Monte-Carlo radiation transport simulation

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I. HIGH LEVEL EXPLANATION

While at $z \gg 10^3$ photon interactions occur on a timescale much shorter than the Hubble time, it is not the case around and after recombination, at $z \lesssim 10^3$. Therefore, one must study the time-dependent evolution of the photon spectrum, and we do so with a Monte Carlo radiative transport simulation, following the temporal and spatial evolution of sub-10 MeV photons.

For a given time-dependent injected photon spectrum $\Psi(E_\gamma, z)$ (such that $\int dE_\gamma \Psi(E_\gamma, z) = 1$), we run a separate simulation for every injection redshift z_i. We assume a matter- and radiation-dominated Universe (i.e. neglect dark energy), with cosmological parameters consistent with the *Planck* 2018 results [2]. We assume a standard ionization history computed with `HyRec` [3, 4], i.e. we do not account for the feedback of a modified ionization history on the energy deposition efficiency.

Initialization – We initialize the simulation at redshift z_i with $N = 10^6$ photons, all located at the origin of coordinates $r = 0$. The photons energies are distributed according to $dN/dE_\gamma = E_{\rm tot}\Psi(E_\gamma, z_{\rm inj})/E_\gamma$, where $E_{\rm tot} = N\left(\int dE_\gamma \Psi(E_\gamma)/E_\gamma\right)^{-1}$ is the total injected energy.

Quantities evolved – In the course of a simulation, we keep track of four phase-space coordinates for each of the N photons, namely their energy E_γ and 3-dimensional comoving vector to the origin $\vec{r}_\gamma$. Note that we do not store these quantities as a function of redshift, but simply update them at each timestep. Since the photons do not interact with one another, we may use a different coordinate system for each photon, and choose it such that, at any given time, the photon's direction of propagation is along the z axis.

Timestep – We take logarithmic time steps in scale factor $d\ln a$, no larger than 0.0025, and such that the probability of any photon to either Compton scatter or photoionize a hydrogen or helium atom is at most 0.005.

Free-streaming step – We account for cosmological redshifting by updating each photon's energy to $E_\gamma := E_\gamma {\rm e}^{-d\ln a}$. We update each photon's position by freely propagating it from its position at the previous timestep along the current direction of propagation $\hat{z}$, i.e. $\vec{r}_\gamma := \vec{r}_\gamma + (d\ln a/aH)\,\hat{z}$.

Interaction step – For each photon, we compute the probability of photoionizing a hydrogen or helium atom, and of Compton scattering during $d\ln a$. Explicitly, for a photon of energy E_γ, the probability for each process X is given by

$$P_X(E_\gamma) = n_X \sigma_X(E_\gamma)\frac{d\ln a}{H(a)}, \tag{1}$$

where the relevant cross sections are given in Appendix A, and n_X is the number density of scatterers relevant to process X – neutral hydrogen or helium abundance for photoionization, total abundance of free and bound electrons for Compton scattering.

We draw a first random number for each photon, uniformly distributed in (0, 1). If this number is less than $P_{\rm ion,H}(E_\gamma)$, the photon photoionizes a hydrogen atom, leading to an electron of energy $E_e = E_\gamma - 13.6$ eV. The original photon is then terminated. We reiterate this procedure with the remaining photons for Helium photoionization. If a photon photoionizes a neutral Helium atom, it is terminated and leads to an electron of energy $E_e = E_\gamma - 24.6$ eV.

With the same procedure, we determine whether each remaining photon Compton scatters. If so, we sample the polar angle θ (with respect to the propagation direction) into which the photon scatters and resulting final energy E'_γ from Eqs. (A1) & (A2), and uniformly sample the azimuthal angle ϕ in $[0, 2\pi)$. This process results in an electron with energy $E_e = E_\gamma - E'_\gamma$. We then update the photon's energy $E_\gamma := E'_\gamma$, and rotate the photon's coordinate system such that the new direction of propagation is along the z direction; explicitly, we update its spatial coordinates $\vec{r}_\gamma := \mathbf{R}(\theta,\phi)\cdot\vec{r}_\gamma$, with the rotation matrix

$$\mathbf{R}(\theta,\phi) \equiv \begin{pmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix}. \tag{2}$$

At the end of each timestep, we thus have an updated table of photon energies and position vectors, for photons that have not been terminated. Moreover, for each photon that interacted during the timestep, we have extracted the energy E_e of the secondary electron produced in the interaction.

Maintaining a large photon sample – As a simulation progresses, photons lose energy to redshifting and Compton scattering, and the gas is increasingly neutral. As a consequence, photons are increasingly likely to be terminated in photoionization events. In order to maintain low statistical errors, we duplicate the remaining photons every time their number decreases by a factor of 2. This procedure is equivalent to having initialized the simulation with twice the original photon number, and

we therefore update $E_{\rm tot} \to 2 \times E_{\rm tot}$ every time we duplicate photons. Depending on the injection energy and redshift, this duplication can happen up to $\mathcal{O}(10)$ times.

Simulation outputs – For a given photon injection spectrum Ψ, the end results of each simulation (with initial scale factor a_i) is a 2-dimensional table of the injection-to-deposition Green's function $G^{\rm inj}_{\rm dep}(a_d, a_i, r_k)$, in predetermined bins in deposition scale factor a_d and comoving distance from the origin r_k. The scale factor bins are logarithmically distributed, in $(6.6 \times 10^{-4}, 0.020)$ with bin width $\Delta \ln a = 0.005$ (this is fixed and not to be confused with the adaptive timestep $d \ln a$). The radial distance bins are logarithmically distributed in $(1,\ 10^3)$ Mpc with bin width $\Delta \ln r = 0.05$; we also include a single bin for $0 < r < 1$ Mpc and a single final bin for $r > 10^3$ Mpc. The Green's function table $G^{\rm inj}_{\rm dep}(a_d, a_i, r_k)$ is initialized to zero; at each timestep in the simulation, if the scale factor a falls within the d-th bin $(a_d - \Delta \ln a/2, a_d + \Delta \ln a/2)$, the relevant table row is incremented by

$$G^{\rm inj}_{\rm dep}(a_d, a_i, r_k) \mathrel{+}= \frac{\sum_{\{r_\gamma \text{ in } k\text{-th bin}\}} E_e F_{\rm dep}(E_e)}{E_{\rm tot}\ \Delta \ln a\ \Delta \ln r}, \quad (3)$$

where the sum goes over all photons that have interacted during the timestep, and the fraction $F_{\rm dep}(E_e)$ of the secondary electron's energy efficiently deposited was described in Sec. II C in the original paper [1].

Appendix A: cross sections and energy loss rates

1. Sub-10 MeV photons

a. Compton Scattering

The Compton cross section $\sigma_{\rm C}(E)$ is the integral of the Klein-Nishina differential cross section computed from tree-level quantum electrodynamics. Namely, for a given initial photon energy E,

$$\frac{{\rm d}\sigma_{\rm C}}{{\rm d}\cos\theta}(E) = \frac{3}{8}\sigma_T \left(\frac{E'}{E}\right)^2 \left(\frac{E}{E'} + \frac{E'}{E} - 1 + \cos^2\theta\right), \quad (A1)$$

where σ_T is the Thomson cross section and the outgoing photon energy, E', is a function of $\cos\theta$ and E,

$$\frac{E'}{E} = \left(1 + \frac{E}{m_e}(1 - \cos\theta)\right)^{-1}. \quad (A2)$$

b. Photoionization

We adopt the following cross sections for photoionization of hydrogen and neutral helium [5],

$$\sigma_{\rm H}(E) = \frac{64\pi}{\alpha^3}\sigma_T (E_I/E)^4 \frac{\exp(-4\eta \arctan(1/\eta))}{1 - \exp(-2\pi\eta)} \quad (A3)$$

$$\eta = \frac{1}{\sqrt{E/E_I - 1}}, \quad (A4)$$

$$\sigma_{\rm HeI}(E) = -12\sigma_{\rm H}(E) + 5.1 \times 10^{-20}\ {\rm cm}^2 \left(\frac{250\ {\rm eV}}{E}\right)^{\Gamma(E)}, \quad (A5)$$

where α is the fine structure constant, and $E_I = 13.6$ eV is the ionization energy of hydrogen. The exponent in the Helium cross section, $\Gamma(E)$, is a broken power-law fit [5]: $\Gamma = 3.30$ for $E > 250$ eV, and $\Gamma = 2.65$ for 50 eV$< E <$ 250 eV, but a posteriori our injected photons do not reach this latter limit even accounting for Hubble expansion and Compton scattering. For comparison to Thomson scattering, when $E \gg E_I$,

$$\sigma_{\rm H}(E) \approx 0.24\,\sigma_T \left(\frac{\alpha m_e}{E}\right)^{7/2}. \quad (A6)$$

2. Electrons

a. Inverse Compton Scattering (ICS)

For ICS we use the general spectrum with no assumptions on the energy regime originally from [6], which we checked matches the asymptotic low- and high-energy approximations (see the appendix of [7] for discussion).

In the situation of interest, electrons interact with CMB photons, with a blackbody spectrum: the number density of photons per energy interval is

$$n_{\rm BB}(\epsilon, T) \equiv \frac{1}{\pi^2\hbar^3}\frac{\epsilon^2}{\exp(\epsilon/k_B T) - 1}. \quad (A7)$$

Given an electron with initial energy E, the doubly differential ICS rate, per initial CMB photon energy ϵ and final photon energy ϵ_1, is then

$$\frac{d^2\Gamma_{\rm ICS}}{d\epsilon d\epsilon_1} = \frac{3\sigma_T n_{\rm BB}(\epsilon)}{32\beta^6\gamma^2\epsilon}\left\{\frac{1}{\gamma^4}\left(\frac{\epsilon}{\epsilon_1} - \frac{\epsilon_1^2}{\epsilon^2}\right) + (1+\beta)\left[\beta(\beta^2+3) + \frac{1}{\gamma^2}(9 - 4\beta^2)\right] + (1-\beta)\left[\beta(\beta^2+3) - \frac{1}{\gamma^2}(9-4\beta^2)\right]\frac{\epsilon_1}{\epsilon} - \frac{2}{\gamma^2}(3-\beta^2)\left(1 + \frac{\epsilon_1}{\epsilon}\right)\log\left(\frac{1+\beta}{1-\beta}\frac{\epsilon}{\epsilon_1}\right)\right\}, \quad (A8)$$

where $\gamma \equiv E/m_e$ and $\beta \equiv \sqrt{1 - 1/\gamma^2}$ are the Lorentz factor and velocity of the incoming electron, respectively.

The expression above holds for $(1-\beta)\epsilon_1/(1+\beta) < \epsilon < \epsilon_1$. In addition, for $\epsilon_1 < \epsilon < (1+\beta)\epsilon_1/(1-\beta)$,

$$\frac{d^2\Gamma_{\rm ICS}}{d\epsilon d\epsilon_1}(\epsilon_1 < \epsilon; \beta) = -\frac{d^2\Gamma_{\rm ICS}}{d\epsilon d\epsilon_1}(\epsilon_1 > \epsilon; -\beta) \tag{A9}$$

All other values of the incoming photon energy are kinematically forbidden. The energy lost by the electron per scattering is $\Delta E = E - E' = \epsilon_1 - \epsilon$. The quantity of interest to us is the rate of electron energy loss to sub-10.2eV photons,

$$\dot{\mathcal{E}}_{\rm sink}(E) = \int d\epsilon \int^{E_{\rm exc}} d\epsilon_1 (\epsilon_1 - \epsilon) \frac{d^2\Gamma_{\rm ICS}}{d\epsilon d\epsilon_1}. \tag{A10}$$

b. *Ionization*

We use the relativistic binary-encounter-dipole model from Ref. [8] for an incident electron ionizing ground-state hydrogen and neutral helium. Taking the liberated electron's outgoing energy as $W = E - E' - E_I$, where E_I is the binding energy of the target atom, the differential ionization cross section per atomic orbital is,

$$\begin{aligned}\frac{d\sigma_{\rm ion}(E)}{dE'} &= \frac{3\sigma_T N m_e}{(\beta_E^2 + \beta_U^2 + \beta_{E_I}^2) 4E_I^2} \\ &\times \left\{ \frac{(N_i/N) - 2}{t+1} \left(\frac{1}{w+1} + \frac{1}{t-w} \right) \frac{1+2t'}{(1+t'/2)^2} \right. \\ &+ [2 - (N_i/N)] \left[\frac{1}{(w+1)^2} + \frac{1}{(t-w)^2} + \frac{(E_I/m_e)^2}{(1+t'/2)^2} \right] \\ &\left. + \frac{1}{N(w+1)} \frac{{\rm d}f}{{\rm d}w} \left[\ln\left(\frac{\beta_E^2}{1-\beta_E^2} \right) - \beta_E^2 - \ln\left(\frac{2E_I}{m_e} \right) \right] \right\},\end{aligned} \tag{A11}$$

where N is the orbital electron occupation number for the relevant atom, $t \equiv E/E_I$, $t' \equiv E/m_e$, $w \equiv W/E_I$, and $u \equiv U/E_I$ where $U = \langle p^2/2m \rangle$ is the average orbital kinetic energy of the target electron. β_i here are the velocities computed for energies $i \in \{E, U, E_I\}$. $N_i \equiv \int_0^\infty ({\rm d}f/{\rm d}w)\, dw$, where ${\rm d}f/{\rm d}w$ is the differential dipole oscillator strength, and is taken from Ref. [9] as a fitted power series

$$\frac{{\rm d}f}{{\rm d}w} = Ay^2 + By^3 + Cy^4 + Dy^5 + Fy^6, \tag{A12}$$

with $y \equiv E_I/(W + E_I) = 1/(1+w)$. The coefficients are given by:

- Hydrogen: $E_I = 13.6$, $U = 13.6$, $N = 1$, $A = 0$, $B = 12.2$, $C = -29.6$, $D = 31.3$, and $F = -12.2$.
- Helium: $E_I = 24.6$, $U = 39.5$, $N = 2$, $A = -0.0225$, $B = 1.18$, $C = -0.463$, $D = 0.0891$, and $F = 0$.

The relevant energy loss is then,

$$\dot{\mathcal{E}}_{\rm ion}(E) = v_E \sum_{i={\rm H,He}} n_i \int {\rm d}E' \, \frac{d\sigma_{{\rm ion},i}(E)}{dE'}(E - E'), \tag{A13}$$

where $v_E = \sqrt{1 - m_e^2/E^2}$ is the velocity of the incoming electron.

c. *Excitation*

We only consider excitations from the ground state to the first excited. We use the fitting functions in Ref. [10],

$$\sigma_{\rm exc}(E) = \frac{3\sigma_T R}{\alpha^4 2\pi (E + E_I + E_{\rm exc})} \left(A \ln\left(\frac{E}{R} \right) + B + C\frac{R}{E} \right) \tag{A14}$$

where $R \approx 13.6$ eV is the Rydberg energy. The coefficients are given by,

- Hydrogen: $E_{\rm exc} = 10.204$, $E_I = 13.6$, $A = 0.5555$, $B = 0.2718$, and $C = 0.0001$.
- Helium: $E_{\rm exc} = 21.218$, $E_I = 24.6$, $A = 0.1656$, $B = -0.07694$, and $C = 0.03331$.

We assume the energy lost by the electron is simply the excitation energy. We therefore obtain the following rate of energy loss through excitation

$$\dot{\mathcal{E}}_{\rm exc}(E) = v_E \sum_{i={\rm H,He}} n_i E_{\rm exc,i} \sigma_{\rm exc,i}(E). \tag{A15}$$

d. *Heating*

An energetic electron propagating in a plasma shares its kinetic energy with ambient electrons, thus heats the plasma. Because we eventually compute the rate of energy loss, we simply use from Ref. [11],

$$\dot{\mathcal{E}}_{\rm heat}(E) = \frac{4\pi(\alpha\hbar c)^2 n_{\rm H} x_e \ln\Lambda}{m_e v_E}, \tag{A16}$$

where v_E is the electron velocity, and the Coulomb logarithm is taken as,

$$\ln\Lambda = \ln\left(\frac{4E}{\zeta_e} \right), \quad \zeta_e \equiv 2\hbar \left(\frac{4\pi n_{\rm H} x_e \alpha\hbar c}{m_e} \right)^{1/2}. \tag{A17}$$

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