Monthly Notices
of the
ROYAL ASTRONOMICAL SOCIETY

MNRAS **509,** 1755–1763 (2022) https://doi.org/10.1093/mnras/stab3102
Advance Access publication 2021 October 28

Non-standard mechanism of recombination in the early Universe

Tamaz Kereselidze,[1]★ Irakli Noselidze[2] and John F. Ogilvie[3,4,5]

[1]*Faculty of Exact and Natural Sciences, Tbilisi State University, Chavchavadze Avenue 3, 0179 Tbilisi, Georgia*
[2]*School of Science and Technology, University of Georgia, Kostava Street 77a, 0171 Tbilisi, Georgia*
[3]*Centre for Experimental and Constructive Mathematics, Department of Mathematics, Simon Fraser University, 8888 University Drive, Burnaby, BC V5A 1S6, Canada*
[4]*Escuela de Quimica, Universidad de Costa Rica, Ciudad Universitaria Rodrigo Facio, San Pedro de Montes de Oca, San Jose 11501-2060, Costa Rica*
[5]*Institute of Quantum Physics, Irkutsk National Research Technical University, 664074 Irkutsk, Russia*

Accepted 2021 October 19. Received 2021 October 1; in original form 2021 August 22

ABSTRACT

In our recent papers, a non-standard quasi-molecular mechanism was suggested and applied to treat the cosmological recombination. It was assumed that, in the pre-recombination stage of evolution of the Universe, an electron combined with two neighbouring protons and created a hydrogen molecular ion, H_2^+ in a highly excited state, which then descended into the lower lying state or dissociated. In this work, we implement a quantitative analysis of this quasi-molecular mechanism of recombination; namely, we elaborate the scheme of calculation for a free–bound radiative transition. We show that the quasi-molecular mechanism played a significant role in the pre-recombination and recombination stages of evolution of the early Universe, and hence must be included into the consideration of the description of a thermal history of the Universe. Together with the earlier developed treatment of bound–bound radiative transitions in H_2^+, the elaborated scheme of calculation can be used for the design of a rapid and complete cosmological recombination code.

Key words: early universe – molecular processes – radiative transfer.

1 INTRODUCTION

This paper is continuation of our previous works (Kereselidze, Noselidze & Ogilvie 2019b, 2021) in which a non-standard quasi-molecular mechanism of recombination (QMR) was suggested and applied to treat the cosmological recombination. According to the QMR, in the pre-recombination stage of evolution of the Universe, when the temperature and density of protons were higher than those of subsequently, the combination of an electron and a proton occurred in the presence of the nearest neighbouring proton, which participated in the process. We assumed that an electron collides with two protons situated one far from another, emits a photon, and creates quasi-molecule H_2^+ in a highly excited state, which then descends into a low-lying state or dissociates.

The influence of the nearest neighbouring proton on the recombination decreases when the density of matter decreases. This effect means that the quasi-molecular mechanism of recombination must transform into the standard mechanism – the recombination of an electron on an isolated proton (Peebles 1968; Zel'dovich, Kurt & Syunyaev 1968) when redshift z decreases. The standard mechanism of recombination is thus a limiting case of the QMR. This statement allows us to expect that the QMR correctly describes the formation of hydrogen in the entire period of the evolution of the Universe from the pre-recombination stage up to the end of recombination era.

As an electron is much less massive than a proton, the velocity of electrons substantially exceeded a velocity of protons in the pre-recombination and recombination stages of evolution of the Universe. We are hence able to treat the cosmological recombination within an adiabatic representation. In this representation, all characteristics of the process depend on distance R between protons participating in the recombination.

A quantitative analysis of the QMR requires a knowledge of wavefunctions that correctly describe an electron involved in the process. For discrete eigenstates, we made use of wavefunctions of H_2^+ that are derived in an algebraic form at large distance R between protons (Kereselidze, Noselidze & Chibisov 2003). More challenging is to obtain the wavefunction that correctly describes an electron in the initial continuous spectral state. Wavefunctions of this type are mostly calculated numerically. An application of numerical wavefunctions to cosmological recombination involves cumbersome and tedious calculations and, accordingly, is time consuming. The application of Coulomb spheroidal wavefunctions obtained in a closed algebraic form for large distances R between the Coulomb centres (Kereselidze, Noselidze & Devdariani 2019a) does not simplify calculations. The problem hence requires an alternative treatment.

The purpose of this work is to obtain the wavefunction of a colliding electron in a form convenient for its further application, and to elaborate a rapid and complete scheme of calculation for cosmological recombination based on the QMR. Furthermore, we calculate the probability of free–bound radiative transitions and compare these results with data obtained within the standard mechanism of recombination; in this way, we reveal the significance of the QMR at various stages of the evolution of the Universe.

★ E-mail: tamaz.kereselidze@tsu.ge

Published by Oxford University Press on behalf of Royal Astronomical Society

Our solution of the problem is based on the use of the non-relativistic Coulomb Green's function (CGF) defined in parabolic coordinates. We apply the CGF to find the wavefunction of an electron that is moving in the field of one Coulomb centre and that experiences the influence of another distant Coulomb centre. The derived wavefunction is applied to calculate probabilities of free–bound transitions as functions of redshift z. An advantage of the developed scheme of calculation is that, in the sevenfold integral arising in the treatment, the fivefold one can be calculated analytically. This fact is crucial for the creation of a rapid and complete cosmological recombination code based on the QMR. To our knowledge, the recombination of an electron and two protons with the subsequent formation of H_2^+ has not been reported in the literature. In our paper (Kereselidze et al. 2021), free–bound transition probabilities were evaluated for a particular case, namely for a linear configuration of particles involved in the recombination.

This paper is organized as follows. After stating our objective, we present the basic equations in Section 2. In Section 3, we perform a qualitative analysis of the hydrogen recombination using the Saha–Boltzmann equation. The wavefunctions of an electron involved in the recombination are derived in Section 4. The results of calculations are presented in Section 5, before a conclusion in Section 6. Unless otherwise indicated, atomic units ($e = m_e = \hbar = 1$) are used throughout the paper.

2 BASIC EQUATIONS

2.1 Energy terms of H_2^+

At large distance R between protons, the energy terms of H_2^+ are representable as (Bates & Reid 1968)

$$U^{(\pm)}_{n_1 n_2 m}(R) = -\frac{1}{2n^2} + \frac{3n(n_1 - n_2)}{2R^2} + O(R^{-3}). \tag{1}$$

Here, n_1 and n_2 are the parabolic quantum numbers that specify electron states in the separate hydrogen atom; m denotes the absolute value of the projected orbital angular momentum of an electron along molecular axis R. The total quantum number n is related to n_1, n_2 and m according to $n = n_1 + n_2 + m + 1$. The superscript ($\pm$) denotes the symmetric and antisymmetric states of H_2^+ with respect to a reflection in the plane normal to and bisecting molecular axis.

As is clear from equation (1), the energy term with $n_2 > n_1$ is attractive, whereas the term with $n_2 < n_1$ is repulsive at large distance R between protons. If H_2^+ is formed in an excited attractive state, it does not dissociate directly. From an attractive state, H_2^+ descends to a lower lying repulsive state with a subsequent dissociation or relaxes down to an attractive state with a subsequent cascade down. Only the repulsive states of H_2^+ thus create the hydrogen atom directly; the attractive states form hydrogen through an intermediate state. The behaviour of the low-lying attractive $\sigma (m = 0)$ and $\pi (m = 1)$ energy terms of H_2^+ in the entire region of R is depicted in Fig. 1.

The formation of H_2^+ in the ground state is also possible from an attractive state. The probability of this process is comparable with the probability of the formation of atomic hydrogen (Kereselidze et al. 2021). As the creation of H_2^+ in an excited repulsive state leads to an immediate dissociation, we consider the transition of a colliding electron into an attractive state with a subsequent formation of H_2^+ in a long-lived vibrational state.

The existence of energy terms that are attractive is thus crucial for the rate of formation of atomic hydrogen, because the colliding particles can bind during a period greater than a collision period.

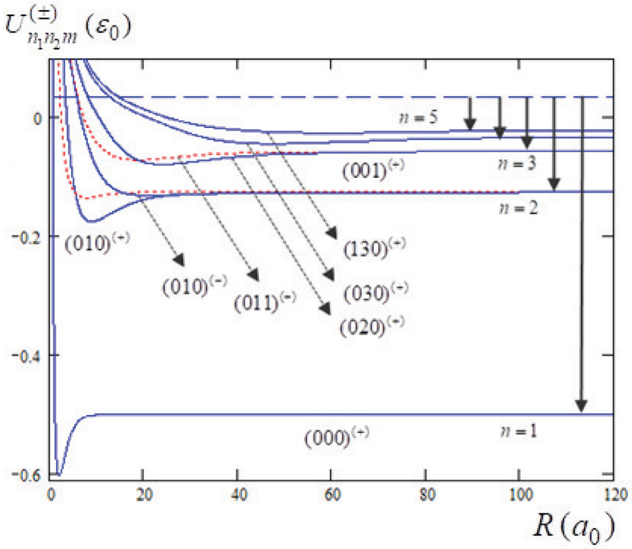

Figure 1. Attractive energy terms of H_2^+ as functions of distance R between protons. The solid and dotted curves correspond to σ and π terms, respectively. The dashed line denotes the energy of a colliding electron. Thick arrows indicate free–bound radiative transitions; $a_0 = \hbar^2/m_e e^2 = 0.529 \times 10^{-8}$ cm is the first Bohr radius of hydrogen and $\varepsilon_0 = m_e e^4/\hbar^2 = 27.21$ eV. Energy term $U^{(-)}_{000}$ that has a shallow minimum at $R = 12.546 a_0$ (Landau & Lifshitz 1977) is not shown.

2.2 Coulomb Green's function

The application of the CGF to investigate various radiative and collisional processes is not new; since the beginning of 1960s, many papers on the properties and applications of the CGF have been published (Hostler 1962, 1964; Hostler & Pratt 1963; Kereselidze & Chibisov 1975; Blinder 1981; Chetouani & Hamman 1987; Swainson & Drake 1991; Maquet, Veniard & Marian 1998; Zaytsev et al. 2020).

The CGF can be constructed from its spectral representation,

$$G^{(+)}(\vec{r}, \vec{r}\,') = \sum_n \frac{\psi_n^*(\vec{r})\psi_n(\vec{r}\,')}{E_n - E}, \tag{2}$$

in which the summation runs over the complete set of discrete and continuum eigenstates; symbol (+) corresponds to an outgoing wave when $r \to \infty$. In the first attempt to evaluate the CGF, Meixner (1933) tried to evaluate this function by explicit summation over eigenfunctions in parabolic coordinates. Further progress was made possible with an integral representation for a product of two Whittaker functions. Hostler (1962) obtained the general closed-form expression for $G^{(+)}(\vec{r}, \vec{r}\,')$ on summing over Coulomb eigenfunctions in spherical polar coordinates. Blinder (1981) showed that summation (2) explicitly written in terms of discrete and continuous eigenstates in parabolic coordinates leads to the integral representation of the CGF.

Making use of the scheme of calculation developed by Blinder, we evaluate the CGF in the form convenient for our calculations:

$$\begin{aligned} G^{(+)}(\vec{r}, \vec{r}\,') = -\frac{\imath k}{2\pi} \sum_{m=-\infty}^{\infty} \mathrm{e}^{\imath m(\varphi - \varphi')} \int_0^\infty \mathrm{d}s\, \mathrm{e}^{\imath \frac{k}{2}(\mu+\nu+\mu'+\nu')\cosh s} \\ \times \sinh s \left(\coth\frac{s}{2}\right)^{\frac{2\imath}{k}} J_m\left(k(\mu\mu')^{1/2}\sinh s\right) \\ \times J_m\left(-k(\nu\nu')^{1/2}\sinh s\right). \end{aligned} \tag{3}$$

In (3), $\mu = r(1 + \cos\vartheta)$, $\nu = r(1 - \cos\vartheta)$, $\varphi = \arctan(y/x)$ are parabolic coordinates, in which r is the radial variable, ϑ is the polar

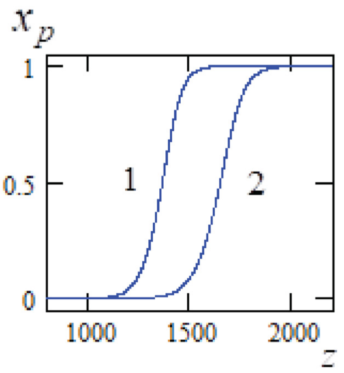

Figure 2. Degree of ionization x_p as a function of redshift z. Curve 1 – standard mechanism of recombination; curve 2 – QMR.

angle, and φ is the azimuthal angle. Details of the derivation of equation (3) are presented in Appendix A.

3 QUALITATIVE ANALYSIS OF THE HYDROGEN RECOMBINATION

We proceed to investigate the question how significant is the influence of a variation of atomic parameters, namely a variation of the binding energy of an electron in atomic hydrogen, on the recombination.

At $R \gg r_n$, where $r_n = 2n^2$ is the radius of the hydrogen atom in the nth excited state, the electron energy in H_2^+ reads

$$\varepsilon_n(R) = -\frac{1}{2n^2} - \frac{1}{R} + O(R^{-2}). \tag{4}$$

Inserting into equation (4) the average distance between protons $R \equiv \overline{R}$, which might be assumed to be no larger than $5r_n = 10n^2$ in the pre-recombination stage of the evolution of the Universe (Kereselidze et al. 2019b), we obtain for the binding energy of an electron that $\overline{I}_n = 1.2I_n$, in which $I_n = 1/2n^2$ is the binding energy of an electron in an isolated hydrogen atom. We thus obtain that in the perturbed hydrogen atom a deviation of the ionization energy from its value in unperturbed atom attains 20 per cent.

Introducing the degree of ionization $x_p = n_p/n$, in which $n = n_H + n_p$ is the number density of all H in both bound and ionized states, and assuming that $n_e = n_p$ in the pre-recombination stage of the evolution of the Universe, we write the Saha–Boltzmann equation [see equation (3) in Kereselidze et al. (2019b)] as

$$\frac{x_p^2}{1 - x_p} = \frac{1}{\overline{n}}\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-\frac{\overline{I}_n}{k_B T}}. \tag{5}$$

With derived equation (5) and $\overline{n} = \text{const} \times (1 + z)^3$ (Zel'dovich & Novikov 1975), we can calculate x_p as a function of redshift z. We find const = 1.4×10^{-7} cm^{-3} on fitting x_p, obtained from (5) in which $\overline{I}_n = 13.6$ eV with x_e presented in a paper of Sunyaev & Chluba (2009) [these authors used equation (5) but with a known $\overline{n}$ for the calculation of x_e]. The results of calculations are depicted in Fig. 2. This figure shows that x_p reaches half of its maximal value at redshift $z = 1359$ according to the standard model of recombination, whereas $x_p = 1/2$ at $z = 1642$ according to the QMR. The obtained values demonstrate clearly that the degree of ionization is sensitive to the binding energy of an electron participating in the recombination. Liu et al. (2019) made the same conclusion on varying the physical and phenomenological parameters in a standard code to compute the recombination history of the Universe.

We thus obtain that, because the binding energy of an electron was greater in the pre-recombination stage of the evolution of the Universe, the recombination began at higher temperatures, i.e. at larger redshift z. The preceding analysis is qualitative: The results of precise calculations would naturally differ from values obtained using the Saha–Boltzmann equation for equilibrium recombination. In what follows, we show that the difference between the standard mechanism of recombination and the QMR persists in a more accurate treatment.

4 WAVEFUNCTIONS OF AN ELECTRON

To begin, we find the wavefunction of an electron that collides with two fixed protons a and b. At large distance R between protons, the wavefunction of an electron is representable as

$$\Psi_i^{(\pm)} = \frac{1}{\sqrt{2}}\left(\psi^{(a)} \pm \psi^{(b)}\right). \tag{6}$$

In (6), $\psi^{(a)}(\psi^{(b)})$ is the wavefunction of an electron moving in the Coulomb field of proton $a(b)$ and that is perturbed by another proton. For definiteness, we derive wavefunction $\psi^{(a)}$ that is centred on proton a. The appropriate Schrödinger equation reads

$$\left(-\frac{1}{2}\Delta_{\vec{r}} - \frac{1}{r} - \frac{k_0^2}{2}\right)\psi^{(a)}(\vec{r}) = \frac{1}{\left|\vec{R} - \vec{r}\right|}\psi^{(a)}(\vec{r}). \tag{7}$$

Here, $\vec{r}$ is the position vector of an electron with respect to proton a, $k_0^2/2$ is the electron energy, and $R \gg 1$ is the distance between protons; $\vec{k}_0$ is the wavevector directed along axis z and vector $\vec{R}$ is directed from proton a to proton b.

Our purpose is to find the solution of equation (7) that is valid in the entire space except the region near proton b. As R is large, one can assume that $r < R$ in this space [far from both nuclei at which $r \sim R \gg 1$ the solution of equation (7) is known – it is a plane wave]. Term $\left|\vec{R} - \vec{r}\right|^{-1}$ on the right-hand side of equation (7) can hence be expanded in powers of r/R. Considering only the first two terms of this expansion, equation (7) takes the form

$$\left(-\frac{1}{2}\Delta_{\vec{r}} - \frac{1}{r} - \frac{k^2}{2}\right)\psi(\vec{r}) = \upsilon(\vec{r})\psi(\vec{r}), \tag{8}$$

in which $k^2 = k_0^2 + 2/R$, $\upsilon = \vec{n}\vec{r}/R^2$, and $\vec{n} = \vec{R}/R$. In (8) and the following equations superscript a is omitted for wavefunction $\psi^{(a)}$.

Introducing the CGF as the solution of the inhomogeneous differential equation

$$\left(-\frac{1}{2}\Delta_{\vec{r}} - \frac{1}{r} - \frac{k^2}{2}\right)G^{(+)}(\vec{r}, \vec{r}\,') = \delta(\vec{r} - \vec{r}\,'), \tag{9}$$

the eigenfunction of equation (8) that satisfies the appropriate boundary conditions is expressible as

$$\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}^{(0)}(\vec{r}) + \int G^{(+)}(\vec{r}, \vec{r}\,')\upsilon(\vec{r}\,')\psi_{\vec{k}}(\vec{r}\,')\mathrm{d}\vec{r}\,'. \tag{10}$$

Here, $\psi_{\vec{k}}^{(0)}(\vec{r})$ is the solution of equation (8) with zero right side. The solution of the homogeneous equation that is normalized with the delta function reads (Landau & Lifshitz 1977)

$$\psi_{\vec{k}}^{(0)}(\vec{r}) = N_i e^{i\vec{k}\vec{r}} F\left(i/k, 1, i(kr - \vec{k}\vec{r})\right),$$
$$N_i = (2\pi)^{-3/2} e^{\pi/2k}\Gamma(1 - i/k), \tag{11}$$

in which $F\left(i/k, 1, i(kr - \vec{k}\vec{r})\right)$ is a confluent hypergeometric function, $\Gamma(1 - i/k)$ is a gamma function, and N_i is a normalizing factor.

In equation (10), function $\upsilon(\vec{r}\,')$ is of order R^{-2} in the region near nucleus a, increases when $r^{'}$ increases, and becomes of order R^{-1} near nucleus b. In contrast, function $\psi(\vec{r}\,')$ is oscillatory with decreasing amplitude as variable $r^{'}$ increases (Kereselidze et al. 2019a). Hence, on the right-hand side of equation (10) the second term is much smaller than the first one, and, accordingly, can be considered as a perturbation. Replacing $\psi_{\vec{k}}(\vec{r}\,')$ by $\psi^{(0)}_{\vec{k}}(\vec{r}\,')$ in (10), we thereby obtain $\psi_{\vec{k}}(\vec{r})$ in the Coulomb–Born approximation

$$\psi_{\vec{k}}(\vec{r}) = \psi^{(0)}_{\vec{k}}(\vec{r}) + \frac{N_i}{R^2}\int G^{(+)}(\vec{r},\vec{r}\,')(\vec{n}\vec{r}\,')\mathrm{e}^{i\vec{k}\vec{r}\,'}F\left(\frac{i}{k},1,i(kr'-\vec{k}\vec{r}\,')\right)\mathrm{d}\vec{r}\,'. \tag{12}$$

The derived wavefunction is valid in the entire space; an exception is a volume in the vicinity of nucleus b. In (12), the first unperturbed term is of order unity, whereas the second perturbed term is much smaller. The wavefunction centred on proton b can be found in an analogous manner.

In parabolic coordinates

$$\vec{n}\vec{r}\,' = \frac{\mu'-\nu'}{2}\cos\vartheta_{\vec{R}} + \sqrt{\mu'\nu'}\cos\varphi'\sin\vartheta_{\vec{R}}, \tag{13}$$

in which $\vartheta_{\vec{R}}$ is the angle between $\vec{R}$ and axis z; azimuthal angles $\varphi^{'}$ and $\varphi_{\vec{R}}$ are measured from plane $(\vec{z},\vec{R})$; accordingly, $\varphi_{\vec{R}}=0$ in (13). Inserting (11), (13), and (3) into (12) and performing the integration over $\varphi^{'}$, we obtain the wavefunction of a colliding electron in parabolic coordinates,

$$\psi_{\vec{k}} = \psi^{(0)}_{\vec{k}}(\mu,\nu) - \frac{ikN_i}{8R}\left[f_1(\mu,\nu)\cos\vartheta_{\vec{R}} + f_2(\mu,\nu)\cos\varphi\sin\vartheta_{\vec{R}}\right], \tag{14}$$

in which

$$\begin{aligned} f_1 = {} & R^{-1}\int_0^\infty \mathrm{d}s\,\sinh s\left(\coth\frac{s}{2}\right)^{2i/k} \\ & \times \int_0^{\mu'_{max}}\int_0^{\nu'_{max}} \mathrm{e}^{i\frac{k}{2}[(\mu+\nu+\mu'+\nu')\cosh s+\mu'-\nu']} \\ & \times J_0\left(k(\mu\mu')^{1/2}\sinh s\right) J_0\left(-k(\nu\nu')^{1/2}\sinh s\right) \\ & \times F(i/k,1,ik\nu')(\mu'^2-\nu'^2)\mathrm{d}\mu'\mathrm{d}\nu', \end{aligned} \tag{15}$$

and

$$\begin{aligned} f_2 = {} & 2R^{-1}\int_0^\infty \mathrm{d}s\,\sinh s\left(\coth\frac{s}{2}\right)^{2i/k} \\ & \times \int_0^{\mu'_{\max}}\int_0^{\nu'_{\max}} \mathrm{e}^{i\frac{k}{2}[(\mu+\nu+\mu'+\nu')\cosh s+\mu'-\nu']} \\ & \times J_1\left(k(\mu\mu')^{1/2}\sinh s\right) J_1\left(-k(\nu\nu')^{1/2}\sinh s\right) \\ & \times F(i/k,1,ik\nu')\sqrt{\mu'\nu'}(\mu'+\nu')\mathrm{d}\mu'\mathrm{d}\nu'. \end{aligned}$$

In (15), the upper limits of integration are chosen from the condition $\mu'_{\max}+\nu'_{\max}=R/2$.

We proceed to find the wavefunctions of a bound electron. For this purpose, we introduce a rotating coordinate system $(\widetilde{x},\widetilde{y},\widetilde{z})$. If we assume that axis $\widetilde{z}$ is directed along $\vec{R}$ and that protons are located on this axis with coordinates $\widetilde{z}_a=0$ and $\widetilde{z}_b=R$, the wavefunction of a bound electron can be written as a sum or difference of the appropriate wavefunctions centred on each nucleus (Bates & Reid 1968)

$$\Psi^{(\pm)}_f = \frac{1}{\sqrt{2}}\left(\psi^{(a)}_{n_1,n_2,\pm m}(\widetilde{\mu}_a,\widetilde{\nu}_a,\widetilde{\varphi}) \pm \psi^{(b)}_{n_1,n_2,\pm m}(\widetilde{\mu}_b,\widetilde{\nu}_b,\widetilde{\varphi})\right). \tag{16}$$

In (16), $\widetilde{\mu},\widetilde{\nu},\widetilde{\varphi}$ are parabolic coordinates defined in the rotating coordinate system.

When the internuclear distance in H_2^+ is greater than the size of the shell on either nucleus, the wavefunction centred on nucleus a is representable as (Kereselidze et al. 2003)

$$\psi_{n_1,n_2,\pm m} = N_f X_{n_1,m}(\widetilde{\mu})Y_{n_2,m}(\widetilde{\nu})\mathrm{e}^{\pm im\widetilde{\varphi}}/\sqrt{2\pi}, \tag{17}$$

with

$$\begin{aligned} X_{n_1,m} = {} & \mathrm{e}^{-\frac{\gamma}{2}\widetilde{\mu}}\widetilde{\mu}^{\frac{m}{2}} \times F\left(-n_1,m+1,\gamma\alpha_1\widetilde{\mu}\right) \\ & \times\left(1+\frac{(2n+2n_2+m)\widetilde{\mu}}{4R}\right)+O(R^{-2}), \\ Y_{n_2,m} = {} & \mathrm{e}^{-\frac{\gamma}{2}\widetilde{\nu}}\widetilde{\nu}^{\frac{m}{2}} \times F\left(-n_2,m+1,\gamma\alpha_2\widetilde{\nu}\right) \\ & \times\left(1+\frac{(2n-2n_1+m)\widetilde{\nu}}{4R}\right)+O(R^{-2}), \end{aligned} \tag{18}$$

in which N_f is a normalizing factor; $\gamma=\sqrt{1/n^2+2/R}$ and $\alpha_{1,2}=\sqrt{1\mp n(2n_{2,1}+m+1\pm 2n)/R}$. The presented wavefunction is valid in the main region of the distribution of a bound electron, i.e. in the region in which $\widetilde{\mu},\widetilde{\nu}\le R/2$.

We rewrite wavefunction (17) in variables μ, ν, and φ that are defined in the fixed coordinate system. Parabolic coordinates in the rotating and fixed coordinate systems are related by relations

$$\begin{aligned} \widetilde{\mu} &= \frac{\mu+\nu}{2}+\frac{\mu-\nu}{2}\cos\vartheta_{\vec{R}}+\sqrt{\mu\nu}\cos\varphi\sin\vartheta_{\vec{R}}, \\ \widetilde{\nu} &= \frac{\mu+\nu}{2}-\frac{\mu-\nu}{2}\cos\vartheta_{\vec{R}}-\sqrt{\mu\nu}\cos\varphi\sin\vartheta_{\vec{R}}, \\ \widetilde{\varphi} &= \arctan\frac{\sqrt{\mu\nu}\sin\varphi}{\sqrt{\mu\nu}\cos\varphi\cos\vartheta_{\vec{R}}-\frac{\mu-\nu}{2}\sin\vartheta_{\vec{R}}}. \end{aligned} \tag{19}$$

In variables μ, ν, and φ, wavefunction (17) reads

$$\begin{aligned} \psi_{n_1,n_2,\pm m} = {} & N_f\mathrm{e}^{-\frac{\gamma}{2}(\mu+\nu)}u^{\frac{m}{2}}F\left(-n_1,m+1,\gamma\alpha_1\widetilde{\mu}\right) \\ & \times F\left(-n_2,m+1,\gamma\alpha_2\widetilde{\nu}\right)\left[1+\frac{1}{2R}Q(\widetilde{\mu},\widetilde{\nu})\right] \\ & \times\mathrm{e}^{\pm im\widetilde{\varphi}}/\sqrt{2\pi}, \end{aligned} \tag{20}$$

in which

$$\begin{aligned} u &= \left(\frac{\mu+\nu}{2}\right)^2-\left(\frac{\mu-\nu}{2}\cos\vartheta_{\vec{R}}+\sqrt{\mu\nu}\cos\varphi\sin\vartheta_{\vec{R}}\right)^2, \\ Q &= n(\mu+\nu)+n_2\widetilde{\mu}-n_1\widetilde{\nu} \\ &\quad +m\left(\frac{\mu-\nu}{2}\cos\vartheta_{\vec{R}}+\sqrt{\mu\nu}\cos\varphi\sin\vartheta_{\vec{R}}\right), \end{aligned} \tag{21}$$

and $\widetilde{\mu},\widetilde{\nu},\widetilde{\varphi}$ are defined with equations (19). We note that, in the wavefunction of a bound electron, the dependence on an orientation of protons arises already in the unperturbed term, whereas this dependence appears in the perturbed term in the wavefunction of a colliding electron.

5 RESULTS OF CALCULATIONS

In the fixed coordinate system, the operator of electric-dipole strength is $\vec{d}=-(\vec{i}x+\vec{j}y+\vec{k}z)$. For convenience, we calculate the matrix elements of operators $d^{(\pm)}=-(x\pm iy)$ and $d=-z$. In parabolic coordinates, these operators read $d^{(\pm)}=-\sqrt{\mu\nu}\mathrm{e}^{\pm i\varphi}$ and $d=-(\mu-\nu)/2$.

Matrix elements $d_{i,f}$ and $d_{i,f}^{(\pm)}$ calculated over wavefunctions (14) and (20) are representable as

$$d_{i,n_1n_2\pm m} = -\frac{N_f}{8}\left[U_{i,n_1n_2\pm m}(\vartheta_{\vec{R}}) + \frac{1}{2R}V_{i,n_1n_2\pm m}(\vartheta_{\vec{R}})\right],$$

$$d^{(\pm)}_{i,n_1n_2\pm m} = -\frac{N_f}{4}\left[U^{(\pm)}_{i,n_1n_2\pm m}(\vartheta_{\vec{R}}) + \frac{1}{2R}V^{(\pm)}_{i,n_1n_2\pm m}(\vartheta_{\vec{R}})\right], \tag{22}$$

in which

$$\begin{aligned} U_{i,n_1n_2\pm m} = &\int_0^\infty\int_0^\infty \mathrm{e}^{-\frac{\gamma}{2}(\mu+\nu)}\psi^{(0)}_{\vec{k}}(\mu,\nu) \\ &\times A_{n_1n_2\pm m}(\mu,\nu)(\mu^2-\nu^2)\mathrm{d}\mu\mathrm{d}\nu, \\ V_{i,n_1n_2\pm m} = &\int_0^\infty\int_0^\infty \mathrm{e}^{-\frac{\gamma}{2}(\mu+\nu)}\left\{\psi^{(0)}_{\vec{k}}(\mu,\nu)B_{n_1n_2\pm m}(\mu,\nu)\right. \\ &-\frac{ikN_i}{4}[f_1(\mu,\nu)A_{n_1n_2\pm m}(\mu,\nu)\cos\vartheta_{\vec{R}} \\ &\left.+f_2(\mu,\nu)C_{n_1n_2\pm m}(\mu,\nu)\sin\vartheta_{\vec{R}}]\right\}(\mu^2-\nu^2)\mathrm{d}\mu\mathrm{d}\nu, \end{aligned} \tag{23}$$

and

$$\begin{aligned} U^{(\pm)}_{i,n_1n_2\pm m} = &\int_0^\infty\int_0^\infty \mathrm{e}^{-\frac{\gamma}{2}(\mu+\nu)}\psi^{(0)}_{\vec{k}}(\mu,\nu)A^{(\pm)}_{n_1n_2\pm m}(\mu,\nu) \\ &\times\sqrt{\mu\nu}(\mu+\nu)\mathrm{d}\mu\mathrm{d}\nu, \\ V^{(\pm)}_{i,n_1n_2\pm m} = &\int_0^\infty\int_0^\infty \mathrm{e}^{-\frac{\gamma}{2}(\mu+\nu)}\left\{\psi^{(0)}_{\vec{k}}(\mu,\nu)B^{(\pm)}_{n_1n_2\pm m}(\mu,\nu)\right. \\ &-\frac{ikN_i}{4}[f_1(\mu,\nu)A^{(\pm)}_{n_1n_2\pm m}(\mu,\nu)\cos\vartheta_{\vec{R}} \\ &\left.+f_2(\mu,\nu)C^{(\pm)}_{n_1n_2\pm m}(\mu,\nu)\sin\vartheta_{\vec{R}}]\right\}\sqrt{\mu\nu}(\mu+\nu)\mathrm{d}\mu\mathrm{d}\nu. \end{aligned}$$

Because the wavefunction of a bound electron exponentially decreases when μ and ν increase, the integration is extended to infinity in (23). Functions $A_{n_1n_2\pm m}, B_{n_1n_2\pm m}, C_{n_1n_2\pm m}$ and $A^{(\pm)}_{n_1n_2\pm m}, B^{(\pm)}_{n_1n_2\pm m}, C^{(\pm)}_{n_1n_2\pm m}$ are defined in Appendix B.

The probability of a free–bound radiative transition depends on the distance R between protons and is defined as (Heitler 1954)

$$W_{i,f}(R) = \frac{4\omega^3_{i,f}(R)}{3c^3}\left|\vec{d}_{i,f}(R)\right|^2. \tag{24}$$

Here, $\omega_{i,f}$ is the frequency of an emitted photon, c is the speed of light, and $\vec{d}_{i,f}$ is the transition matrix element. Taking into account that

$$\left|\vec{d}_{i,f}\right|^2 = \left|d_{i,f}\right|^2 + \frac{1}{2}\left|d^{(+)}_{i,f}\right|^2 + \frac{1}{2}\left|d^{(-)}_{i,f}\right|^2, \tag{25}$$

and assuming that $R \equiv \overline{R}$ in (24), with $\overline{R}$ as the average distance between protons [equation (5) with $n_{\mathrm{H}} = n_e$ in Kereselidze et al. (2019b)], we thereby determine the free–bound transition probability as a function of redshift.

We calculate the free–bound transition probabilities in σ and π attractive states of H_2^+ with $n \leq 5\,(n_1+n_2+m \leq 4)$ at the parallel ($\vartheta_{\vec{R}} = 0$) and perpendicular ($\vartheta_{\vec{R}} = \pi/2$) orientations of protons with respect to the direction of propagation of a colliding electron. In the transition matrix elements, integrals over φ, φ' and μ, μ', ν are calculated analytically; the appropriate explicit expressions are presented in Appendixes B and C. The integration over ν' and s is performed numerically.

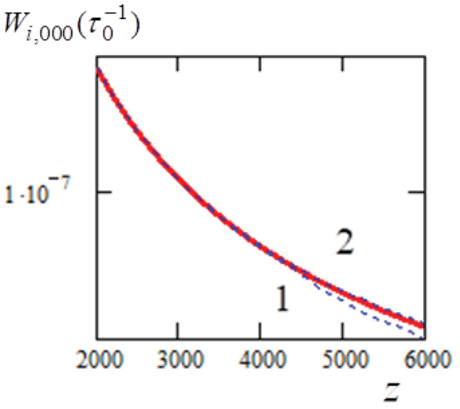

Figure 3. Probabilities $W_{i,\,000}$ as functions of redshift z. Red solid curve – influence of a second proton is neglected and blue dotted curves – influence of a second proton is taken into account; curve 1 – $\vartheta_{\vec{R}} = 0$ and curve 2 – $\vartheta_{\vec{R}} = \pi/2$; $\tau_0 = \hbar^3/m_e e^4 = 2.42 \times 10^{-17}$ s.

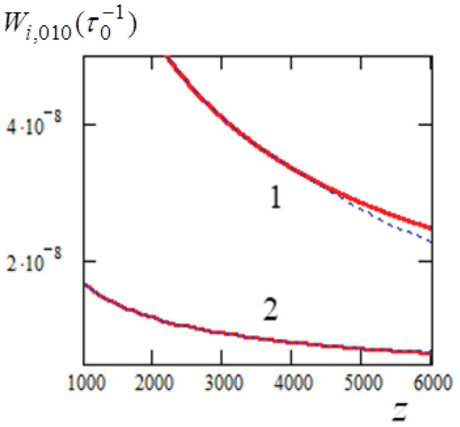

Figure 4. As in Fig. 3 but for probabilities $W_{i,\,010}$.

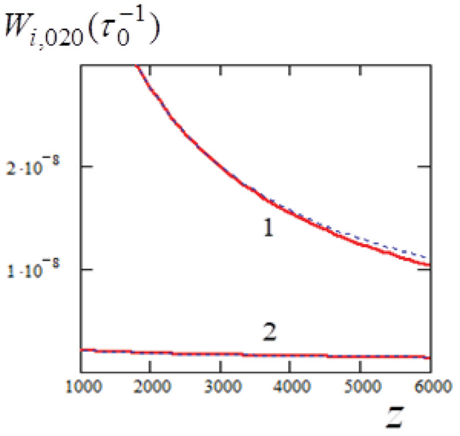

Figure 5. As in Fig. 3 but for probabilities $W_{i,\,020}$.

Probabilities as functions of redshift z are shown in Fig. 3 – for a transition into the ground state, and in Figs 4, 5, and 6 – for a transition into the excited states of H_2^+. Transition probabilities calculated using the standard mechanism of recombination, that is when the influence of the neighbouring proton is ignored ($R = \infty$), are shown as red solid curves. Probabilities calculated using the QMR are depicted with blue dotted curves. Curves 1 and 2 correspond to probabilities at the parallel and perpendicular orientations of protons with respect to a colliding electron. Concerning these probabilities, the following should be stated. As the wavefunction of a colliding

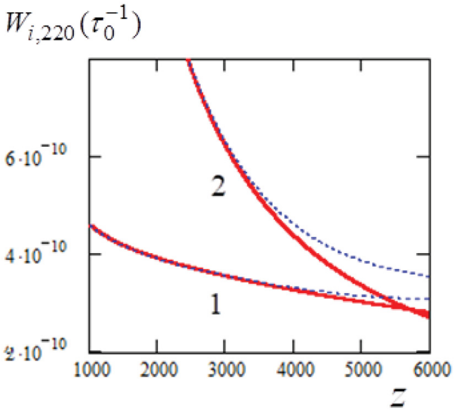

Figure 6. As in Fig. 3 but for probabilities $W_{i,\,220}$.

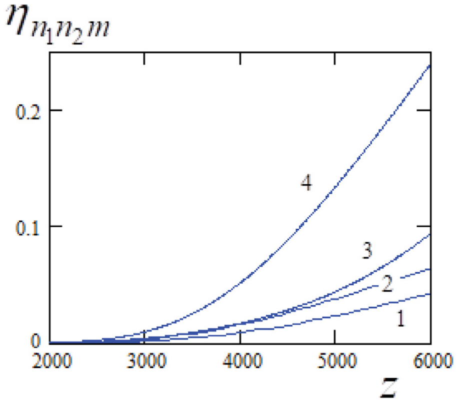

Figure 7. Ratios $\eta_{n_1n_2m}$ as functions of redshift z. Curve 1 – η_{010}, curve 2 – η_{020}, and curve 3 – η_{220}; in all these cases, $\vartheta_{\vec{R}} = 0$. Curve 4 –η_{220}, $\vartheta_{\vec{R}} = \pi/2$.

electron is defined in parabolic coordinates with a distinctive direction, transition probabilities depend on this direction even in a case when the influence of a second proton is neglected (red solid curves in Figs 4, 5, and 6). Only the transition probability into the ground state of hydrogen does not depend on a distinctive direction (red solid curve in Fig. 3). The reason is that the wavefunction of an electron in the ground state of H does not depend on a distinctive direction.

Figs 3–6 show that all transition probabilities decrease when z increases, and that the most probable is a transition into the ground state of H_2^+. We note that the direct radiative recombination into the ground state of H_2^+ is inefficient because the resulting photon has energy greater than that sufficient to ionize an adjacent H_2^+ that must hence dissociate, leaving no net result. For the formation of atomic hydrogen in the early Universe, a crucial factor was thus the recombination into the excited states of H_2^+.

Figs 4, 5 and 6 demonstrate clearly that the transition probabilities with and without inclusion of an influence of a second proton coincide completely for $z < 1500$, differ negligibly for $1500 < z < 3000$ but differ perceptibly for $z > 4000$. The latter statement is especially evident for the recombination into the excited state of H_2^+ with $n_1 = n_2 = 2$ and $m = 0$ (the corresponding attractive energy term is not shown in Fig. 1). We note that all calculated probabilities, which are not shown in Figs 4–6, exhibit a similar behaviour. In matrix elements $V_{i,n_1n_2\pm m}$ and $V^{(\pm)}_{i,n_1n_2\pm m}$, the main contribution gives the first terms in equations (23). The obtained results thus confirm that the QMR correctly describes the radiative recombination in the pre-recombination stage of the evolution of the Universe and naturally transforms into the standard mechanism of recombination when z decreases.

To make more apparent the difference between the transition probabilities, calculated with the QMR and with the standard mechanism of recombination, we present in Fig. 7 the ratio $\eta_{n_1n_2m} = |W_{n_1n_2m}(\overline{R}) - W_{n_1n_2m}(\infty)|/W_{n_1n_2m}(\infty)$ as a function of redshift z for three sets of parabolic quantum numbers. Fig. 7 shows that $\eta_{n_1n_2m}$ is minute for $z < 1500$ and increases when z increases. At $z = 4000$, $\eta_{n_1n_2m}$ increases from 0.9 per cent for $n_1 = 0$, $n_2 = 1$, $m = 0$, and $\vartheta_{\vec{R}} = 0$ to 5.2 per cent for $n_1 = n_2 = 2$, $m = 0$, and $\vartheta_{\vec{R}} = \pi/2$. These obtained values show that the influence of a second proton on the recombination was significant, especially for the radiative transitions into the excited states of H_2^+.

The scheme of calculation elaborated in this paper together with equations derived in Kereselidze et al. (2021) allows us to calculate the total probability as a function of z, which is a product of free–bound and bound–bound transition probabilities. Depending on z, the calculation of one free–bound transition probability W_{i,n_1n_2m} takes from several to several tens of seconds on a standard computer. Probabilities of bound–bound transitions occurring in H_2^+ do not depend on z.

6 CONCLUSIONS

In this work, we implement a quantitative analysis of the recombination of an electron and a proton when the nearest neighbouring proton participates in the process. The system of colliding particles is considered as a quasi-molecule, H_2^+, temporarily formed during a collision and is described in an adiabatic representation. We elaborate a rapid and complete scheme of calculation, which allows us to determine the probability of free–bound transition, in principle, into an arbitrary state of H_2^+. Our calculations demonstrate clearly that the participation of a second proton in the recombination alters the probability of a free–bound transition, especially in the pre-recombination stage of the evolution of the Universe. This elaborated scheme of calculation, with the earlier developed algorithm for bound–bound transitions in H_2^+, enables a revelation of details of the cosmological radiative recombination.

The main result of the quasi-molecular approach is that in this case the formation of H_2^+ in its ground state is available and that the probability of this process is comparable with the probability of the formation of atomic hydrogen. The formation of H_2^+ decreases the rate of recombination of hydrogen relative to the recombination of an electron on an isolated proton. Because the binding energy of an electron in H_2^+ is greater than that in H, the cosmological recombination began at higher temperatures, i.e. at larger redshift ($z \simeq 2000$–5000). The participation of a second proton in the process thus stretched the recombination compared with the standard mechanism. This effect can lead to a larger value of the present rate of expansion of the Universe obtained using the cosmic microwave background data, and thus might contribute to resolving the problem of the Hubble tension (Beradze & Gogberashvili 2021).

In this work, we have calculated the probability of a free–bound transition into quasi-molecular states with $n \leq 5$. The objective is to extend calculations on including in the treatment a free–bound and a bound–bound radiative transition into an optimally maximal number of excited states.

The hydrogen molecular ions formed in the ground state are destroyed through photoionization, photoexcitation in a repulsive quasi-molecular state, or a collision with other particles. We recognize that analysing the process of the formation of H_2^+ is insufficient and the destruction processes should also be studied. A treatment of the destruction processes is complicated and requires a separate consideration.

The results obtained in this paper thus make obvious that the quasi-molecular mechanism of recombination played a significant role in the formation of atomic hydrogen in the early Universe, and hence must be taken into account at the designing of a complete cosmological recombination code.

ACKNOWLEDGEMENTS

TK thanks Professor Jens Chluba for helpful discussion of problems considered in this paper.

DATA AVAILABILITY

The data underlying this article are available in the article and in its online supplementary material.

REFERENCES

Bates D. R., Reid R. H. G., 1968, in Bates D. R., Esterman I., eds, Advances in Atomic and Molecular Physics, Vol. IV. Academic Press, New York, USA

Beradze R., Gogberashvili M., 2021, Phys. Dark Universe, 32, 100841

Blinder S. M., 1981, J. Math. Phys., 22, 306

Buchholz H., 1969, The Confluent Hypergeometric Function. Springer, Berlin

Chetouani L., Hamman T. F., 1987, J. Math. Phys., 28, 598

Gradshtein I. S., Ryzhik I. M., 1980, Table of Integrals, Series and Products. Academic Press, New York, USA

Heitler W., 1954, The Quantum Theory of Radiation, 3rd edn. Clarendon Press, Oxford

Hostler L., 1962, Am. Phys. Soc., 7, 609

Hostler L., 1964, J. Math. Phys., 5, 591

Hostler L., Pratt R., 1963, Phys. Rev. Lett., 10, 469

Janke E., Emde F., Lösch F., 1960, Tables of Higher Functions. McGraw-Hill, New York, USA

Kereselidze T. M., Chibisov M. I., 1975, Zh. Eksp. Teor. Fiz., 68, 12

Kereselidze T. M., Noselidze I. L., Chibisov M. I., 2003, J. Phys. B: At. Mol. Opt. Phys., 36, 853

Kereselidze T., Noselidze I., Devdariani A., 2019a, J. Phys. B: At. Mol. Opt. Phys., 52, 105003

Kereselidze T., Noselidze I., Ogilvie J. F., 2019b, MNRAS, 488, 2093

Kereselidze T., Noselidze I., Ogilvie J. F., 2021, MNRAS, 501, 1160

Landau L. D., Lifshitz E. M., 1977, Quantum Mechanics: Non-Relativistic Theory, 3rd edn. Pergamon, Oxford

Liu M., Huang Z., Luo X., Miao H., Singh N. K., Huang L., 2019, Sci. China Phys. Mech. Astron., 63, 290405

Maquet A., Veniard V., Marian T. A., 1998, J. Phys. B: At. Mol. Opt. Phys., 31, 3743

Meixner J., 1933, Math. Z., 36, 677

Peebles P. J. E., 1968, ApJ, 153, 1

Sunyaev R. A., Chluba J., 2009, Astron. Nachr., 330, 657

Swainson R. A., Drake G. W. F., 1991, J. Phys. A, 24, 95

Zaytsev S. A., Ancarani L. U., Zaytsev A. S., Kouzakov K. A., 2020, Eur. Phys. J. Plus, 135, 655

Zel'dovich Y. B., Novikov I. D., 1975, Structure and Evolution of the Universe. Isdatel'stvo Nauka, Moscow, USSR

Zel'dovich Y. B., Kurt V. G., Syunyaev R. A., 1968, Zh. Eksp. Teor. Fiz., 55, 278

APPENDIX A

In parabolic coordinates, the CGF can be represented as this expansion (Blinder 1981)

$$G^{(+)}(\vec{r},\vec{r}\,') = \frac{i}{2\pi^2 k}\sum_{m=-\infty}^{\infty} \mathrm{e}^{im(\varphi-\varphi')} \times \int_{-\infty}^{\infty} \mathrm{d}\lambda\, g_m^{(+)}(\beta-\lambda,\mu,\mu')\, g_m^{(+)}(\lambda,\nu,\nu') \tag{A1}$$

in which

$$g_m^{(+)}(\lambda,x,x') = \frac{\Gamma\left((m+1)/2-i\lambda\right)}{\Gamma(m+1)}\,\frac{M_{i\lambda,m/2}\left(-ikx_<\right)}{(x_<)^{1/2}} \times \frac{W_{i\lambda,m/2}\left(-ikx_>\right)}{(x_>)^{1/2}}, \tag{A2}$$

$M_{i\lambda,m/2}(-ikx_<)$ and $W_{i\lambda,m/2}(-ikx_>)$ represent Whittaker functions of the first and second kinds, respectively, $\beta = 1/k$ and $x_< = \min(x, x')$, $x_> = \max(x, x')$.

Using the integral representation of the product of Whittaker functions (Buchholz 1969; Gradshtein & Ryzhik 1980), we obtain

$$g_m^{(+)}(\lambda,x,x') = (-1)^{\frac{m+1}{2}} k \times \int_0^{\infty} \mathrm{d}s\,\mathrm{e}^{i\frac{k}{2}(x+x')\cosh s}\left(\coth\frac{s}{2}\right)^{2i\lambda} \times J_m\left(k\sqrt{xx'}\sinh s\right), \tag{A3}$$

in which J_m is a Bessel function.

Returning to equation (A1), integral representation (A3) becomes applicable to each factor $g_m^{(+)}(\beta-\lambda,\mu,\mu')g_m^{(+)}(\lambda,\nu,\nu')$. As a result, we obtain that

$$\begin{aligned} G^{(+)}(\vec{r},\vec{r}\,') = {} & -\frac{ik}{2\pi^2}\sum_{m=-\infty}^{\infty}(-1)^m\mathrm{e}^{im(\varphi-\varphi')} \times \int_0^{\infty}\mathrm{d}s\,\mathrm{e}^{i\frac{k}{2}(\mu+\mu')\cosh s} \\ & \times J_m\left(k\sqrt{\mu\mu'}\sinh s\right)\left(\coth\frac{s}{2}\right)^{2i\beta} \\ & \times \int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{i\frac{k}{2}(\nu+\nu')\cosh t} J_m\left(k\sqrt{\nu\nu'}\sinh t\right) \\ & \times \int_{-\infty}^{\infty}\mathrm{d}\lambda\left(\coth\frac{s}{2}\right)^{-2i\lambda}\left(\coth\frac{t}{2}\right)^{2i\lambda}. \end{aligned} \tag{A4}$$

The integral over λ gives a delta function,

$$\begin{aligned} G^{(+)}(\vec{r},\vec{r}\,') = {} & -\frac{ik}{2\pi^2}\sum_{m=-\infty}^{\infty}(-1)^m\mathrm{e}^{im(\varphi-\varphi')} \times \int_0^{\infty}\mathrm{d}s\,\mathrm{e}^{i\frac{k}{2}(\mu+\mu')\cosh s} \\ & \times J_m\left(k\sqrt{\mu\mu'}\sinh s\right)\sinh s\left(\coth\frac{s}{2}\right)^{2i\beta} \\ & \times \int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{i\frac{k}{2}(\nu+\nu')\cosh t} J_m\left(k\sqrt{\nu\nu'}\sinh t\right)\delta(t-s). \end{aligned} \tag{A5}$$

Performing an integration over t and taking into account that $(-1)^m J_m(x) = J_m(-x)$, we arrive at equation (3).

APPENDIX B

Here are defined functions that appear in equation (23):

$$
\begin{aligned}
A_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}} F\left(-n_1, m_f+1, \gamma\alpha_1\widetilde{\mu}\right)\\
&\quad\times F(-n_2, m_f+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
B_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}} Q\left(\widetilde{\mu}, \widetilde{\nu}\right)\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
C_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}} F\left(-n_1, m+1, \gamma\alpha_1\widetilde{\mu}\right)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\cos\varphi\mathrm{d}\varphi,\\
A^{(\pm)}_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}}\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
B^{(\pm)}_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}} Q\left(\widetilde{\mu}, \widetilde{\nu}\right)\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
C^{(\pm)}_{n_1n_2\pm m} &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\mathrm{e}^{\mp im\widetilde{\varphi}} u^{\frac{m}{2}}\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\cos\varphi\mathrm{d}\varphi.
\end{aligned}
\tag{B1}
$$

When $\vartheta_{\vec{R}} = 0$, these integrals are readily solvable:

$$
\begin{aligned}
A_{n_1n_2\pm m}(0) &= \sqrt{2\pi}(\mu\nu)^{\frac{m}{2}} F(-n_1, m+1, \gamma\alpha_1\mu)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\nu)\delta_{m,0},\\
B_{n_1n_2\pm m}(0) &= \sqrt{2\pi}(\mu\nu)^{\frac{m}{2}} Q(\mu, \nu)F(-n_1, m+1, \gamma\alpha_1\mu)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\nu)\delta_{m,0},\\
C_{n_1n_2\pm m}(0) &= \sqrt{\frac{\pi}{2}}(\mu\nu)^{\frac{m}{2}} Q(\mu, \nu)F(-n_1, m+1, \gamma\alpha_1\mu)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\nu)\delta_{m,1},\\
A^{(\pm)}_{n_1n_2\pm m}(0) &= \sqrt{2\pi}(\mu\nu)^{\frac{m}{2}} F(-n_1, m+1, \gamma\alpha_1\mu)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\nu)\delta_{m,1},\\
B^{(\pm)}_{n_1n_2\pm m}(0) &= \sqrt{2\pi}(\mu\nu)^{\frac{m}{2}} Q(\mu, \nu)F(-n_1, m+1, \gamma\alpha_1\mu)\\
&\quad\times F(-n_2, m+1, \gamma\alpha_2\nu)\delta_{m,1},\\
C^{(\pm)}_{n_1n_2\pm m}(0) &= \sqrt{\frac{\pi}{2}}(\mu\nu)^{\frac{m}{2}} F\left(-n_1, m+1, \gamma\alpha_1\mu\right)\\
&\quad\times F\left(-n_2, m+1, \gamma\alpha_2\nu\right)\left(\delta_{m,0}+\delta_{m,2}\right).
\end{aligned}
\tag{B2}
$$

When $\vartheta_{\vec{R}} = \pi/2$, integrals can be substantially simplified in (B1) on making the appropriate transformations:

$$
\begin{aligned}
A_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
B_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F\left(-n_1, m+1, \gamma\alpha_1\widetilde{\mu}\right) F\left(-n_2, m+1, \gamma\alpha_2\widetilde{\nu}\right)\\
&\quad\times Q\left(\widetilde{\mu}, \widetilde{\nu}\right)\mathrm{d}\varphi,\\
C_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F\left(-n_1, m+1, \gamma\alpha_1\widetilde{\mu}\right) F\left(-n_2, m+1, \gamma\alpha_2\widetilde{\nu}\right)\\
&\quad\times \cos\varphi\mathrm{d}\varphi,\\
A^{(\pm)}_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\mathrm{d}\varphi,\\
B^{(\pm)}_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\\
&\quad\times Q(\widetilde{\mu}, \widetilde{\nu})\mathrm{d}\varphi,\\
C^{(\pm)}_{n_1n_2\pm m}\left(\frac{\pi}{2}\right) &= \frac{1}{2^m\sqrt{2\pi}}\int_0^{2\pi} \mathrm{e}^{\pm i\varphi}\left(\mu-\nu\pm 2i\sqrt{\mu\nu}\sin\varphi\right)^m\\
&\quad\times F(-n_1, m+1, \gamma\alpha_1\widetilde{\mu})F(-n_2, m+1, \gamma\alpha_2\widetilde{\nu})\\
&\quad\times \cos\varphi\mathrm{d}\varphi.
\end{aligned}
\tag{B3}
$$

For given quantum numbers n_1, n_2, and m, these integrals become a sum of analytically solvable integrals.

APPENDIX C

Integrals over μ that appear in equation (23) in terms proportional to R^{-1} can be reduced to this integral,

$$
\upsilon_\tau^{(p)}(s, \mu') = \int_0^\infty \mathrm{e}^{-\frac{\gamma-ik\cosh s}{2}\mu} J_\tau\left(k(\mu\mu')^{1/2}\sinh s\right)\mu^p\mathrm{d}\mu, \tag{C1}
$$

in which $\tau = 0$ or 1; $p = 0, 1, 2, \ldots$ for $\tau = 0$ and $p = 1/2, 3/2, 5/2, \ldots$ for $\tau = 1$. This integral is analytically solvable (Gradshtein & Ryzhik 1980)

$$
\begin{aligned}
\upsilon_\tau^{(p)}\left(s, \mu'\right) &= \frac{2^{p+1-\frac{\tau}{2}}\Gamma\left(p+1+\frac{\tau}{2}\right)(k\sinh s)^\tau \mu'^{\frac{\tau}{2}}}{\Gamma(\tau+1)(\gamma-ik\cosh s)^{p+1+\frac{\tau}{2}}}\\
&\quad\times F\left(p+1+\frac{\tau}{2}, \tau+1, -\frac{(k\sinh s)^2\mu'}{2(\gamma-ik\cosh s)}\right).
\end{aligned}
\tag{C2}
$$

In the confluent hypergeometric function, the first parameter is equal to the second one or is greater by an integer, $p + 1 + \tau/2 = \tau + 1 + l$ with $l = 0, 1, 2. \ldots$ Taking into account that $F(\tau + 1, \tau + 1, x) = \mathrm{e}^x$ and making use of a recurrence relation (Janke, Emde & Lösch 1960)

$$
\begin{aligned}
F(a+1, \tau+1, x) &= a^{-1}[(2a-\tau-1+x)F(a, \tau+1, x)\\
&\quad+(\tau+1-a)F(a-1, \tau+1, x)],
\end{aligned}
\tag{C3}
$$

$F(\tau + 1 + l, \tau + 1, x)$ becomes represented as a product of e^x and a polynomial function of order l.

Inserting $\upsilon_\tau^{(p)}(s, \mu')$ into integrals over $\mu^{'}$, we arrive at a sum of analytically solvable integrals of this type,

$$
\chi_\tau^{(p')}(s) = \int_0^{R/2} \mathrm{e}^{-\frac{1}{2}\left(\frac{(k\sinh s)^2}{\gamma-ik\cosh s}-ik(1+\cosh s)\right)\mu'} \mu'^{(p'+\tau/2)}\mathrm{d}\mu', \tag{C4}
$$

in which $p^{'} + \tau/2 = 0, 1, 2, \ldots.$

Integrals over ν that appear in equation (23) in terms proportional to R^{-1}

$$h_{\tau}^{(\rho)}(s,\nu')=\int_0^{\infty}\mathrm{e}^{-\frac{\gamma-ik\cosh s}{2}\nu}J_{\tau}\left(-k(\nu\nu)^{1/2}\sinh s\right)\nu^{\rho}\mathrm{d}\nu, \tag{C5}$$

in which $\rho = 0, 1, 2, \dots$ for $\tau = 0$ and $\rho = 1/2, 3/2, 5/2, \dots$ for $\tau = 1$, can be solved as (C1). Taking into account that $J_{\tau}(-x) = (-1)^{\tau}J_{\tau}(x)$, we obtain

$$h_{\tau}^{(\rho)}(s,\nu')=(-1)^{\tau}\frac{2^{\rho+1-\tau/2}\Gamma\left(\rho+1+\tau/2\right)(k\sinh s)^{\tau}\,\nu'^{\tau/2}}{\Gamma(\tau+1)(\gamma-ik\cosh s)^{\rho+1+\tau/2}}$$
$$\times F\left(\rho+1+\frac{\tau}{2},\tau+1,-\frac{(k\sinh s)^2\nu'}{2(\gamma-ik\cosh s)}\right). \tag{C6}$$

In (C6), the confluent hypergeometric function can be represented as a product of an exponential function and a polynomial function.

Inserting $h_{\tau}^{(\rho)}(s,\nu')$ into integrals over $\nu^{'}$, we obtain a sum of integrals of this type,

$$g_{\tau}^{(\rho')}(s)=\int_0^{\frac{R}{2}}\mathrm{e}^{-\frac{1}{2}\left(\frac{(k\sinh s)^2}{\gamma-ik\cosh s}+ik(1-\cosh s)\right)\nu'}$$
$$\times F\left(\frac{i}{k},1,ik\nu'\right)\nu'^{(\rho'+\tau/2)}\mathrm{d}\nu', \tag{C7}$$

in which $\rho^{'} + \tau/2 = 0, 1, 2, \dots$. These integrals we calculate numerically.

This paper has been typeset from a TEX/LATEX file prepared by the author.