Formation of hydrogen in the early Universe: quasi-molecular mechanism of recombination

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Epoch	Time	Temperature
Plank epoch	$<10^{-43}\,s$	$10^{32}\,K$
Quark epoch	$10^{-12}\,s \sim 10^{-5}\,s$	$10^{15}\,K \sim 10^{12}\,K$
Hadron epoch	$10^{-5}\,s \sim 1s$	$10^{12}\,K \sim 10^{10}\,K$
Nucleosynthesis epoch	$10s \sim 10^{3}\,s$	$10^{9}\,K \sim 10^{7}\,K$
Recombination epoch	$\sim 3.7\times10^{5}$ *years after the Big Bang*	$1500K \sim 4000K$
Dark Ages	$3.8\times10^{5} \sim 10^{6}$ *years after the Big Bang*	$4000K \sim 60K$

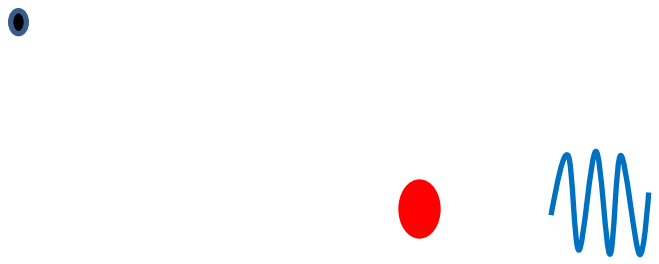
$$T = 2.725(1+z)K$$

Electron-proton recombination

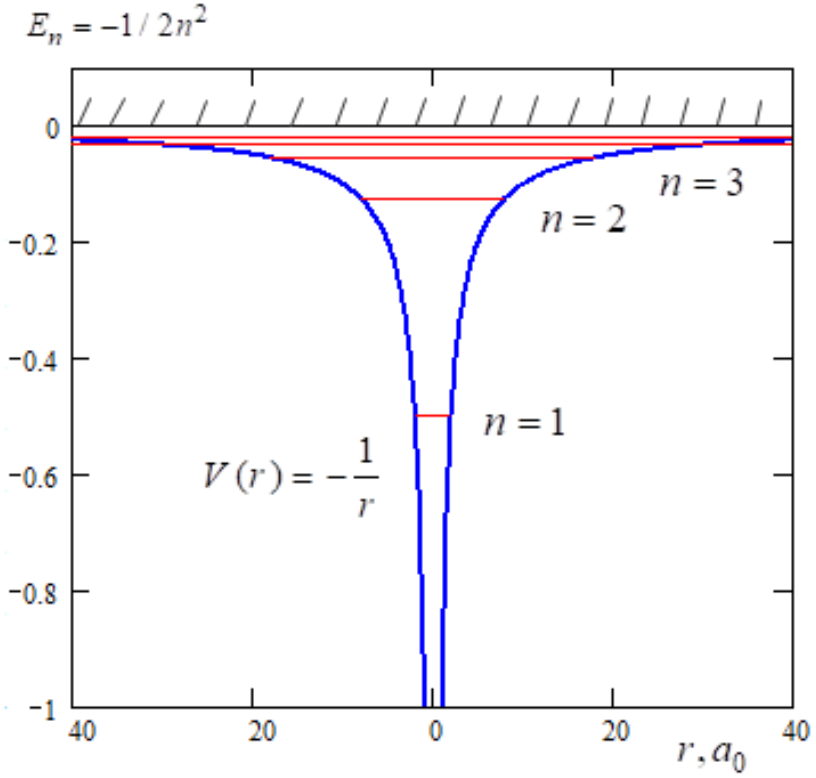
$$e + p \rightarrow H^{*}(n \gg 1) + \hbar\omega$$

Zel'dovich Y. B., Kurt V. G. and Syunyaev R. A. 1968 *ZhETF* **55** 278

Peebles P J E 1968 *Astrophysical Journal* **153** 1



$$e + p \rightarrow H^{*}(n \gg 1) + \hbar\omega$$



Energy levels in the hydrogen atom

$2p \rightarrow 1s$ - one-photon decay

$2s \rightarrow 1s$ - two-photon decay

Chluba J., Ali- Haïmoud Y., 2016, MNRAS, 456, 3494

Glover S. C. O., Cluba J., Furlanetto S. R., Pritchard J. R., Savin D. W., 2014, Advances in Atomic, Molecular and Optical Physics, 63, 135

Chluba J., Thomas R. M., 2011, MNRAS, 412, 748

Grin D., Hirata C. M., 2010, Phys. Rev. D, 81, 083005

Ali-Haïmoud Y, Hirata C. M., 2010, Phys. Rev. D, 82, 063521

Hirata C. M., 2008, Phys. Rev. D, 78, 023001

Dubrovich V. K., Grachev S. I., 2005, Astron. Lett., 32,359

Nowadays “COSMOSPEC” is the most promoted code, which was elaborated by J. Chluba and Ali- Haïmoud (2016).

$$e + p \rightleftarrows H + \hbar\omega$$

The average distance between protons in the recombination stage of evolution of the Universe is estimable if one assumes that, before recombination, the reaction $e + p \rightleftarrows H + \hbar\omega$ was in statistical equilibrium, i.e. the rate of radiative recombination was balanced with the rate of photoionization.

In statistical equilibrium at temperate T, the number density n_a of particles with mass m_a is given according to the Maxwell-Boltzmann equation

$$n_a = g_a \left(\frac{m_a k_B T}{2\pi\hbar^2} \right)^{3/2} \mathbf{e}^{-\frac{m_a c^2}{k_B T}}$$

The Saha equation

$$\frac{n_\mathrm{p} n_\mathrm{e}}{n_\mathrm{H}} = \left(\frac{m_\mathrm{e} k_B T}{2\pi\hbar^2} \right)^{3/2} \mathbf{e}^{-\frac{I}{k_B T}}$$

The average distance between protons

Introducing degree of ionization

$$\eta = \frac{n_p}{n_p + n_H},$$

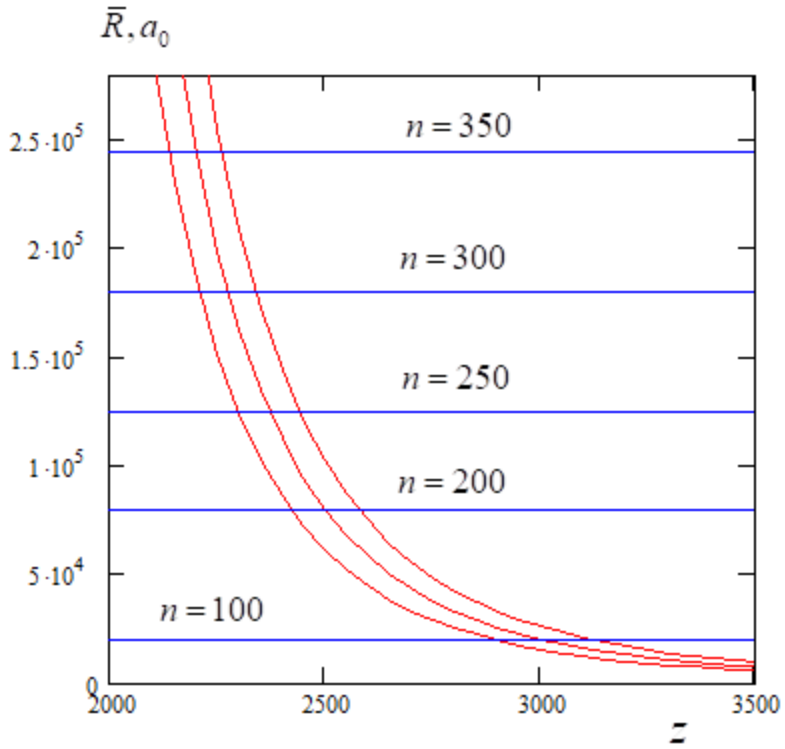
and making use of equality $n_e \simeq n_p$, which assumes the charge neutrality of the Universe , we obtain that

$$n_p = \frac{1-\eta}{\eta}\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-\frac{I}{k_B T}},$$

in which $0 \le \eta \le 1.$

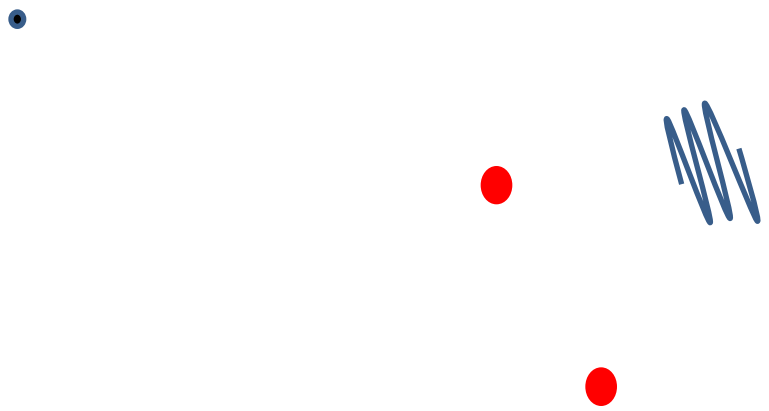
$$\bar{R} / cm = \frac{1}{\sqrt[3]{n_p}} = 7.45\times 10^{-6}\left(\frac{\eta}{1-\eta}\right)^{1/3} \frac{e^{\frac{52606}{T}}}{T^{1/2}}$$

The average distance between protons as a function of Z. Straight lines correspond to the linear size $d_n = 2n^2$ of the hydrogen atom in the excited state with principal quantum number n .



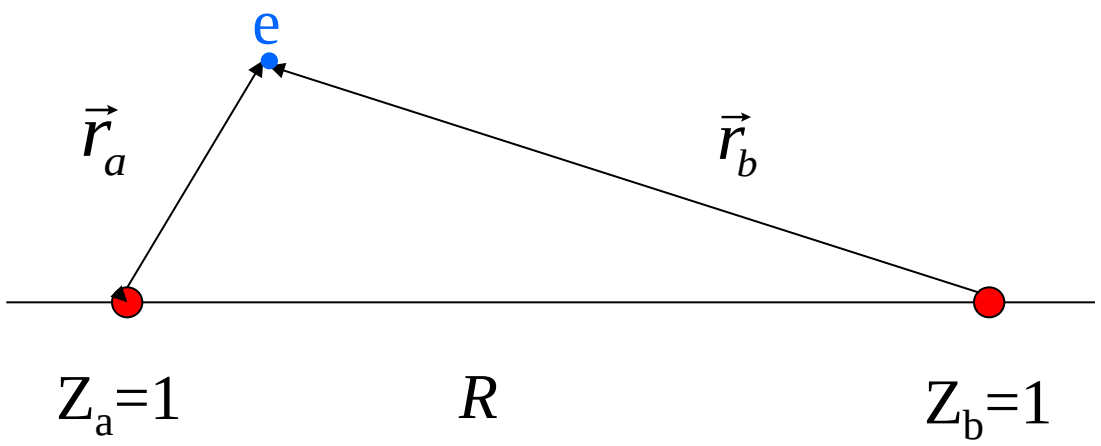
Recombination of an electron on two protons

$$e + p + p \rightarrow H_2^{+*} + \hbar\omega$$



The two-Coulomb centre problem (adiabatic approxmation)

$$\left(-\frac{1}{2}\Delta-\frac{1}{r_a}-\frac{1}{r_b}\right)\Psi = E\Psi$$



$$e = m = \hbar = 1$$

The Coulomb Green's function in parabolic coordinates

$$G^{(+)}(\vec{r},\vec{r}^{\,'}) = -\frac{ik}{2\pi}\sum_{\bar{m}=-\infty}^{\infty} e^{i\bar{m}(\varphi-\varphi')}\int_0^{\infty} ds e^{i\frac{k}{2}(\mu+\nu+\mu'+\nu')\cosh s}$$

$$\times \sinh s\left(\coth\frac{s}{2}\right)^{2i/k} J_{\bar{m}}\left(b(\mu\mu')^{1/2}\right) J_{\bar{m}}\left(-b(\nu\nu')^{1/2}\right).$$

$\mu,\ \nu, \varphi$ are parabolic coordinates and

$J_{\bar{m}}(x)$ is a Bessel function

$\sinh s,\ \cosh s$ are hyperbolic sine and cosine

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

The wave function of a colliding electron in parabolic coordinates

$$\psi_{\vec{k}}^{a} = \psi_{\vec{k}}^{(0)}(\mu,\nu) - \frac{ik}{4R}\sum_{l,m} A_{l,m}(\mu,\nu) e^{im\varphi} P_l^m(\cos\vartheta_{\vec{R}})$$

$$A_{l,m} = \frac{1}{(2R)^l}\frac{(l-m)!}{(l+m)!}\int_0^{\infty}\chi(s)\int_0^{\mu'_{\max}}\int_0^{\nu'_{\max}} e^{i\frac{k}{2}\left(\mu+\nu+\mu'+\nu'\right)\cosh s} P_l^m\left(\frac{\mu'-\nu'}{\mu'+\nu'}\right)$$

$$\times J_m\left(b(\mu\mu')^{1/2}\right) J_m\left(-b(\nu\nu')^{1/2}\right)\psi_{\vec{k}}^{(0)}(\mu',\nu')(\mu'+\nu')^{l+1}\,d\mu'\,d\nu'\,ds,$$

$$\chi = e^{i\frac{k}{2}(\mu+\nu+\mu'+\nu')\cosh s}\sinh s\left(\coth\frac{s}{2}\right)^{2i/k}$$

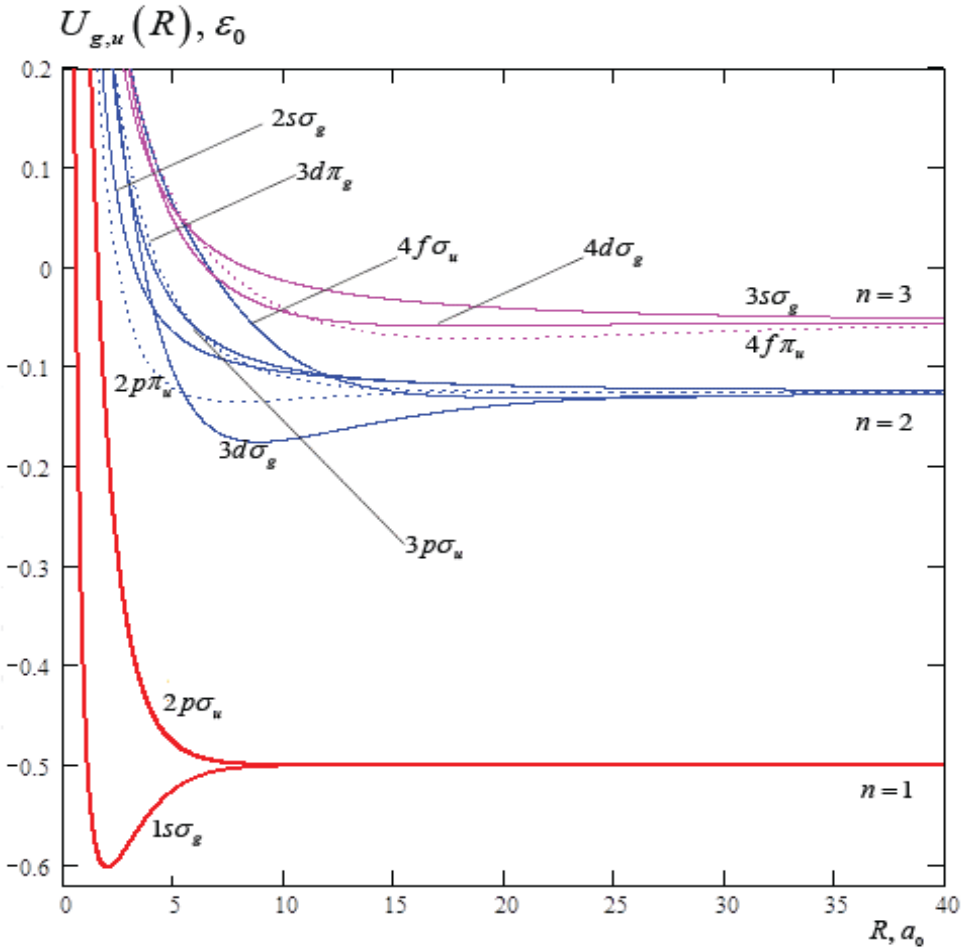
$P_l^m(x)$ is a Legendre polynomial

$$b = k\sinh s \qquad k = \sqrt{2E}$$

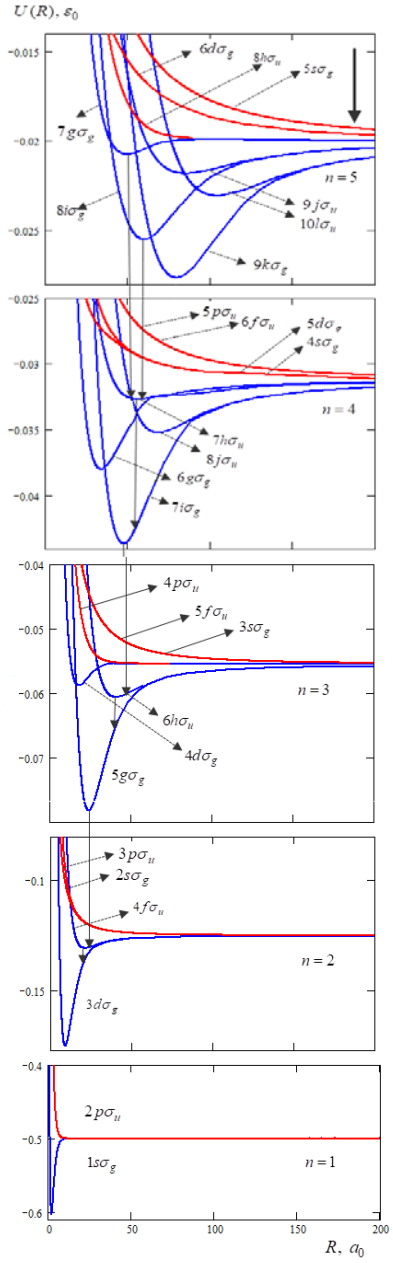
The quasi-molecular mechanism of recombination

$$e + p + p \rightarrow H_2^+(n > 2) + \hbar\omega,$$
$$\hookrightarrow H^* + p,$$

$$H_2^+(n > 2) \rightarrow H_2^+(n-1) + \hbar\omega$$



Energy terms of H_2^+ as functions of distance R between protons



The thick arrow indicates the initial free-bound transition, the thin arrows show bound-bound transitions in H_2^+

Energy terms of H_2^+ with $n \leq 5$ and $m = 0$

The probability of a free-bound and bound-bound radiative transition

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

$\omega_{i,f}$ is the frequency of an emitted photon

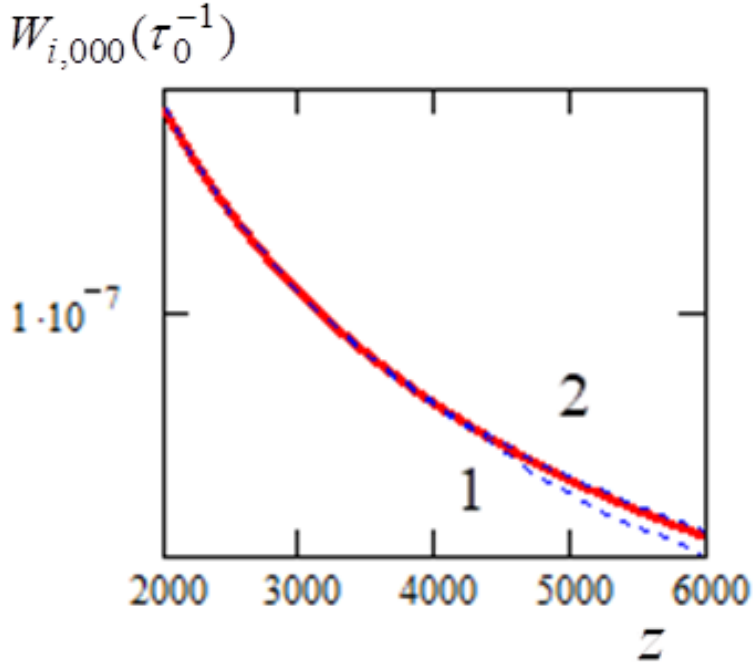
c is the speed of light

The dipole moment matrix element

$$\vec{d}_{if}(R) \sim \int \Psi^*_f(\mu,\nu,\varphi,R)(e\vec{d})\Psi_i(\mu,\nu,\varphi,R)dV$$

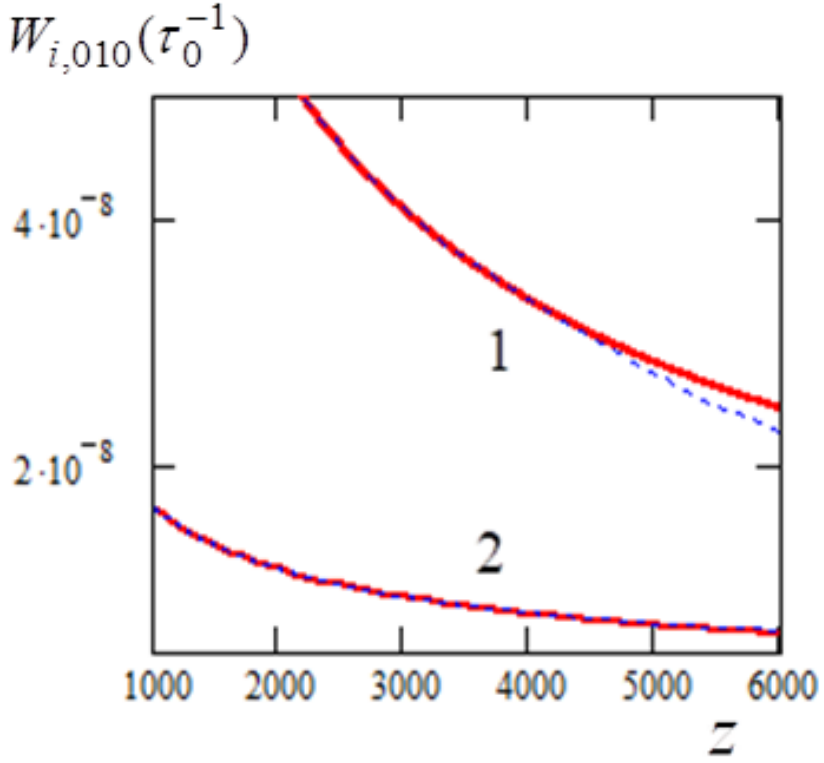
$$\vec{d} = -(\vec{i}x + \vec{j}y + \vec{k}z) \qquad d^{(\pm)} = -(x \pm iy), \quad d^{(z)} = -z$$

Free-bound transitions probabilities



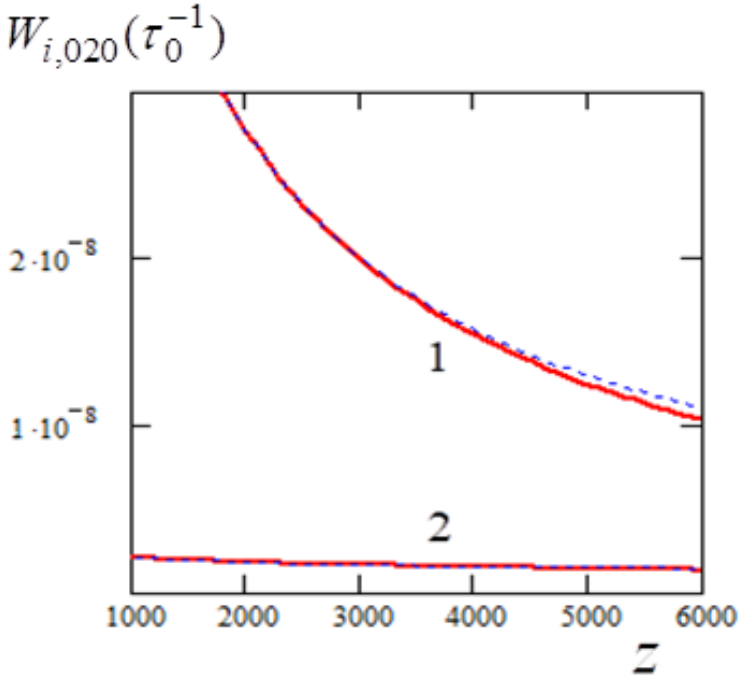
Probabilities $W_{i,000}$ as functions of redshift. Red curve – influence of a second proton is neglected and blue dotted curves – influence of a second proton is taken into account; Curve 1 – parallel and curve 2 – perpendicular orientation of protons.

Free-bound transitions probabilities



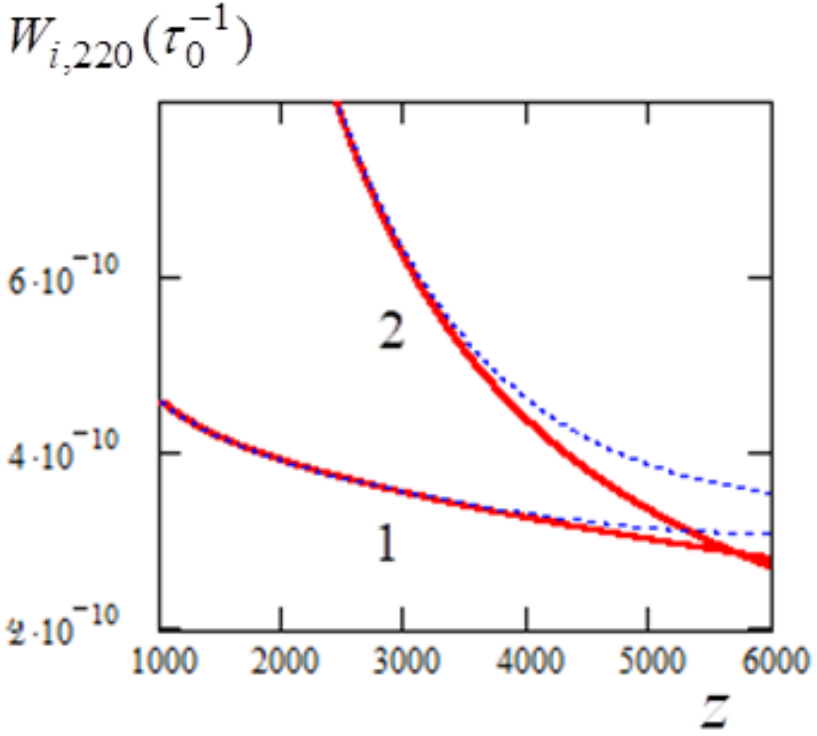
Probabilities $W_{i,010}$ as functions of redshift. Red curve – influence of a second proton is neglected and blue dotted curves – influence of a second proton is taken into account; Curve 1 – parallel and curve 2 – perpendicular orientation of protons.

Free-bound transitions probabilities



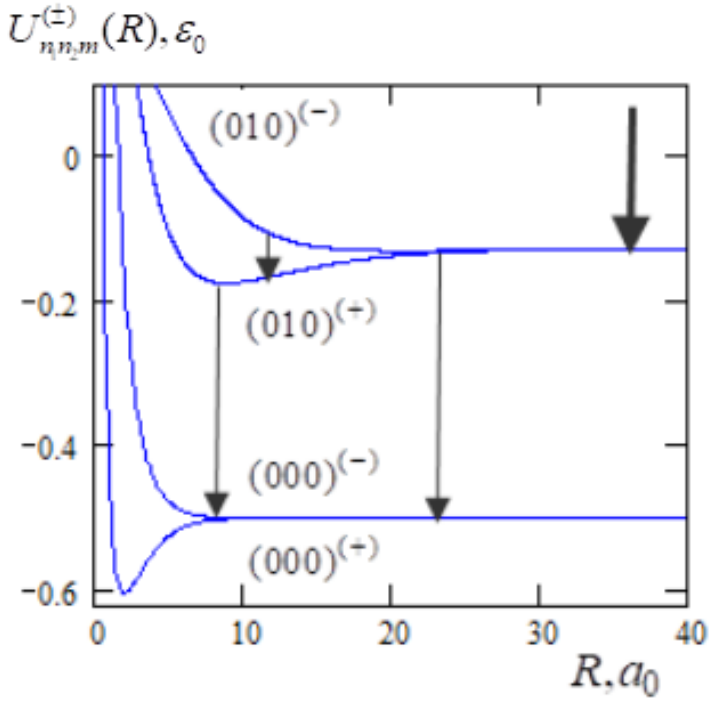
Probabilities $W_{i,020}$ as functions of redshift. Red curve – influence of a second proton is neglected and blue dotted curves – influence of a second proton is taken into account; Curve 1 – parallel and curve 2 – perpendicular orientation of protons.

Free-bound transitions probabilities

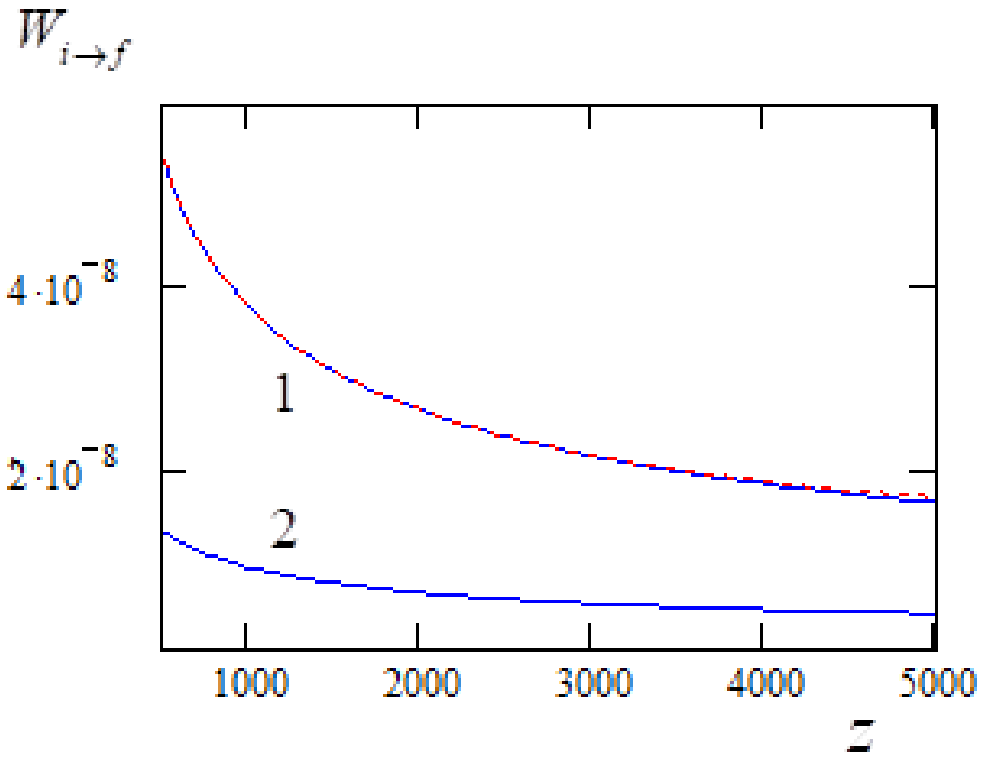


Probabilities $W_{i,220}$ as functions of redshift. Red curve – influence of a second proton is neglected and blue dotted curves – influence of a second proton is taken into account; Curve 1 – parallel and curve 2 – perpendicular orientation of protons.

Formation of H_2^+ in the ground state



The thick arrow indicates the initial radiative transition of a free electron into excited attractive state of H_2^+. Thin arrows indicate radiative transitions between quasi-molecular states.



Probabilities $W_{i\to 2s}$ as functions of redshift. Blue solid curve 1 - the standard model, blue solid curve 2 - the non-standard model. Protons are oriented parallel to the direction of propagation of a colliding electron.

References

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Conclusions

Our investigations show clearly that the quasi-molecular mechanism of recombination (QMR) 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

The QMR shifts the beginning of recombination to the earlier period and increases the rate of the formation of hydrogen in comparison with the standard model

The QMR leads to the formation of the hydrogen molecular ion in the ground state, and hence changes the chemical content of the primordial plasma.

The QMR transforms into the standard mechanism when distances between protons increase. The standard mechanism of recombination is thus the limiting case of the QMR

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Thank you for the attention!