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Multipole and relativistic effects in radiative recombination process in hot plasmas

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On the basis of the fully relativistic Dirac-Fock treatment of photoionization and radiative recombination processes with regard to all multipoles of the radiative field, we have assessed the influence of nondipole effects on the radiative recombination rate coefficients. A formula for the rate coefficient has been derived using the relativistic Maxwell-Boltzmann distribution of continuum electrons instead of the commonly used nonrelativistic distribution. This decreases the recombination rate coefficient considerably in hot thermal plasmas.

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The radiative recombination rate coefficients along with the radiative recombination cross sections (RRCSs) and photoionization cross sections (PCSs) are required for estimates of ionization equilibria and thermal balance in terrestrial and astrophysical plasmas contaminated by various ions. In fusion reactors, core plasmas is expected to have electron temperature about 25 keV at which impurity ions of various elements may be stripped to bare nuclei. Data on highly charged ions will be important in performance of future fusion devices developed, for example, in the framework of the tungsten program [1]. In astrophysical objects such as stellar black-hole binaries and Seyferrt galaxies, the plasma temperature may reach 150 keV [2].

As is well known (see, for example, Refs. [3–7], and references therein), the multipole and relativistic effects are of great importance in calculations of PCS and RRCS at high electron energies. Nevertheless, these effects were usually neglected in study of the photoionization and radiative recombination processes in plasmas with the exception of pioneering works [8,9] on rate coefficients for highly charged ions. Previous work on radiative recombination in thin plasmas for elements H to Ni has been summarized in Ref. [10]. The most extensive advanced calculations of PCS, RRCS, and rate coefficients by Badnell (ADAS database) [11] were performed using the semirelativistic and electric dipole approximation for electron energies to $1.36Z^2$ keV and for $Z \leqslant 54$, that is, to $\sim$4 MeV. The widely used tables of hydrogenic recombination rate coefficients were calculated within the nonrelativistic dipole approximation for temperatures up to $T=\infty$ [12].

In the present paper, we assess the influence of multipole effects on the radiative recombination rate coefficients and relevant PCS and RRCS as well as certain of relativistic effects such as the relativistic transformation coefficient between PCS and RRCS and the relativistic correction factor for the recombination rate coefficient. A formula for recombination rate coefficient has been derived using the relativistic Maxwell-Boltzmann distribution of continuum electrons instead of the usual nonrelativistic distribution. With allowance made for the relativistic transformation coefficient, the formula is factorized giving rise to the temperature-dependent relativistic correction factor for which the usual nonrelativistic expression is multiplied. This factor is absent in all previous calculations and all available databases although rate coefficients have been calculated at temperature to 1000 keV and higher [11–13]. The factor is shown to change rate coefficients considerably at enough high temperatures.

We consider the case of thin plasmas for which we take the basic processes as for free atoms and ions. The fully relativistic treatment of the photoionization and recombination processes is used [7]. All significant multipole orders of the radiative field are taken into account in the calculations. Electron wave functions are generated in the framework of the self-consistent Dirac-Fock (DF) method. It should be noted that the calculations performed by the DF method and by the commonly used Dirac-Slater method where the exchange is taken into consideration approximately, may differ significantly even at high energies, especially for the low excited electron states of low-charged ions. For example, in the W^{6+} case, the difference between the two calculations of RRCS is 20–35 % for the excited s, p, and d shells with $n=5-8$ at energies $E_k \gtrsim 50$ keV and reaches 83% for the 6f shells [7]. The shells with $n=5-8$ and $l \leqslant 3$ make a contribution more than 80% to the total RRCS at $E_k=50.3$ keV.

The relativistic PCS in the ith subshell per one electron can be written in the form

$$\sigma_{\rm ph}^{(i)} = \frac{4\pi^2\alpha}{\tilde{k}(2j_i+1)} \sum_L \sum_\kappa [(2L+1)Q_{LL}^2(\kappa) + LQ_{L+1L}^2(\kappa) + (L+1)Q_{L-1L}^2(\kappa) - 2\sqrt{L(L+1)}Q_{L-1L}(\kappa)Q_{L+1L}(\kappa)]. \quad (1)$$

Here $\tilde{k}$ is the photon energy in m_0c^2, L is the multipolarity of the radiative field, $\kappa=(l-j)(2j+1)$, l and j are the orbital and total angular momenta of the electron, α is the fine structure constant, and $Q_{\Lambda L}(\kappa)$ is the reduced matrix element.

The cross section of the recombination process with the capture of an electron with energy $\tilde{E}_k$ to the ith subshell of the ion is expressed in terms of the corresponding PCS as follows:

$$\sigma_{\rm RR}^{(i)} = A q_i \sigma_{\rm ph}^{(i)}, \tag{2}$$

where q_i is the number of vacancies in the ith subshell prior to recombination. The transformation coefficient A can be derived from the principle of the detailed balance. The exact relativistic expression for the coefficient is written as [3,6]

$$A_{\rm rel} = \frac{\tilde{k}^2}{2\tilde{E}_k + \tilde{E}_k^2}, \quad \tilde{E}_k = \frac{E_k}{m_0 c^2}. \tag{3}$$

However in the RRCS calculations, the coefficient is used in the form

$$A_{\rm nrel} = \frac{k^2}{2 m_0 c^2 E_k}, \quad k = m_0 c^2 \tilde{k}, \tag{4}$$

which may be obtained in the nonrelativistic approximation from Eq. (3). The discrepancy between $\sigma_{\rm RR}$ obtained with Eqs. (3) and (4) which is equal to $E_k/2m_0c^2$ depends only on the electron kinetic energy E_k with the difference $\sim 5\%$ at $E_k = 50$ keV and reaching $\sim 100\%$ at $E_k = 1000$ keV. Consequently, at high electron energy, the relativistic expression [Eq. (3)] should be used in the RRCS calculations.

The radiative recombination rate coefficient is calculated using the thermal average over RRCS. In the present paper, the continuum electrons are described by the relativistic Maxwell-Boltzmann (or the term Maxwell-Jüttner is used sometimes) distribution function $f(E)$ normalized to unity as follows [14,15]:

$$f(E)dE = \frac{E(E^2-1)^{1/2}}{\theta e^{1/\theta} K_2(1/\theta)} e^{-(E-1)/\theta} dE. \tag{5}$$

Here E is the total electron energy in units of m_0c^2 including the rest energy, $\theta = k_\beta T / m_0 c^2$ is the characteristic dimensionless temperature, T is the temperature, and k_β is the Boltzmann constant. The function K_2 denotes the modified Bessel function of the second order. Taking into account the relativistic distribution in the form of Eq. (5) and the relativistic transformation coefficient $A_{\rm rel}$ [Eq. (3)], we arrive to the expression for the relativistic radiative recombination rate coefficient

$$\alpha_{\rm rel}^{(i)}(T) = \langle v \sigma_{\rm RR}^{(i)} \rangle = F_{\rm rel}(\theta) \alpha^{(i)}(T). \tag{6}$$

Here $v = (p/E)c$ is the electron velocity with the momentum $p = \sqrt{E^2 - 1}$ and $\alpha^{(i)}(T)$ is the usual rate coefficient with the nonrelativistic electron distribution which may be written as [8]

$$\alpha^{(i)}(T) = (2/\pi)^{1/2} c^{-2} (m_0 k_\beta T)^{-3/2} q_i \int_{\varepsilon_i}^{\infty} k^2 \sigma_{\rm ph}^{(i)}(k) e^{(\varepsilon_i - k)/(k_\beta T)} dk, \tag{7}$$

where k is the photon energy and ε_i is the binding energy of the ith subshell. In Eq. (7), $F_{\rm rel}(\theta)$ is the relativistic factor

$$F_{\rm rel}(\theta) = \sqrt{\frac{\pi}{2}\theta} \Bigg/ K_2(1/\theta) e^{1/\theta}. \tag{8}$$

This is just the factor which has been disregarded in all previous calculations.

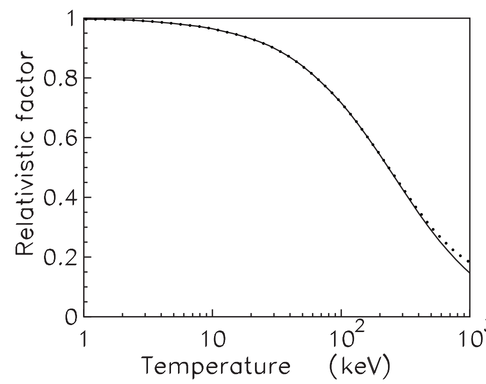

FIG. 1. Exact relativistic factor $F_{\rm rel}(T)$ (full) and approximate factor $\tilde{F}_{\rm rel}(T)$ (dotted).

It follows from Eq. (8) that the relativistic factor for the recombination rate coefficient depends on temperature only. The T dependence of the factor is demonstrated in Fig. 1. As is seen, the factor $F_{\rm rel}(\theta)$ differs noticeably from unit beginning with several tens of keV. Adopting the relativistic distribution of continuum electrons instead of the nonrelativistic one results in a decrease of the rate coefficient values by a factor of 1.2 at plasma temperature $k_\beta T = 50$ keV and up to a factor of 7 at $k_\beta T = 1000$ keV. It should be noted that the hydrogenic recombination rate coefficients tabulated for temperatures up to $T = \infty$ [12] were calculated for the nonrelativistic Maxwellian electron velocity distribution.

One may easily obtain an approximate expression for the relativistic factor $F_{\rm rel}(\theta)$. Using the asymptotic expansion of the Bessel function $K_2(1/\theta)$ at large $1/\theta$ [16], that is, at low temperature, we arrive at the factor $\tilde{F}_{\rm rel}(\theta)$, an approximation to $F_{\rm rel}(\theta)$

$$\tilde{F}_{\rm rel}(\theta) = 1 \Bigg/ \left(1 + \frac{15}{8}\theta + \frac{105}{128}\theta^2 + \cdots\right). \tag{9}$$

Equation (9) provides an excellent approximation for $F_{\rm rel}(\theta)$ with the terms through order θ^2 at $\theta \lesssim 1$. The factors $F_{\rm rel}(\theta)$ and $\tilde{F}_{\rm rel}(\theta)$ are compared in Fig. 1. The full curve refers to the exact factor [Eq. (8)] and the dashed curve refers to the approximate factor [Eq. (9)]. As can be seen, there is a little difference between the two curves, the relative error is $\sim 4\%$ at $k_\beta T = 500$ keV and 25% at $k_\beta T = 1000$ keV.

Let us next consider the influence of the multipole effects. The electric dipole approximation takes into account only terms with $L = 1$ in Eq. (1). In Fig. 2, we compare RRCS obtained in the dipole approximation $\sigma_{\rm RR}(\text{dip})$ (dashed curves) with RRCS calculated including all multipoles $\sigma_{\rm RR}(L)$ (full curves) for bare nuclei of two representative elements Fe ($Z = 26$) and W ($Z = 74$). The energy range under consideration is 1 keV $\leqslant E_k \leqslant$ 1000 keV.

As is seen, the curves begin to diverge noticeably even at several keV. At the highest energy 1000 keV, in the case of W^{74+}, $\sigma_{\rm RR}(\text{dip})$ is smaller than the exact value $\sigma_{\rm RR}(L)$ by a factor of ~ 5 for the $1s$ shell and by a factor of ~ 40 for the $4f_{5/2}$ subshell. Our calculations showed that the relative difference between the exact calculation of RRCS and the dipole approximation

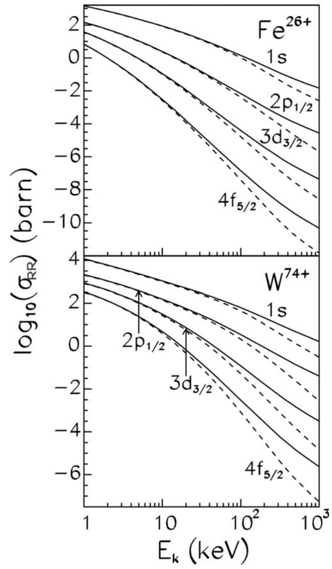

FIG. 2. Subshell RRCS calculated taking into account all multipoles L (full) and in the dipole approximation (dashed).

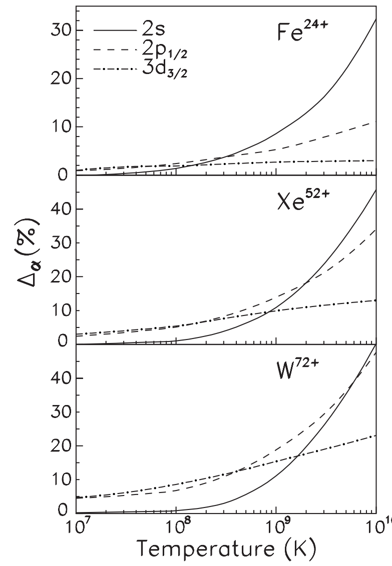

FIG. 3. Difference Δ_α between rate coefficients calculated involving all multipoles and in the dipole approximation for the $2s$ (full), $2p_{1/2}$ (dashed), and $3d_{3/2}$ (chain) shells.

$$\Delta_{\mathrm{RRCS}} = \frac{\sigma_{\mathrm{RR}}(L) - \sigma_{\mathrm{RR}}(\mathrm{dip})}{\sigma_{\mathrm{RR}}(L)} \times 100\% \qquad (10)$$

varies in the range ~3–20 % for shells with different orbital momenta l_i at E_k=10 keV, ~15–50 % at E_k=50 keV and reaches several multiples at E_k=1000 keV. The dependence of Δ_{RRCS} on l_i is shown to be considerable, Δ_{RRCS} being larger with increasing l_i. The difference Δ_{RRCS} was found to be practically independent on Z, the ion charge, and the principal quantum number n_i of a subshell.

In Table I, we compare our present PCS calculations with the dipole results by Badnell [11] for the $1s$ shell of the H-like ion Xe^{53+}. The case of an one-electron ion is particularly convenient for checking the influence of higher multipoles and a method of calculation because there are no inter-electron interactions. In this case, the PCS must be independent of the gauge used in calculations for correct wave functions.

TABLE I. Comparison of our PCS with results by Badnell [11] for the $1s$ shell of the H-like ion Xe^{53+}. $\Delta_{\mathrm{PCS}}=\{[\sigma_{\mathrm{ph}}(\mathrm{present}) - \sigma_{\mathrm{ph}}(\mathrm{Badnell})]/\sigma_{\mathrm{ph}}(\mathrm{present})\}\times 100\%$.

	σ_{ph} (Mb)		
E_k (keV)	Badnell	Present	Δ_{PCS} (%)
0.00083	2.246(−3)	1.937(−3)	−16
0.03967	2.240(−3)	1.935(−3)	−16
0.3967	2.186(−3)	1.892(−3)	−16
3.967	1.734(−3)	1.523(−3)	−14
39.67	3.256(−4)	3.114(−4)	−4.5
83.31	9.095(−5)	9.206(−5)	1.2
182.4	1.539(−5)	1.740(−5)	12
396.7	1.894(−6)	2.802(−6)	32
833.1	2.071(−7)	5.495(−7)	62
1824.0	1.730(−8)	1.318(−7)	87
3967.0	1.350(−9)	4.117(−8)	97

We found that our results are in excellent agreement with values from exact relativistic calculations of RRCS for bare nuclei [3] where all multipoles L were involved. Specifically, for the $1s$ shell of the H-like ion Xe^{53+}, the two calculations coincide with an accuracy of the three significant digits presented in Ref. [3] in the wide energy range 1 eV$\leqslant E_k \leqslant$6000 keV. By contrast, PCS obtained by Badnell exceed our values and results from Ref. [3] by ~16% in the energy range $E_k \lesssim 4$ keV and diminish progressively at higher energies becoming lower by a factor of ~8 at $E_k \approx 1800$ keV and a factor of ~30 at $E_k \approx 4000$ keV compared with our values. The comparison of our PSC values and results from [3] with calculation by Badnell [11] for the lighter ion Fe^{23+} reveals a similar tendency, but smaller in magnitude at low energies.

The reason of the difference at low energies is unclear for us because the nondipole terms make a small contribution in this range (see Fig. 2). It is possible that the difference arises from the methods of calculation used in Ref. [11]. The difference at high energies (>100 keV) must be due to neglect of the higher multipoles and possibly also due to the semi-relativistic approximation adopted in Ref. [11].

From the discussion above, it would be expected that the dipole approximation would also fail in calculations of rate coefficients at a high temperature T. In Fig. 3, we present the difference Δ_α between the exact $\alpha^{(i)}(L)$ and the dipole $\alpha^{(i)}(\mathrm{dip})$ values of partial rate coefficients. The difference is defined in the same way as in Eq. (10). The difference Δ_α is given for the $2s$, $2p_{1/2}$, and $3d_{3/2}$ electrons recombining with the He-like ions Fe^{24+}, Xe^{52+}, and W^{72+}. These shells are the lowest ones making a large contribution to the total rate coefficients. As is evident from the figure, the difference Δ_α is larger for the heavy, highly charged ions. The inclusion of all multipoles may change partial rate coefficients by ~7% at temperature $T=10^8$ K, by $\sim$20% at $T=10^9$ K, and by $\sim$50% at $T=10^{10}$ K for W^{72+}. This means that total rate coefficients obtained within the dipole approximation have to be smaller considerably at high temperature than the accurate values obtained with regard to all multipoles L.

It is of interest to compare our total recombination rate coefficients for the highly charged tungsten ions with results by Kim and Pratt [9] obtained in the framework of an approximate theoretical method using tip bremsstrahlung cross sections together with only few direct calculations of RRCS. The authors performed the relativistic Dirac-Slater calculations of the RRCS with regard to all multipoles L. All other cross sections for each a state $n\kappa$ were obtained by interpolation using the quantum defect method. As was noted, the nonrelativistic distribution, therefore omitting the factor $F_{\rm rel}(\theta)$, was used. Because of the approximations, the difference between our exact calculations and values from Ref. [9] reaches 11% for the bare nucleus and 36% for the Ar-like tungsten ion.

In conclusion, we showed that a contribution of multipole effects in the recombination rate coefficients is significant (within 10–50 %) at electron energies of the order of 10 keV and higher. We showed also that the relativistic Maxwell-Boltzmann distribution of continuum electrons must be used instead of the nonrelativistic one in the rate coefficient calculations in hot plasmas.

It is significant that the relativistic rates for processes of dielectronic recombination and the electron impact ionization in hot plasmas may be similarly obtained with the relativistic distribution. In a recent debate [17] about "the correct generalization of Maxwell's velocity distribution in special relativity" which was put forward by Jüttner [18] in 1911, the importance of the relativistic Maxwell-Jüttner distribution for proper interpretation of some relativistic effects in astrophysics and in experiments with ultrarelativistic plasma beams was particularly emphasized.

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[1] R. Neu *et al.*, Nucl. Fusion **45**, 209 (2005).
[2] A. A. Zdziarski, J. Poutanen, and W. N. Johnson, Astrophys. J. **542**, 703 (2000).
[3] A. Ichihara and J. Eichler, At. Data Nucl. Data Tables **74**, 1 (2000).
[4] M. B. Trzhaskovskaya, V. K. Nikulin, V. I. Nefedov, and V. G. Yarzhemsky, J. Phys. B **34**, 3221 (2001).
[5] M. B. Trzhaskovskaya, V. I. Nefedov, and V. K. Nikulin, Atomic Spectrosc. **91**, 569 (2001).
[6] M. B. Trzhaskovskaya and V. K. Nikulin, Atomic Spectrosc. **95**, 537 (2003).
[7] M. B. Trzhaskovskaya, V. K. Nikulin, and R. E. H. Clark, At. Data Nucl. Data Tables **94**, 71 (2008).
[8] W. D. Barfield, J. Phys. B **13**, 931 (1980).
[9] Young Soon Kim and R. H. Pratt, Phys. Rev. A **27**, 2913 (1983).
[10] P. Mazzotta, G. Mazzitelli, S. Colafrancesco, and N. Vittorio, Astron. Astrophys. Suppl. Ser. **133**, 403 (1998).
[11] N. R. Badnell, Astrophys. J., Suppl. Ser. **167**, 334 (2006).
[12] A. Burgess, Mem. R. Astron. Soc. **60**, 1 (1964).
[13] D. A. Verner and G. J. Ferland, Astrophys. J., Suppl. Ser. **103**, 467 (1996).
[14] Moorad Alexanian, Phys. Rev. **165**, 253 (1968).
[15] J. L. Synge, *The Relativistic Gas* (North-Holland, Amsterdam, 1957).
[16] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards, Washington, D.C., 1964).
[17] D. Cubero, J. Casado-Pascual, J. Dunkel, P. Talkner, and P. Hänggi, Phys. Rev. Lett. **99**, 170601 (2007).
[18] F. Jüttner, Ann. Phys. **34**, 856 (1911).