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Radiative recombination rates with different statistical distributions

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Abstract. We deduce radiative recombination rates for any two recombining particles of charge Ze and $-Z'e$ with non-relativistic velocities and reduced mass Mc^2 , useful in a great variety of problems, averaged over Maxwellian and non-Maxwellian distributions and give their parametrization which is valid over the whole range of temperatures for which relativistic effects can be neglected. This has been accomplished using a recent parametrization, obtained by us, of the non-relativistic, radiative recombination cross section in the dipole approximation, valid for any value of the principal quantum number n and for all values of the energy.

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I. Introduction

In these last years there has been a refurbished activity in the field of radiative recombination due to the experimental and theoretical research on electron cooling [1, 2] and its applications to particle accelerators [3, 4], antimatter and exotic atoms production, laser enhanced recombination [5, 6] and highly charged ions physics mainly developed at G.S.I. Laboratory [7, 8].

Since the discover of the Stobbe formula in the early 30's [9], a large number of published papers has given analytical and numerical approximations to evaluate the radiative recombination rates for Maxwellian distributions. In particular we wish to recall the work of Seaton [10], based on an asymptotic expansion of the Kramers-Gaunt factors, and the work of Burgess [11] based on the use of simple recursion relations. These rates have been used extensively in the fields of astrophysics and plasma physics and its diagnostics.

With the development of new and more powerful computing facilities, the radiative recombination cross sections have been calculated more and more precisely also for very large values of the principal quantum number n and in the very low energy region. These new

computational efforts have produced some new analytical expressions that parametrize more precisely the cross sections [12–14]. Recently we have obtained a very precise parametrization of the cross section based on the exact computation of the non-confluent hypergeometrical functions and also derived high energy and low energy approximations to the cross section [15]. Reference [15] is the starting point of the present work (see also our previous works of [16, 17] for further details), in which we are interested in computing and giving a parametrization of the radiative recombination rates averaged over Maxwellian and non-Maxwellian distributions of velocities. In fact, radiative recombination can occur in the presence of an electromagnetic field, for instance laser radiation or simply a static electric field (Druyvenstein effect [18, 19]), or generally in the presence of an average external field in such a way that non-Maxwellian distributions must be used [20, 21]. There is also another reason to be interested in non-Maxwellian distributions: recent studies [22, 23] of stationary distributions obtained as solutions of the Fokker-Planck equation show that in addition to the Maxwell distribution there is also a set of solutions that describes stationary non-Maxwellian distributions.

At the moment we are not interested in a specific physical system, our results are general and can be applied to a variety of processes involving the radiative recombination of two non-relativistic particles with ground state energy E_{1s} (in the bound state) and are valid over the range of temperatures $0 \leq kT \leq \infty$. For $kT \geq Mc^2$ one should also consider relativistic effects, which become important at those temperatures. Our calculations are valid only for the pure Coulomb field of point charges, not for complex ions.

In Sect. II we recall our parametrization of the radiative recombination cross section and we report the distribution functions [20] we will use in our calculations. In Sect. III we define the rates and show how we are going to parametrize them. In Sect. IV we show the results and we discuss their features and give their parametrization. Conclusions are in Sect. V.

II. Radiative recombination cross section and statistical distributions

The total non-relativistic radiative recombination cross section $\sigma_{\text{tot}}(\varepsilon)$, in the dipole approximation, is given by:

$$\sigma_{\text{tot}}(\varepsilon) = \sum_n \sum_{l,j} \sigma_{n,l,j}(\varepsilon) \quad (\text{II.1})$$

where $\sigma_{n,l,j}(\varepsilon)$ is the cross section for recombination in the state of quantum numbers n, l, j and

$$\varepsilon = E_k/E_{1s} \quad (\text{II.2})$$

$$E_{1s} = \frac{1}{2} \left(\frac{ZZ' e^2}{\hbar c} \right)^2 M c^2 \quad (\text{II.3})$$

where M is the reduced mass; the kinetic energy E_k in the center of mass frame is:

$$E_k = \frac{1}{2} M v^2 \quad (\text{II.4})$$

where v is the velocity in the center of mass frame. We can write $\sigma_{\text{tot}}(\varepsilon)$ as [15]:

$$\sigma_{\text{tot}}(\varepsilon) = \sum_{n=1}^{\infty} \frac{\sigma_{1s}(\varepsilon)}{n^{\bar{X}(n,\varepsilon)}} = \sigma_{1s}(\varepsilon) s(\varepsilon) \quad (\text{II.5})$$

where:

$$s(\varepsilon) = \sum_{n=1}^{\infty} \frac{1}{n^{\bar{X}(n,\varepsilon)}} \quad (\text{II.6})$$

where the function $\bar{X}(n, \varepsilon)$ has been studied in detail by Erdas et al. [15] and where $\sigma_{1s}(\varepsilon)$ is the cross section for recombination in the $n=1$ level, and is given by:

$$\sigma_{1s}(\varepsilon) = \frac{8\pi}{3\sqrt{3}} (ZZ')^4 \frac{(\hbar c)^2}{(1+\varepsilon)\varepsilon} \left(\frac{e^2}{\hbar c} \right)^5 \frac{g_1(\varepsilon)}{E_{1s}^2} \quad (\text{II.7})$$

where $g_1(\varepsilon)$ is the Gaunt factor:

$$g_1(\varepsilon) = 8\pi\sqrt{3} \frac{1}{\varepsilon+1} \frac{e^{-4 \frac{\arctan \sqrt{\varepsilon}}{\sqrt{\varepsilon}}}}{1 - e^{-\frac{2\pi}{\sqrt{\varepsilon}}}} \quad (\text{II.8})$$

The function $s(\varepsilon)$ is parametrized in the following way (Erdas et al. [15])

$$s(\varepsilon) = \begin{cases} -1.38133 \log \varepsilon + 0.480383 & \text{if } \varepsilon \leq 10^{-2}; \\ 0.259387 \log^2 \varepsilon - 0.421437 \log \varepsilon + 1.39636 & \text{if } 10^{-2} < \varepsilon \leq 10; \\ 1.2020569 & \text{if } \varepsilon > 10. \end{cases} \quad (\text{II.9})$$

We use the statistical distributions given by Mora et al. [20]:

$$\phi_l(v) = 4\pi v^2 \left(\frac{C_l M}{2kT} \right)^{\frac{3}{2}} \frac{l}{4\pi \Gamma(3/l)} \exp \left[- \left(\frac{C_l M v^2}{2kT} \right)^{1/2} \right] \quad (\text{II.10})$$

$$C_l = \frac{2\Gamma(5/l)}{3\Gamma(3/l)} \quad (\text{II.11})$$

where $\Gamma(z)$ is the gamma function (Euler's integral of the second kind). When $l=2$ (II.10) gives the Maxwell distribution, when $l>2$ the distributions obtained from (II.10) have a depleted tail compared to the Maxwell one, and, when $l=1$, the tail is enhanced.

III. The recombination rates

We define the recombination rate as:

$$\alpha_l = \int \sigma_{\text{tot}}(v) \phi_l(v) v dv \quad (\text{III.1})$$

where v is the relative velocity of the recombining particles and where l refers to the specific distribution used. After changing the variable of integration to ε , which is defined in (II.2), and using (II.10), we obtain:

$$\alpha_l = \left(\frac{1}{2Mc^2} \right)^{\frac{1}{2}} \left(\frac{C_l}{kT} \right)^{\frac{3}{2}} \frac{l}{\Gamma(3/l)} c E_{1s}^2 \cdot \int_0^{\infty} \sigma_{\text{tot}}(\varepsilon) \varepsilon \exp \left[- \left(\frac{C_l \varepsilon E_{1s}}{kT} \right)^{1/2} \right] d\varepsilon \quad (\text{III.2})$$

where c is the speed of light. Using the expression of $\sigma_{\text{tot}}(\varepsilon)$ from (II.4), we obtain:

$$\alpha_l = A_l(kT) \int_0^{\infty} \frac{1}{(1+\varepsilon)} g_1(\varepsilon) s(\varepsilon) \cdot \exp \left[- \left(\frac{C_l \varepsilon E_{1s}}{kT} \right)^{1/2} \right] d\varepsilon \quad (\text{III.3})$$

where $s(\varepsilon)$ is given by (II.9), $g_1(\varepsilon)$ is given by (II.8) and $A_l(kT)$ is given by:

$$A_l(kT) = \frac{8\pi}{3\sqrt{3}} (ZZ')^4 \left(\frac{e^2}{\hbar c} \right)^5 \left(\frac{1}{2Mc^2} \right)^{\frac{1}{2}} \cdot \left(\frac{1}{E_{1s}} \right)^{\frac{3}{2}} \left(\frac{E_{1s}}{kT} \right)^{\frac{3}{2}} \frac{C_l^{\frac{3}{2}} l}{\Gamma(3/l)} c (\hbar c)^2 \quad (\text{III.4})$$

Considering the integration in (III.3), we have:

$$\int_0^{\infty} \frac{1}{(1+\varepsilon)} \exp \left(- \frac{\varepsilon E_{1s}}{kT} \right) d\varepsilon = -e^{E_{1s}/kT} Ei(-E_{1s}/kT) \quad (\text{III.5})$$

where $Ei(x)$ is the exponential-integral function. In view of (III.5) we may write:

$$\int_0^{\infty} \frac{1}{(1+\varepsilon)} g_1(\varepsilon) s(\varepsilon) \exp \left[- \left(\frac{C_l \varepsilon E_{1s}}{kT} \right)^{1/2} \right] d\varepsilon = -e^{E_{1s}/kT} Ei(-E_{1s}/kT) S_l(kT/E_{1s}) \quad (\text{III.6})$$

where $S_l(x)$ is, for now, an unknown function. We have evaluated numerically the integral on the left-hand side of (III.6) for all values of the temperature, and therefore we have obtained the exact values of the functions $S_l(x)$ for $l=1, 2, 3$, which are plotted in Fig. 1. We remark the behaviour of the three functions $S_l(x)$: at $\log x > 5$ their values are more or less the same, but they are very differ-

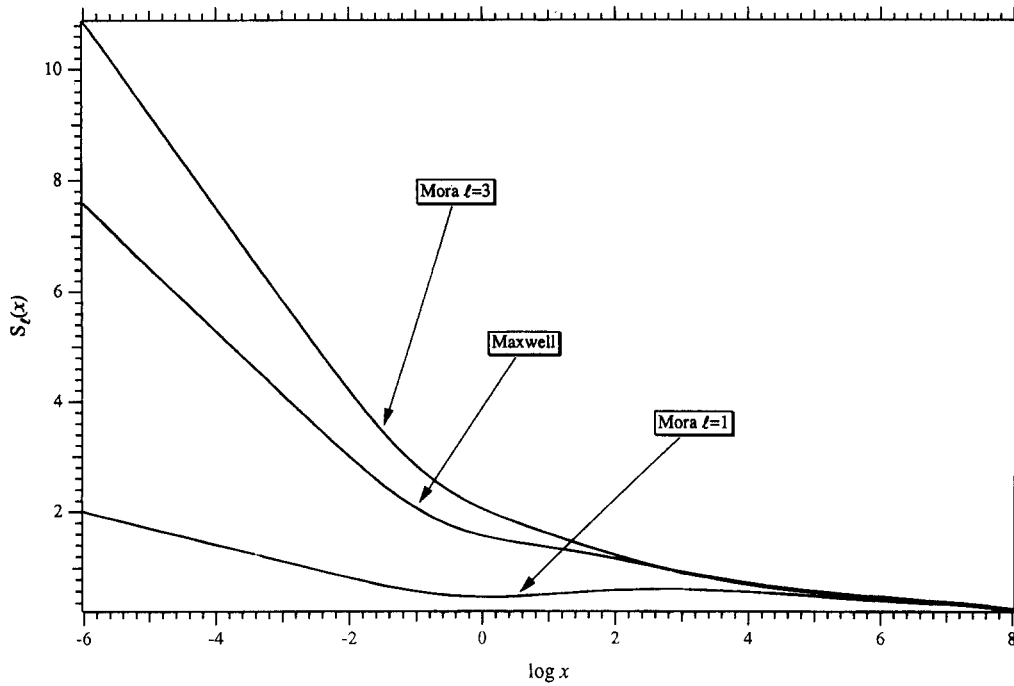


Fig. 1. The functions $S_l(x)$ for $l=1, 2, 3$ as a function of $\log x$, where $x = kT/E_{1s}$

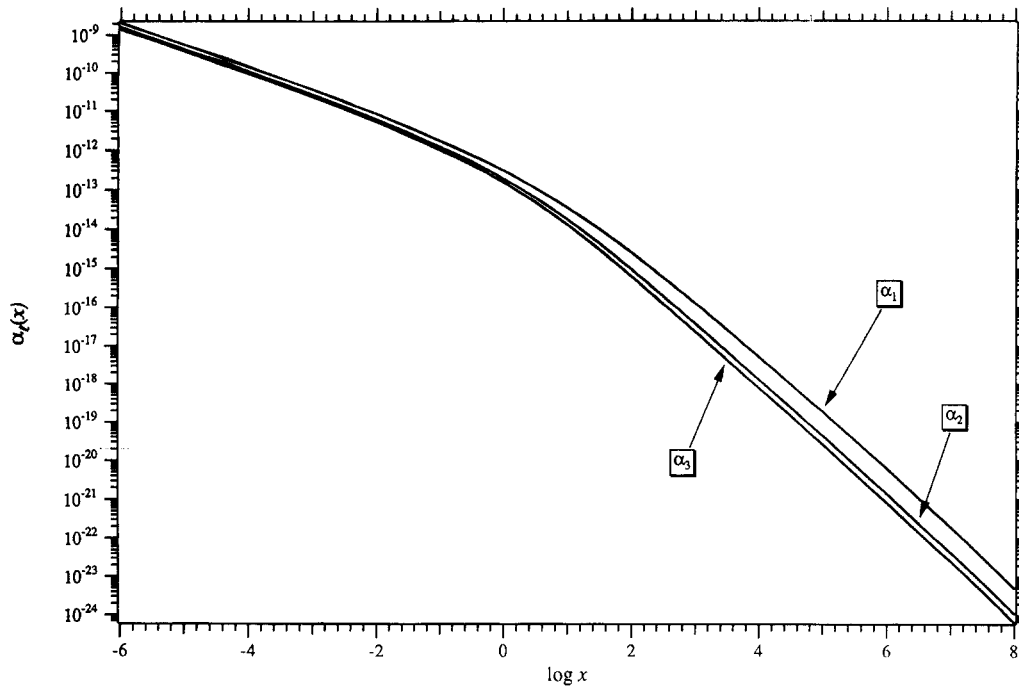


Fig. 2. The radiative recombination rates in the case of positronium recombination, α_l^P (in $\text{cm}^3 \text{s}^{-1}$) for $l=1, 2, 3$ as a function of $\log x$

ent for $kT < E_{1s}$. Using these functions we may write the rates as:

$$\alpha_l = -A_l(kT)e^{E_{1s}/kT} Ei(-E_{1s}/kT) S_l(kT/E_{1s}) \quad (\text{III.7})$$

In Fig. 2 we plot the rates α_l^P for $l=1, 2, 3$ in the case of $e^+ - e^-$ recombining to form positronium and for a wide range of temperatures. For a fixed value of x , the relation between α_l^P and α_l (the recombination rate for any system of reduced mass Mc^2 and charges Ze and $-Z'e$) is the following:

$$\alpha_l = \alpha_l^P \left(\frac{m_e c^2}{2Mc^2} \right)^2 (ZZ') \quad (\text{III.8})$$

where $m_e c^2$ is the electron mass. Caution should be used for very high temperature, because relativistic effects become important for $kT \geq Mc^2$, non-relativistic velocities correspond to

$$x = \frac{kT}{E_{1s}} \ll \frac{Mc^2}{E_{1s}} = 2 \left(\frac{\hbar c}{ZZ' c^2} \right)^2 < 4 \times 10^4 \quad (\text{III.9})$$

IV. Parameterization of the recombination rates

After introducing the variable

$$x = \frac{kT}{E_{1s}} \quad (IV.1)$$

we now report the parametrizations we found for the functions $S_l(x)$ for $l=1, 2, 3$:

$$\begin{aligned} S_1(x) &= \begin{aligned} &0.250 - 0.291 \log x \\ &0.516 + 0.002 \log x + 0.051 \log^2 x - 0.017 \log^3 x + 0.001 \log^4 x \\ &1.713 x^{-0.095} \end{aligned} & \begin{aligned} &\text{if } x \leq 10^{-2} \\ &\text{if } 10^{-2} < x \leq 10^6 \\ &\text{if } x > 10^6 \end{aligned} & (IV.2) \\ S_2(x) &= \begin{aligned} &0.704 - 1.146 \log x \\ &1.592 - 0.340 \log x + 0.113 \log^2 x - 0.031 \log^3 x + 0.003 \log^4 x \\ &2.302 x^{-0.107} \end{aligned} & \begin{aligned} &\text{if } x \leq 10^{-2} \\ &\text{if } 10^{-2} < x \leq 10^6 \\ &\text{if } x > 10^6 \end{aligned} & (IV.3) \\ S_3(x) &= \begin{aligned} &0.854 - 1.666 \log x \\ &2.063 - 0.618 \log x + 0.153 \log^2 x - 0.030 \log^3 x + 0.002 \log^4 x \\ &2.186 x^{-0.107} \end{aligned} & \begin{aligned} &\text{if } x \leq 10^{-2} \\ &\text{if } 10^{-2} < x \leq 10^6 \\ &\text{if } x > 10^6 \end{aligned} & (IV.4) \end{aligned}$$

We also report the well-known expansion of the exponential-integral function

$$-e^{1/x} Ei\left(-\frac{1}{x}\right) = e^{1/x} \left[\ln x - \gamma - \sum_{k=1}^{\infty} \frac{(-1)^k}{k k! x^k} \right] \quad (IV.5)$$

where $\gamma = 0.5772156649\dots$ is Euler's constant. This expansion converges very rapidly for $x \geq 1$. When $0 < x < 1$, instead of using the expansion of (IV.5), it is better to use the following polynomial approximation [24]

$$-e^{1/x} Ei\left(-\frac{1}{x}\right) \approx x \left[\frac{1 + 2.334733x + 0.250621x^2}{1 + 3.30657x + 1.681534x^2} \right] \quad (IV.6)$$

that gives a percentage error which, for all x in the considered range, is less than 5×10^{-5} .

The values of the $A_l(kT)$ are:

$$\begin{aligned} A_1(kT) &= 9.3468(Z)^4 (Mc^2)^{-\frac{1}{2}} (kT)^{-\frac{3}{2}} \times 10^{-12} \text{ cm}^3 \text{ s}^{-1} \\ A_2(kT) &= 1.8645(Z)^4 (Mc^2)^{-\frac{1}{2}} (kT)^{-\frac{3}{2}} \times 10^{-12} \text{ cm}^3 \text{ s}^{-1} \\ A_3(kT) &= 1.1572(Z)^4 (Mc^2)^{-\frac{1}{2}} (kT)^{-\frac{3}{2}} \times 10^{-12} \text{ cm}^3 \text{ s}^{-1} \end{aligned} \quad (IV.7)$$

where Mc^2 is in MeV and kT is in eV. Therefore using (III.7–III.8) and (IV.2–IV.7) one can easily compute the numerical values of the radiative recombination rates α_l for all values of the temperature. In Table 1 we report the exact numerical values of α_l^P for $10^{-6} \leq x \leq 10^8$. Table 1, together with (III.8), can be used to calculate exact values of the recombination rates for any recombining system.

A discussion on the precision of the different approximations for the rates which one can find in the literature is reported in [3]. Our parametrization has a percentage error which is always less than 2% (in most cases of the order of few tenths of a percent) over the whole range of temperature, while the other approximations reported in [3], are valid on a limited range of tempera-

tures and have a percentage error of several percent, in particular the low energy approximation given by Bell and Bell [3] has a percentage error up to ten percent.

V. Conclusions

Recently the interest in non-Maxwellian distributions has increased, in order to have a better understanding

Table 1. The exact numerical values of α_l^P , in $\text{cm}^3 \text{ s}^{-1}$, for $10^{-6} \leq x \leq 10^8$. This table, together with (III.8), allows one to calculate the exact values of the rates for any recombining system

$\log x$	α_1^P	α_2^P	α_3^P
-6.00	2.084×10^{-9}	1.577×10^{-9}	1.401×10^{-9}
-5.75	1.505×10^{-9}	1.138×10^{-9}	1.010×10^{-9}
-5.50	1.086×10^{-9}	8.196×10^{-10}	7.272×10^{-10}
-5.25	7.823×10^{-10}	5.894×10^{-10}	5.226×10^{-10}
-5.00	5.626×10^{-10}	4.231×10^{-10}	3.749×10^{-10}
-4.75	4.038×10^{-10}	3.031×10^{-10}	2.683×10^{-10}
-4.50	2.892×10^{-10}	2.167×10^{-10}	1.916×10^{-10}
-4.25	2.067×10^{-10}	1.545×10^{-10}	1.365×10^{-10}
-4.00	1.474×10^{-10}	1.099×10^{-10}	9.697×10^{-11}
-3.75	1.048×10^{-10}	7.793×10^{-11}	6.868×10^{-11}
-3.50	7.432×10^{-11}	5.507×10^{-11}	4.846×10^{-11}
-3.25	5.252×10^{-11}	3.877×10^{-11}	3.406×10^{-11}
-3.00	3.697×10^{-11}	2.718×10^{-11}	2.383×10^{-11}
-2.75	2.591×10^{-11}	1.896×10^{-11}	1.659×10^{-11}
-2.50	1.807×10^{-11}	1.315×10^{-11}	1.147×10^{-11}
-2.25	1.253×10^{-11}	9.062×10^{-12}	7.885×10^{-12}
-2.00	8.638×10^{-12}	6.201×10^{-12}	5.378×10^{-12}
-1.75	5.913×10^{-12}	4.209×10^{-12}	3.636×10^{-12}
-1.50	4.017×10^{-12}	2.833×10^{-12}	2.437×10^{-12}
-1.25	2.706×10^{-12}	1.889×10^{-12}	1.617×10^{-12}
-1.00	1.806×10^{-12}	1.246×10^{-12}	1.061×10^{-12}
-0.75	1.191×10^{-12}	8.101×10^{-13}	6.854×10^{-13}
-0.50	7.747×10^{-13}	5.172×10^{-13}	4.335×10^{-13}
-0.25	4.951×10^{-13}	3.223×10^{-13}	2.665×10^{-13}
0.00	3.097×10^{-13}	1.949×10^{-13}	1.583×10^{-13}
0.25	1.890×10^{-13}	1.138×10^{-13}	9.039×10^{-14}
0.50	1.122×10^{-13}	6.406×10^{-14}	4.956×10^{-14}
0.75	6.466×10^{-14}	3.471×10^{-14}	2.610×10^{-14}
1.00	3.615×10^{-14}	1.813×10^{-14}	1.323×10^{-14}
1.25	1.961×10^{-14}	9.147×10^{-15}	6.479×10^{-15}
1.50	1.033×10^{-14}	4.475×10^{-15}	3.080×10^{-15}
1.75	5.293×10^{-15}	2.131×10^{-15}	1.429×10^{-15}
2.00	2.644×10^{-15}	9.910×10^{-16}	6.491×10^{-16}
2.25	1.290×10^{-15}	4.519×10^{-16}	2.900×10^{-16}
2.50	6.167×10^{-16}	2.028×10^{-16}	1.279×10^{-16}
2.75	2.893×10^{-16}	8.982×10^{-17}	5.581×10^{-17}
3.00	1.335×10^{-16}	3.935×10^{-17}	2.415×10^{-17}

Table 1 (continued)

log x	α_1^P	α_2^P	α_3^P
3.25	6.069×10^{-17}	1.709×10^{-17}	1.038×10^{-17}
3.50	2.724×10^{-17}	7.366×10^{-18}	4.442×10^{-18}
3.75	1.208×10^{-17}	3.154×10^{-18}	1.890×10^{-18}
4.00	5.351×10^{-18}	1.354×10^{-18}	8.072×10^{-19}
4.25	2.339×10^{-18}	5.766×10^{-19}	3.424×10^{-19}
4.50	1.015×10^{-18}	2.449×10^{-19}	1.450×10^{-19}
4.75	4.375×10^{-19}	1.036×10^{-19}	6.120×10^{-20}
5.00	1.879×10^{-19}	4.381×10^{-20}	2.583×10^{-20}
5.25	8.020×10^{-20}	1.847×10^{-20}	1.087×10^{-20}
5.50	3.397×10^{-20}	7.744×10^{-21}	4.555×10^{-21}
5.75	1.421×10^{-20}	3.214×10^{-21}	1.889×10^{-21}
6.00	6.238×10^{-21}	1.399×10^{-21}	8.216×10^{-22}
6.25	2.638×10^{-21}	5.883×10^{-22}	3.454×10^{-22}
6.50	1.109×10^{-21}	2.462×10^{-22}	1.445×10^{-22}
6.75	4.614×10^{-22}	1.021×10^{-22}	5.988×10^{-23}
7.00	1.976×10^{-22}	4.356×10^{-23}	2.555×10^{-23}
7.25	8.202×10^{-23}	1.804×10^{-23}	1.058×10^{-23}
7.50	3.322×10^{-23}	7.294×10^{-24}	4.278×10^{-24}
7.75	1.317×10^{-23}	2.889×10^{-24}	1.694×10^{-24}
8.00	5.095×10^{-24}	1.116×10^{-24}	6.546×10^{-25}

of many different physical processes in astrophysics, plasma physics and nuclear physics. In addition to the [20–23] we wish to recall the works of Langdon [25] and of Whitney and Pulsifer [26] concerning the conditions under which non-Maxwellian distributions must be used when analyzing inverse bremsstrahlung and heated-electron, laser produced plasmas and high current discharges.

Non-Maxwellian distribution are important also in the field of nuclear physics, where, on one side we have the proposal by Clayton [27] to use non-Maxwellian distributions in the solar plasma in order to explain the solar neutrino puzzle, and on the other side we have studies on non-Maxwellian distributions of nucleons in nuclear matter with momentum-dependent effective interaction [28, 29].

Since the process of radiative recombination is important in atomic physics, plasma physics and astrophysics, we have provided in this paper a useful parametrization of the recombination rates valid at any temperature for which relativistic effects can be neglected. This work reports for the first time a parametrization of α_i valid for both low temperature and high temperature. These results have been obtained using the precise parametrization of the non-relativistic radiative recombination cross sections that we have calculated previously [15].

While the difference between the values of α_2 (Maxwellian distribution) and α_3 (depleted tail) is quite small and only at very high temperature there is a difference of a factor of two, on the contrary the difference between α_2 or α_3 and α_1 (enhanced tail) increases with the temperature and at high temperature can be of the order of a factor of ten.

At very high temperature the difference among the three different α_i is due to the different values of the functions $A_i(kT)$. At low temperature the difference is mainly due to both S_i and A_i however their product compensates some of the differences.

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