and the final result is insensitive to this initialization. The hydrogen and helium neutral fractions are both initialized to unity. In the code, we inserted hydrogen \( (\sim 10^{-4}) \) and helium residuals \( (\sim 10^{-7}) \) before reionization for numerical reasons; these do not affect the final temperature (Ali-Haïmoud & Hirata 2011).

Using Equation (8), it is straightforward to show that \( M \) has the form
\[
M = \begin{pmatrix}
-\sum_{\alpha=1}^{5} \nu_{1\alpha} & \nu_{12} & \nu_{13} & \nu_{14} & \nu_{15} \\
-\sum_{\beta=2}^{5} \nu_{2\beta} & -\nu_{23} & \nu_{24} & \nu_{25} \\
-\nu_{31} & -\sum_{\beta=4}^{5} \nu_{3\beta} & -\sum_{\beta=4}^{5} \nu_{4\beta} & \nu_{45} \\
-\nu_{51} & -\nu_{52} & -\nu_{53} & -\sum_{\beta=4}^{5} \nu_{5\beta} & -\sum_{\beta=4}^{5} \nu_{6\beta} \\
\end{pmatrix},
\]
The row summations vanish because \( dT_{\alpha}/dt' = 0 \) whenever all of the components are in equilibrium at the same temperature.

The abovementioned stiff solver is implemented in the code by alternating between the energy injection/photoionization step, and a thermalization step. The energy injection/photoionization step is a forward Euler step using Equations (1)–(3), which form a system of \( 3N_{\text{grid}} \) ordinary differential equations. The added energy is deposited into the electrons. The second step is a thermalization step, using the stiff integration method (Equation (8)) to distribute energy among the species. To save computation time, \( M \) is computed using the temperatures at time \( t' \).

To implement this, we need to compute the thermalization rates, i.e., the entries of \( M \). We discuss the interactions between different IGM components in the following four categories.

3.1. Ionized + Ionized

Ionized particles include \( e^{-}, \text{H II}, \) and \( \text{He II} \). For the two-body system, the corresponding energy-transfer rate is (Anders 1990)
\[
\nu_{\alpha\beta} = \left( m_{\alpha}m_{\beta}/Z_{\alpha}^{2}Z_{\beta}^{2}n_{\beta}\ln\Lambda_{\alpha\beta}\right)/\left( m_{\alpha}T_{\alpha} + m_{\beta}T_{\beta}\right)^{2}/1.8 \times 10^{-19} \text{ s}^{-1},
\]
where \( m_{\alpha/\beta} \) are the particle masses of \( \alpha \) and \( \beta \), respectively, \( Z_{\alpha/\beta} \) are their atomic numbers, \( n_{\beta} \) is the particle density of \( \beta \), and temperature is in eV. We fix the value of the Coulomb logarithm \( \ln\Lambda_{\alpha/\beta} = \ln(b_{\text{max}}/b_{\text{min}}) \) to a typical value, \( \ln\Lambda \approx 28 \), since it varies slowly with parameters. This value is taken from setting the maximum impact parameter \( b_{\text{max}} \) equal to the Debye length, and the minimum to \( b_{\text{min}} = (2\pi c_{\text{e}}m_{\alpha}v_{\alpha}^{-2}) \) (Book 1983) at a temperature of \( 10^{4} \) K.

3.2. Ions + Neutrals

For ions (H II and He II, denoted as \( \alpha \)) and neutrals (H I and He I, denoted as \( \beta \)), their mutual interactions are primarily caused by the polarization of neutrals induced by the electric field of ions, and resonant exchange for species with the same atomic number. The energy-transfer rate \( \nu_{\alpha\beta} \) is related to the interaction cross section \( \sigma_{\alpha\beta} \) through
\[
\nu_{\alpha\beta} = n_{\beta} m_{\beta}^{2}/(m_{\alpha} + m_{\beta}) \cdot \sigma_{\alpha\beta} v,
\]
where \( n_{\beta} \) is the neutral density, \( \nu_{\alpha\beta} = \langle \sigma_{\alpha\beta} v \rangle \) is the momentum transfer rate, \( v \) is relative speed, and the factor of
mass ratio is introduced by the conversion from momentum to
energy-transfer rate.
Assuming the polarization potential is in an ideal $r^{-4}$ form, the
momentum transfer rate coefficient is constant (Draine 2011).
For resonant exchange ($\text{HI} + \text{II}, \text{He I} + \text{He II}$), we fit the total
cross section as a function of temperature in a power-law form,
using data from Hunter & Kuriyan (1977) and Maiorov et al.
(2017).

3.3. Electrons + Neutrals
For interactions between electrons and neutrals, we also use
a power-law fitting for the elastic collisions cross section.
Experimental data is measured by Brackmann et al. (1958) and
Golden et al. (1984).

3.4. Neutrals + Neutrals
Due to the van der Waals interaction caused by dipole
moment fluctuations, neutrals repulse each other at small range
and weekly attract at larger separation. We do the power-law
fitting for the elastic scattering cross section according to the
measurements from Gengenbach et al. (1973).
The interpolated interaction rates between IGM pairs as a
function of temperature are shown in Figure 1. Electron–ion
and ion–ion interactions dominate in the low-temperature
region (less than $10^{4}$ K) and decrease to become comparable
with electron/ion–neutral rate.

4. Results
We aim to quantify the dependence of $T_{\text{re}}$ on the incident
spectrum temperature $T_{bb}$ and front velocity $v_{f}$ when none-
quilibrium interactions are present. The results are summarized
from Figures 2–6. In Figure 2, $T_{\text{re}}$ gets higher with higher velocity
(lower density) because of the smaller ratio of the Ly$\alpha$ cooling
process to photoionization heating, where our choice of velocities
refers to the typical range found in D’Aloisio et al. (2019).
The galaxy-driven I-fronts stay within the nonrelativistic region
($v_{f} < 10^{10}$ cm s$^{-1}$) and a quasar may generate relativistic I-front
(White et al. 2003; Shapiro et al. 2006; Alvarez & Abel 2007;
Cantalupo et al. 2008; Davies et al. 2016). With the discovery
of high-redshift quasars at $z > 5.7$ (Fan et al. 2004), these sources
are thought to be surrounded by ionized IGM bubbles. In the early
phase of the expansion of the Stromgren sphere around a quasar,
we expect that the ionization front moves out at nearly the speed
of light. White et al. (2003) proposed an I-front speed model in
which the radius of the Stromgren sphere scales with roughly
one-third of the radius of the expansion timescale. This suggests
that the I-front could reach around $0.3 c$ halfway in the relativistic
expansion phase. To provide an additional sense of scale, in the
Haardt & Madau (2012) model, hydrogen reionization completes
at $z = 6.7$; the background intensity implies an ionization front
velocity of $v_{f} \approx F/(0.1 + n_{\text{bb}}) = 1.7 \times 10^{8} \Delta^{-1}$ cm s$^{-1}$,
where $\Delta = \rho_{b}/\rho_{\text{bb}}$ is the baryon overdensity. A very luminous
quasar can provide a higher flux: the ionizing flux model for
the $z = 7.1$ quasar ULAS J1120 + 0641 from Barnett et al.
(2015, Section 3.1) can produce an ionization front velocity
$v_{f}/(1 - v_{f}/c) \approx 6 \times 10^{8}(r/50 \text{ Mpc})^{-2} \Delta^{-1}$ cm s$^{-1}$.

Figure 3 illustrates a few examples of the equilibration
process for a range of model parameters. The ionizing sources
inject radiation from the left of the plot, and the ionization front
propagates toward the right. High-energy photons stream ahead
of the ionization front, resulting in a temperature increase.
The energy of photoionization goes into the electrons, with
the result that the electrons in the mostly neutral region
(right side of the plot) are hotter than the ions or neutrals.
Their temperature may be quite high ($>5 \times 10^{4}$ K in panel (c)) but
because of the low ionization fraction they carry little thermal
energy.

In general, all species stay in equilibrium at the fully ionized
region (roughly $N_{\text{II}} \lesssim 25 \times 10^{18}$ cm$^{-2}$ in Figure 3). Note
that interaction rates are proportional to the density, so when written
in terms of the rescaled time they are inversely with $v_{f}$. Therefore,
nonequilibrium effects are most important for the fastest ionization fronts.
The sign of the effect is that in nonequilibrium, more of the thermal energy is in electrons that
can cause Ly$\alpha$ cooling, thus compared with the equilibrium case (solid green curve in Figure 3), $T_{\text{re}}$ gets lowered when
nonequilibrium interactions (the rest curves) are present. At the highest-velocity ($v_{f} \gtrsim 10^{9}$ cm s$^{-1}$) region, temperatures of
electrons and ions decouple from neutral species in the
ionization front, and nonequilibrium effects become important.

\footnote{The flux of ionizing photons incident on a planar front due to the
background radiation is $F = \int \frac{1}{\lambda} \frac{I_{\lambda}}{4\pi} \lambda d\lambda$, where $I = 13.6$ eV is the
ionization energy of hydrogen. This corresponds to $F = 1.6 \times 10^{4}$ cm$^{-2}$ s$^{-1}$.}
We can understand the nonequilibrium temperature of the electrons in the mostly neutral region by using order-of-magnitude arguments for the energy balance. As an example, consider the case of $T_{bb} = 8 \times 10^4$ K and $v_i = 5 \times 10^7$ cm/s. In the mostly neutral part of the front ($N_H > 3 \times 10^{19}$ cm$^{-2}$ in Figure 3(f)), electrons reach a temperature of $\sim 5 \times 10^4$ K, even though few ionizing photons have been absorbed. This is because the injection of energy into the electrons is fast and the electrons do not have time to transfer all of this energy to other species. The electron temperature in this region thus depends on the ionization front velocity $v_i$ and the average interaction rate $\bar{\nu}$ between electron and other species.

In the mostly neutral part of the front ($N_H > 3 \times 10^{19}$ cm$^{-2}$ in Figure 3(f)), electrons reach a temperature of $\sim 5 \times 10^4$ K, even though few ionizing photons have been absorbed. This is because the injection of energy into the electrons is fast and the electrons do not have time to transfer all of this energy to other species. The electron temperature in this region thus depends on the ionization front velocity $v_i$ and the average interaction rate $\bar{\nu}$ between electron and other species.

Although there are incident photons between 1 to 4 Ry that contribute to the photoionization (at >4 Ry, the radiation is blocked by He II), the medium to the right of the I-front is optically thick to low-energy photons, so that the photons that contribute to the heating are mostly the higher-energy photons (~4 Ry). We estimate that the average photon energy deposited into an electron is $E_{\text{inject}} = 2.2$ Ry subtracting He I ionization energy from 4 Ry. The energy present in the electrons is then related to the energy injected by these hard photons, and the ratio of the cooling time to the front time (the timescale on which this energy is injected):

$$E_{\text{remain}} = E_{\text{inject}} \cdot \frac{\Delta t_{\text{cool}}}{\Delta t_{\text{front}}} = E_{\text{inject}} \cdot \frac{\delta N_{\text{cool}}}{\delta N_{\text{front}}}. \quad (12)$$

We take $\Delta t_{\text{cool}} \equiv 1/(n_e \bar{\nu})$ as the average time that electrons cool down due to collisional interactions with other species,
and Δνfront as the e-folding time of the ionized electron fraction, which would be

\[
\delta N_{\text{front}} \equiv \frac{1}{\sigma_{\text{HI}} + \bar{\nu}\sigma_{\text{He}}} = \frac{1}{(0.12 + 0.079 \times 1.7) \times 10^{-18}} \approx 4.0 \times 10^8 \text{ cm}^{-2}
\]

(13)

using the H I and He I cross section at 3 Ry. Then \(\delta N_{\text{cool}} \equiv \nu_{\text{cool}}n_{\text{H}} = \nu_{\text{H}}/\bar{\nu}\) is the average change of column density when electron transfer heats to the rest species, where \(\nu_{\text{H}} = 5 \times 10^9 \text{ cm s}^{-1}\). The transfer rate coming from elastic collisions in a mostly neutral medium is \(\bar{\nu} \sim \nu_{\text{e,HI}}/n_{\text{H}} \times 10^{10} \text{ cm}^3 \text{s}^{-1}\) (see Figure 1). However, the actual cooling rate of the electrons is dominated by inelastic collisions where the hydrogen atoms are excited: for H \((n = 2)\) cooling this is given by \(\bar{\nu} \sim \nu_{\text{e,HI}}n_{\text{H}} \times 10^{10} \text{ cm}^3 \text{s}^{-1}\) (see Figure 1). However, the actual cooling rate of the electrons is dominated by inelastic collisions where the hydrogen atoms are excited: for H \((n = 2)\) cooling this is given by \(\bar{\nu} \sim \nu_{\text{e,HI}}/n_{\text{H}} = \nu_{\text{H}}/\bar{\nu}\), which is \((1.4, 3.8, 5.8) \times 10^{-9} \text{ cm}^3 \text{s}^{-1}\) at \(T_e = (3, 5, 7.5) \times 10^4 \text{ K}\). This gives \(\delta N_{\text{cool}} \approx (3.7, 1.3, 0.9) \times 10^{18} \text{ cm}^{-2}\) and hence \(2E_{\text{cool,small}}/k = (21, 7.5, 5.2) \times 10^4 \text{ K}\). Setting this equal to \(T_e\), we see that there will be a solution between \(T_e = 5 \times 10^4 \text{ K}\) and \(7.5 \times 10^4 \text{ K}\); this is indeed consistent with the numerical result that \(T_e = 6 \times 10^4 \text{ K}\) in Figure 3(f). We thus interpret the electron temperature in the mostly neutral region to be the result of a balance between energy injection from photoionization by hard photons, and energy loss due to inelastic collisions that excite H I and emit energy by Lyα and H(2s) two-photon emission.

In the temperature and velocity range of interest, ions (H II and He II) stay in equilibrium all the time since their mutual interaction rate is high enough compared with the front propagation speed.

Naturally, the final temperature within the reionization bubble increases as the incident spectrum becomes harder (Tbb increases). However, the importance of nonequilibrium effects exhibits a nonmonotonic behavior with Tbb (Figure 6) at small I-front velocity \(\nu_i \lesssim 5 \times 10^9 \text{ cm s}^{-1}\), when the collisional process overcomes radiative effects. This is because ion–neutral interaction and electron–ion interactions scale differently with temperature: ion/electron–neutral interaction rate scales with \(T^{3/2}\) while electron–ion interaction rate scales with \(T^{-3/2}\). Therefore, for low-temperature incident radiation \((T_{bb} \lesssim 7 \times 10^4 \text{ K})\) electron–ion interaction rate is the larger in I-front, and electron/ion–neutral interaction becomes more significant at higher temperature \((T_{bb} \gtrsim 9 \times 10^4 \text{ K})\). At \(T_{bb} \approx 8 \times 10^4 \text{ K}\), both interaction rates are relatively low compared with timescale that particles stay in the I-front, so \(T_{re}\) decreases the most compared with the equilibrium case. At higher I-front velocity \(\nu_i \gtrsim 5 \times 10^9 \text{ cm s}^{-1}\), Lyα and β cooling, which are exponential in temperature, dominates over the collisional process, so the final temperature decreases as \(T_{bb}\) goes up.

The bounds of the heat map are limited by our choice of energy sources for reionization. The upper limit of temperature we adopt \((10^5 \text{ K})\) corresponds to the effective blackbody temperature of the generic spectra for metal-free stars above 100M⊙ (Bromm et al. 2001). We have not considered even harder spectra, which might arise from ionization fronts dominated by AGN radiation. (See McQuinn 2012, Puchwein 2019 and D’Aloisio et al. 2019 for examples of such studies. Note that when X-ray radiation is included, one must also follow the energy loss of the secondary electrons prior to thermalization, as described in Furlanetto & Stoever 2010.)

5. Summary and Conclusions

We have presented a model of post-ionization-front temperatures \(T_{re}\), taking into account deviations from thermal equilibrium among the species in the IGM. Existing reionization simulations typically assume that photoelectrons thermalize baryon gas within an I-front in a timescale much shorter than the time over which the baryon species stays inside the front.

To verify equilibration assumption and better predict \(T_{re}\), this paper made a first attempt to combine a density-dependent ionization front model with an implicit stiff solver to include baryons’ elastic interactions. Our main results are as follows:

1. The equilibrium assumption is valid for ionization fronts slower than \(10^9 \text{ cm s}^{-1}\). However, baryon species start to thermally decouple at the higher-velocity (lower-density) region, where the momentum and energy-transfer rates are comparable with the front speed. This can be illustrated by Figures 3(c) and (f). Photoelectrons first heat up ions and H I through elastic collisions, and He I is the last to be thermalized due to its small momentum transfer cross section.

2. Adding nonequilibrium effects, this density-dependent model still predicts final temperature \(T_{re}\) decreases as local density \(\Delta\) decreases (or I-front velocity \(\nu_i\) increases), because of the greater importance of the collisional cooling effects (Figure 2). \(T_{re}\) ranges from \(1.7 \times 10^4 \text{ K}\) to \(3.2 \times 10^4 \text{ K}\) in our parameter space.

3. We demonstrated that during the EoR, the nonequilibrium interactions will affect \(T_{re}\) up to a level of 30%. The higher-velocity (lower-density) region has a smaller momentum transfer rate, so baryon species have lower temperatures than photoelectrons in the ionization front. Therefore, photoelectrons will be averaged to a lower density-dependent ionization front model with an implicit stiff solver to include baryons’ elastic interactions. Our main results are as follows:

- \(T_{re}\) increases as the incident spectrum becomes harder (Tbb increases).
- The importance of nonequilibrium effects exhibits a nonmonotonic behavior with Tbb (Figure 6) at small I-front velocity (νi ≲ 5 × 10⁹ cm s⁻¹), when the collisional process overcomes radiative effects. This is because ion–neutral interaction and electron–ion interactions scale differently with temperature: ion/electron–neutral interaction rate scales with T³/² while electron–ion interaction rate scales with T⁻³/². Therefore, for low-temperature incident radiation (Tbb ≲ 7 × 10⁴ K) electron–ion interaction rate is the larger in I-front, and electron/ion–neutral interaction becomes more significant at higher temperature (Tbb ≳ 9 × 10⁴ K). At Tbb ≈ 8 × 10⁴ K, both interaction rates are relatively low compared with timescale that particles stay in the I-front, so T_re decreases the most compared with the equilibrium case. At higher I-front velocity (νi ≳ 5 × 10⁹ cm s⁻¹), Lyα and β cooling, which are exponential in temperature, dominates over the collisional process, so the final temperature decreases as Tbb goes up.
during the early expansion phase of the IGM around high-redshift quasars at $z > 6$.

Future improvements include a better interpolation of the momentum transfer cross section and using a realistic incident spectrum (e.g., quasar spectrum) instead of blackbody, and a two-dimensional grid model to better describe the inhomogeneous ionized bubble.

We have seen that nonequilibrium effects can substantially affect the structure of an ionization front, especially for the electron temperature. But from an astrophysical perspective, these corrections are smaller than, but not entirely negligible compared to, the observational errors in IGM temperature determination at $z \sim 4$ (e.g., Becker et al. 2011).

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