The impact of multipole and relativistic effects on photoionization and radiative recombination cross sections in hot plasmas

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It is shown in the framework of the fully relativistic Dirac-Fock treatment of photoionization and radiative recombination processes that taking into account all significant multipoles of the radiative field is of considerable importance at electron energy higher than several keV. For the first time, we show that the relativistic Maxwell-Bolzmann distribution of continuum electrons should be used in hot thermal plasmas. This decreases the radiative recombination rate coefficient up to several multiplies compared to the non-relativistic distribution commonly used.

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The photoionization and radiative recombination cross sections as well as the radiative recombination rate coefficients are required for estimates of ionization equilibria and thermal balance in terrestrial and astrophysical plasmas contaminated by various ions. In fusion reactors at temperatures above several keV, impurity atoms of various elements may be stripped to bare nuclei. At temperatures around 1000 keV, tungsten atoms are fully stripped [1]. In astrophysical objects such as stellar black-hole binaries and Seyfert galaxies, the plasma temperature may reach 150 keV [2].

At sufficiently high kinetic electron energy $E_k$ and for highly charged ions, multipole and relativistic effects should be taken into account in calculations of photoionization cross sections (PCS), radiative recombination cross sections (RRCS) and radiative recombination rate coefficients. The effects were considered beginning with pioneering works [3, 4, 5]. Nevertheless, these effects are
usually neglected in the application of these processes in plasmas (see Refs. in [6, 7]). The most extensive advanced calculations by Badnell [7] were performed using the electric dipole and semi-relativistic approximations for electron energies to 1.36Z^2 keV and for Z ≤ 54, that is up to ∼ 4 MeV.

We used the fully relativistic treatment of the photoionization process in recent calculations of PCS and RRCS for 31 ions of elements from the range 26 ≤ Z ≤ 74 [6]. Electron wave functions were generated in the self-consistent Dirac-Fock (DF) framework. We took into account all significant multipole orders of the radiative field. Previously, we performed relativistic calculations of total and differential RRCS for recombination of an electron with the H-, He- and Li-like uranium ions using this model with regard to the Breit electron interaction and the main quantum electrodynamic corrections [8]. The influence of the multipole effects was also considered in our studies of the total and differential PCS [9, 10, 11].

Exact relativistic benchmark calculations of RRCS including all significant multipoles were carried out by Ichihara and Eichler [12] for radiative recombination of the K, L and M electrons with bare nuclei with charge numbers 1 ≤ Z ≤ 112. The results for a few representative cases were compared with those derived from the widely used non-relativistic dipole approximation in order to assess the accuracy of the latter.

In the present paper, we discuss the influence of multipole effects on PCS, RRCS and rate coefficients as well as the influence of the relativistic effects such as the relativistic transformation coefficient between PCS and RRCS and the relativistic correction factor for the non-relativistic rate coefficient. This temperature depend factor is reported for the first time in this paper.

The relativistic PCS in the i-th subshell per one electron can be written in the form

\[ \sigma_{\text{ph}}^{(i)} = \frac{4\pi^2\alpha}{\hat{k}(2j_i + 1)} \sum_L \sum_\kappa \left[ (2L + 1)Q_{L,\kappa}^2 + LQ_{L+1,\kappa}^2 \right] \]

(1)

Here \( \hat{k} \) is the photon energy in \( m_0c^2 \), \( L \) is the multipolarity of the radiative field, \( \kappa = (\ell - j)(2j + 1) \), \( \ell \) and \( j \) are the orbital and total angular momenta of the electron, \( \alpha \) is the fine structure constant and \( Q_{\ell L}(\kappa) \) is the reduced matrix element (for detailed expressions see [6]).

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

$$\sigma_{rr}^{(i)} = A q_i \sigma_{ph}^{(i)},$$

where $q_i$ is the number of vacancies in the $i$-th 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

$$A_{rel} = \frac{\tilde{k}^2}{2\tilde{E}_k + \tilde{E}_k^2}, \quad \tilde{E}_k = \frac{E_k}{m_0c^2},$$

(3)

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

$$A_{nrel} = \frac{k^2}{2m_0c^2 E_k}, \quad k = m_0c^2 \tilde{k},$$

(4)

which may be obtained in the non-relativistic approximation from Eq. (3). The difference between $\sigma_{rr}$ obtained with Eq. (3) and Eq. (4) depends only on the electron kinetic energy $E_k$ and can be written as

$$\frac{A_{nrel} - A_{rel}}{A_{rel}} = \frac{E_k}{2m_0c^2}$$

(5)

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 (3) should be used in the RRCS calculations.

The relativistic recombination rate coefficients $\alpha_{rel}^{(i)}(T)$ can be calculated using the thermal average over RRCS. In the present paper, the continuum electrons are described by the relativistic Maxwell-Boltzmann distribution function $f(E)$ normalized to unity as follows

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

(6)

Here $E$ is the total electron energy in units of $m_0c^2$ including the rest energy, $\theta = k_B T/m_0c^2$ is the characteristic dimensionless temperature, $T$ is the temperature and $k_B$ is the Boltzmann constant. The function $K_2$ denotes the modified Bessel function of the second order. The relativistic rate coefficient may be written as

$$\alpha_{rel}^{(i)}(T) = \langle \nu \sigma_{rr}^{(i)} \rangle = F_{rel}(\theta) \cdot \alpha^{(i)}(T),$$

(7)
where \( v = (p/E)c \) is the electron velocity with the momentum \( p = \sqrt{E^2 - 1} \) and \( \alpha^{(i)}(T) \) is the usual non-relativistic rate coefficient [14].

\[
\alpha^{(i)}(T) = \frac{(2/\pi)^{1/2}c^{-2}(m_0k_\beta T)^{-3/2}}{\varepsilon_i} \int_{\varepsilon_i}^{\infty} k^2 \sigma_{ph}^{(i)}(k) e^{(\varepsilon_i - k)/(k_\beta T)} dk,
\]

where \( k \) is the photon energy and \( \varepsilon_i \) is the binding energy of the \( i-th \) shell. In Eq. (7), \( F_{\text{rel}}(\theta) \) is the relativistic factor

\[
F_{\text{rel}}(\theta) = \sqrt{\frac{\pi}{2}} \theta / K_2(1/\theta) e^{1/\theta}.
\]

Using the asymptotic expansion of the Bessel function \( K_2(1/\theta) \) at large \( 1/\theta \) [15], that is at low temperature, we arrive at the factor \( \tilde{F}_{\text{rel}}(\theta) \), an approximation to \( F_{\text{rel}}(\theta) \)

\[
\tilde{F}_{\text{rel}}(\theta) = 1 \left( 1 + \frac{15}{8} \theta + \frac{105}{128} \theta^2 + \ldots \right).
\]

Eq. (10) provides an excellent approximation for \( F_{\text{rel}}(\theta) \) with the terms through order \( \theta^2 \) at \( \theta \lesssim 1 \). The factors \( F_{\text{rel}}(\theta) \) and \( \tilde{F}_{\text{rel}}(\theta) \) are compared in Fig. 1. The solid curve refers to the exact factor (Eq. (9)) and the dashed curve refers to the approximate factor (Eq. (10)). As can be seen, there is little difference between the two curves, the relative error is \( \sim 4\% \) at \( k_\beta T = 500 \text{ keV} \) and \( 25\% \) at \( k_\beta T = 1000 \text{ keV} \).

![Fig. 1: Exact factor \( F_{\text{rel}}(T) \) (solid) and approximate factor \( \tilde{F}_{\text{rel}}(T) \) (dashed).](image)

As is seen from Fig. 1, the use of the relativistic distribution instead of non-relativistic one results in a decrease of rate coefficients by a factor of 1.2 at plasma temperature \( k_\beta T = 50 \text{ keV} \).
and up to factor of 7 at $k_\beta T = 1$ MeV.

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). As is well known, the dipole approximation holds at a low electron energy $E_k$ but breaks down at a higher energy.

![Subshell RRCS (in barns) calculated taking into account all multipoles $L$ (solid) and in the dipole approximation (dashed).](image)

**FIG. 2:** Subshell RRCS (in barns) calculated taking into account all multipoles $L$ (solid) and in the dipole approximation (dashed).

In Fig. 2, we compare RRCS obtained in the dipole approximation $\sigma_{rr}(\text{dip})$ (dashed curves) with RRCS calculated with all multipoles $\sigma_{rr}(L)$ making significant contribution (solid curves) for bare nuclei of two representative elements Fe ($Z=26$) and W ($Z=74$). The energy range under consideration is $1 \text{ keV} \leq E_k \leq 1000 \text{ keV}$. As is seen in Fig. 2, the curves begin to diverge noticeably even at several keV. At the highest energy 1000 keV, in the case of W$^{74+}$, $\sigma_{rr}(\text{dip})$ is smaller than the exact value $\sigma_{rr}(L)$ by a factor of $\sim 5$ for the 1s shell and by a factor of $\sim 40$ for the 4f$5/2$ subshell. Our calculations showed that the relative difference between the exact calculation of RRCS and the dipole approximation

$$\Delta_{\text{RRCS}} = \frac{\sigma_{rr}(L) - \sigma_{rr}(\text{dip})}{\sigma_{rr}(L)} \cdot 100\%$$

(11)
varies in the range $\sim 3$-$20\%$ for shells with different orbital momenta $\ell_i$ at $E_k=10$ keV, $\sim 15$-$50\%$ at $E_k=50$ keV and reaches several multiples at $E_k=1000$ keV. The dependence of $\Delta_{RRCS}$ on $\ell_i$ is shown to be considerable, $\Delta_{RRCS}$ being larger with increasing $\ell_i$. The difference $\Delta_{RRCS}$ was found to increase with $Z$, especially for high energy.

Calculations show that to achieve accuracy $\sim 0.01\%$ in the PCS, e.g., for the $1s$ and $3d$ shells of the ion $W^{73+}$ one has to take into account all terms in Eq. (1) up to $L=5$ and $L=8$, respectively at $E_k=10$ keV, to $L=7$ and $11$ at $E_k=100$ keV and to $L=19$ and $31$ at $E_k=1000$ keV.

Table I. Comparison of our PCS with results by Badnell [7] for the $1s$ shell of the H-like ion $Xe^{53+}$. $\Delta_{PCS} = \left[\frac{\sigma_{ph}(\text{present}) - \sigma_{ph}(\text{Badnell})}{\sigma_{ph}(\text{present})}\right] \cdot 100\%$.

| $E_k$, keV | $\sigma_{ph}$, Mb | Badnell | Present | $\Delta_{PCS}$, % |
|------------|-------------------|---------|---------|------------------|
| 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.      | 1.730(-8)         | 1.318(-7) | 87      |
| 3967.      | 1.350(-9)         | 4.117(-9) | 97      |

In Table I, we compare our present PCS calculations with the corresponding results of Badnell [7] for the $1s$ shell of the H-like ion $Xe^{53+}$. The case of the one-electron ion is particularly convenient for checking the influence of the higher multipoles and the method of calculation because there are no any inter-electron interactions. In this case, the PCS must be independent of the gauge used in calculations for correct wave functions.

We found that our calculation is in excellent agreement with values from [12] where all multipoles $L$ were involved. 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 [12] in the wide energy range $1 \text{ eV} \leq E_k \leq 6000 \text{ keV}$. By contrast, PCS obtained by Badnell exceed our values and results from [12] by $\sim 16\%$ in the energy range $E_k \lesssim 4 \text{ keV}$ and diminish progressively at higher energies becoming lower by a factor of $\sim 8$ at $E_k \approx 1800 \text{ keV}$ and a factor of $\sim 30$ at $E_k \approx 4000 \text{ keV}$ compared with our values. The comparison of our PSC values and results from [12] with calculation by Badnell [7] for the lighter ion Fe$^{23+}$ reveals a similar tendency, but smaller in magnitude.

The reason of the difference at low energies is unclear for us because the non-dipole terms make a small contribution at low energies (see Fig. 2). It is possible that the difference arises from the methods of calculation used in [7]. The difference at high energies ($> 100 \text{ keV}$) must be due to neglect of the higher multipoles and possibly also due to the semi-relativistic approximation adopted in [7].

FIG. 3: Difference $\Delta \alpha$ between rate coefficients calculated with using all multipoles and in the dipole approximation for the $2s$ (solid), $2p_{1/2}$ (dashed), and $3d_{3/2}$ (dash-dotted) shells.

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 $\Delta \alpha$ between the exact $\alpha^{(i)}(L)$ and the dipole $\alpha^{(i)}(\text{dip})$ values of partial rate coefficients. The difference is defined in the same way as in Eq. (11). The difference $\Delta \alpha$ 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 $\Delta \alpha$ is larger for the heavy, highly charged ions. The inclusion of higher multipoles may change partial rate coefficients by $\sim 7\%$ 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 considerably smaller than the accurate values obtained with regard to all multipoles $L$.

In conclusion we have clearly demonstrated the importance of multipole effects to the PCS, RRCS and rate coefficient calculations at electron energy of the order of 10 keV and higher. We have also showed that in hot plasmas, the relativistic Maxwell-Bolzmann distribution of continuum electrons must be used in the rate coefficient calculations. It should be noted that the relativistic rates may be similarly obtained for processes of dielectronic recombination and the electron impact ionization in hot plasmas.

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