Degeneracy and relativistic microreversibility relations for collisional-radiative equilibrium models

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(Received 28 February 2017; published 1 June 2017)

We present the relativistic expressions of standard nonrelativistic microreversibility relations that can be used in collisional-radiative equilibrium models to calculate the transition rates including the free electron degeneracy for collisional excitation and deexcitation, collisional ionization and three-body recombination, dielectronic capture and autoionization, photoexcitation and photodeexcitation, and radiative recombination and photoionization. Semiempirical expressions or more refined calculations can be used for the cross sections of interest as long as they are calculated by taking into account either nonrelativistic, relativistic, or ultrarelativistic effects for both the bound and free electrons. The bound and the free electrons should be treated on the same footing. This is crucial for the internal consistency of the approach valid at arbitrary degeneracy and relativistic degrees.

DOI: 10.1103/PhysRevE.95.063201

I. INTRODUCTION

The description of nonlocal thermodynamic-equilibrium (NLTE) plasmas has become an important and active field of research, especially due to the kind of plasmas encountered on Earth in x-ray lasers, ultrashort-pulse (USP) lasers, the National Ignition Facility (NIF) or the Laser Mégajoule (LMJ), Z-pinch machines, the International Thermonuclear Experimental Reactor (ITER), or x-ray free electron (XFEL) lasers. NLTE plasmas can also be of interest in astrophysics, i.e., in the corona of a star, the intergalactic medium, or the accretion disk near a supermassive black hole in a luminous quasar. The characterization of these plasmas is not an easy task, especially if they belong to the warm and hot dense matter for which the lifetime can be short. We speak of highly transient states of matter. Indeed, the widespread approach to describe these plasmas consists in using a collisional-radiative equilibrium (CRE) model [1–9].

The atomic data we need to run a CRE code are usually nonrelativistic but not always [10,11]. Recently, Sampson *et al.* [12] proposed a detailed review of their fully relativistic approach to calculate atomic data for highly charged ions. Unfortunately, they focused on atomic structure calculations and cross sections of some specific processes needed in CRE models. Moreover, they averaged over nonrelativistic or relativistic nondegenerate free-electron distribution functions to get the transition rates from the cross sections, making their approach questionable from a relativistic point of view. In LTE plasma, it has been shown [13] that it is crucial to describe in the same way bound and free electrons, i.e., either in a nonrelativistic or relativistic way but not treating the bound electrons in one way and the free electrons in another way. Finally, Sampson *et al.* [12] did not consider degenerate free electrons.

In the present work, we extend to the relativistic regime the calculation of the nonrelativistic rates up to the ultrarelativistic regime by treating explicitly the degeneracy of the free electrons. Using the detailed balance when LTE is applied, we find the relativistic version of the microreversibility relations such as the Klein-Rosseland formula for collisional excitation and deexcitation, the Fowler formula for collisional ionization and three-body recombination, and the Einstein-Milne formula for radiative electron capture and photoionization. We show how the dielectronic capture cross section is related to the autoionization rate. By relativity, we mean the special theory of relativity. The paper is organized as follows. First, we show how to obtain the relativistic extension of the microreversibility relations. We check that we recover the nonrelativistic and ultrarelativistic limits. We summarize the main results in two tables. The last part is the conclusion.

II. METHOD

The starting point is the calculation of N_e which is given by the formula

$$N_e = 2\int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\frac{1}{1+e^{\beta_e\varepsilon-\eta}}, \tag{1}$$

where $\hbar$ is the reduced Planck constant and $\eta = \beta_e\mu$ the reduced chemical potential. μ is the chemical potential and $\beta_e = 1/k_BT_e$ where k_B is the Boltzmann constant and T_e the electron temperature. The relation between the kinetic energy ε and the momentum p is more complicated in the relativistic regime than in the nonrelativistic and ultrarelativistic regimes. Taking the electron rest-mass energy m_ec^2 as the reference of energies, i.e., for ε and μ, one has

$$\varepsilon = \sqrt{p^2c^2 + m_e^2c^4} - m_ec^2. \tag{2}$$

c is the speed of light and m_e the electron mass. With this convention, the chemical potential μ does not contain the electron rest-mass energy and $\varepsilon = 0$ when $p = 0$. In the nonrelativistic regime $\varepsilon \approx p^2/2m_e$ and in the ultra-relativistic regime $\varepsilon \approx pc$. The question is to see what happens in the intermediate regime and to study the transition between the nonrelativistic and the ultrarelativistic regimes. To do so, one puts m_ec^2 on the left-hand side of Eq. (2), takes the square of the two members of this equation, and differentiates. One finds that

$$pdpc^2 = (\varepsilon + m_ec^2)d\varepsilon. \tag{3}$$

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Developing the square of the left-hand side of Eq. (2), one finds that

$$pc = \sqrt{\varepsilon}\sqrt{\varepsilon + 2m_e c^2}. \tag{4}$$

We are now ready to calculate N_e. We find that

$$N_e = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^{+\infty} d\varepsilon\, \lambda(\varepsilon)\frac{1}{1+e^{\beta_e\varepsilon-\eta}}, \tag{5}$$

where

$$\lambda(\varepsilon) = \sqrt{\varepsilon}\sqrt{1+\frac{\varepsilon}{2m_e c^2}}\left(1+\frac{\varepsilon}{m_e c^2}\right). \tag{6}$$

Equation (5) is the relativistic expression of the electronic density N_e from which the rates of interest can be calculated. It is interesting to find the nonrelativistic and ultrarelativistic expressions of $\lambda(\varepsilon)$. When $\varepsilon \ll m_e c^2$, we are in the nonrelativistic regime and

$$\lambda(\varepsilon) \approx \sqrt{\varepsilon}, \tag{7}$$

whereas when $\varepsilon \gg m_e c^2$, we are in the ultrarelativistic regime and

$$\lambda(\varepsilon) \approx \frac{\varepsilon^2}{\sqrt{2}(m_e c^2)^{3/2}}. \tag{8}$$

As an illustration, we plot in Fig. 1 $\lambda(\varepsilon)$ as a function of ε. We clearly see at low energy the nonrelativistic behavior (7) and at high energy the ultrarelativistic behavior (8). There is a small range around $m_e c^2 \approx 0.511$ MeV that interpolates between these two limits. Indeed, the two asymptotic curves intersect at $\varepsilon = \sqrt[3]{2}m_e c^2$.

In the nonrelativistic regime, we have the well-known expression

$$N_e = \frac{\sqrt{2}(m_e k_B T_e)^{3/2}}{\pi^2\hbar^3} I_{1/2}(\eta), \tag{9}$$

where $I_{1/2}(\eta)$ is the Fermi-Dirac integral of order 1/2. By definition, the Fermi-Dirac integral [14,15] of order k is

$$I_k(\eta) = \int_0^{+\infty} dx \frac{x^k}{1+e^{x-\eta}}. \tag{10}$$

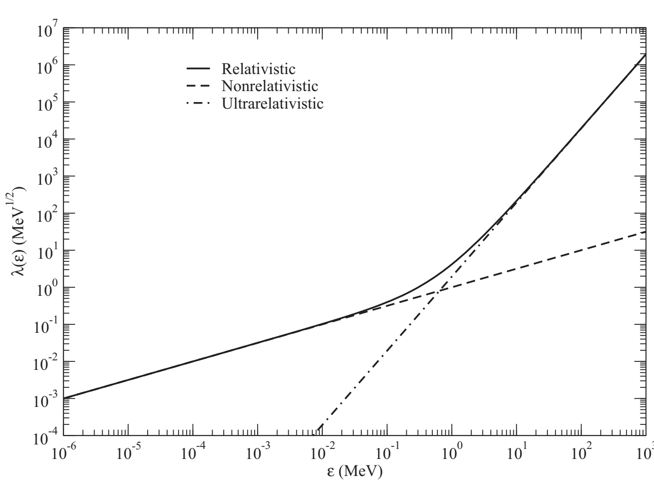

FIG. 1. $\lambda(\varepsilon)$ as a function of ε.

In the relativistic regime, we have

$$N_e = \frac{\sqrt{2}m_e^3 c^3\theta^{3/2}}{\pi^2\hbar^3}[F_{1/2}(\eta,\theta) + \theta F_{3/2}(\eta,\theta)], \tag{11}$$

where

$$F_k(\eta,\theta) = \int_0^{+\infty} dx \frac{x^k\sqrt{1+\frac{\theta x}{2}}}{1+e^{x-\eta}} \tag{12}$$

and

$$\theta = \frac{k_B T_e}{m_e c^2}. \tag{13}$$

Obviously, $F_k(\eta,0) = I_k(\eta)$ and

$$F_k(\eta,\theta) \approx \frac{\theta^{1/2}}{\sqrt{2}} I_{k+1/2}(\eta) \tag{14}$$

when $\theta \to +\infty$. In the ultrarelativistic regime, we find that

$$N_e = \frac{(k_B T_e)^3}{\pi^2\hbar^3 c^3} I_2(\eta), \tag{15}$$

where $I_2(\eta)$ is the Fermi-Dirac integral of order 2. It can be useful to have also the nondegenerate expressions of Eqs. (9), (11), and (15). In the nonrelativistic regime, we have the well-known expression

$$N_e \approx 2e^\eta\left(\frac{m_e k_B T_e}{2\pi\hbar^2}\right)^{3/2}, \tag{16}$$

in the relativistic regime

$$N_e \approx e^\eta \frac{m_e^3 c^3}{\pi^2\hbar^3}\theta e^{1/\theta} K_2(1/\theta), \tag{17}$$

where K_2 is the modified Bessel function of the second kind [16,17], and in the ultrarelativistic regime

$$N_e \approx 2e^\eta \frac{(k_B T_e)^3}{\pi^2\hbar^3 c^3}. \tag{18}$$

Associated to Eqs. (16), (17), and (18), we have the well-known Maxwell-Boltzmann distribution function

$$F_{ndg}^{nr}(\varepsilon) = \frac{2\beta_e^{3/2}}{\sqrt{\pi}}\sqrt{\varepsilon}e^{-\beta_e\varepsilon} \tag{19}$$

in the nonrelativistic regime, the Jüttner distribution function [18]

$$F_{\rm ndg}^{\rm rel}(\varepsilon) = \frac{\sqrt{2}}{m_e c^2}\frac{e^{-1/\theta}}{\theta K_2(1/\theta)}\sqrt{\frac{\varepsilon}{m_e c^2}} \times\sqrt{1+\frac{\varepsilon}{2m_e c^2}}\left(1+\frac{\varepsilon}{m_e c^2}\right)e^{-\beta_e\varepsilon}, \tag{20}$$

in the relativistic regime, and

$$F_{\rm ndg}^{\rm ur}(\varepsilon) = \frac{\beta_e^3}{2}\varepsilon^2 e^{-\beta_e\varepsilon} \tag{21}$$

in the ultrarelativistic regime. All these distribution functions are normalized to unity, i.e.,

$$\int_0^{+\infty} F_{\rm ndg}^{\rm nr}(\varepsilon)d\varepsilon = \int_0^{+\infty} F_{\rm ndg}^{\rm rel}(\varepsilon)d\varepsilon = \int_0^{+\infty} F_{\rm ndg}^{\rm ur}(\varepsilon)d\varepsilon = 1. \tag{22}$$

Equations (16)–(21) are given because they are needed to derive the nonrelativistic expressions when the electrons are nondegenerate from the general case when the electrons are degenerate.

To calculate the collisional rates, we need the relativistic expression of the velocity as a function of the energy ε. Since by definition,

$$\varepsilon = \frac{m_e c^2}{\sqrt{1-\frac{v^2}{c^2}}} - m_e c^2, \tag{23}$$

we find that

$$v = c\vartheta(\varepsilon), \tag{24}$$

where

$$\vartheta(\varepsilon) = \sqrt{\frac{\frac{\varepsilon}{m_e c^2}\left(\frac{\varepsilon}{m_e c^2}+2\right)}{\left(\frac{\varepsilon}{m_e c^2}+1\right)^2}}. \tag{25}$$

This is the relativistic expression of the velocity as a function of energy ε. One can check that in the nonrelativistic domain, we have $v \approx \sqrt{2\varepsilon/m_e}$, i.e.,

$$\vartheta(\varepsilon) \approx \sqrt{\frac{2\varepsilon}{m_e c^2}}; \tag{26}$$

whereas in the ultrarelativistic domain, we have $v \approx c$, i.e.,

$$\vartheta(\varepsilon) \approx 1 \tag{27}$$

as expected. As an illustration, we plot in Fig. 2. We clearly see the nonrelativistic behavior at low energy and the asymptotic limit at high energy corresponding to the ultrarelativistic regime. As for $\lambda(\varepsilon)$, the transition between the two regimes is around $m_e c^2$. Indeed, the two asymptotic curves intersect at $\varepsilon = m_e c^2/2$.

A. Collisional excitation and deexcitation

Let us consider a collisional excitation from level j to level k for which the cross section is σ_{jk}^{ce}. The cross section of the collisional deexcitation from level k to level j is σ_{kj}^{cd}. The transition energy is $\Delta E_{jk} = E_k - E_j$ with $E_k > E_j$. E_j and E_k are the energies of levels j and k, respectively. From Equations (5) and (25), we can now write the relativistic expression of the collisional excitation rate which reads

$$\tau_{jk}^{ce} = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_{\Delta E_{jk}}^{+\infty} d\varepsilon\,\lambda(\varepsilon)\frac{1}{1+e^{\beta_e\varepsilon-\eta}}c\vartheta(\varepsilon)\sigma_{jk}^{ce}(\varepsilon) \times \frac{1}{1+e^{-\beta_e(\varepsilon-\Delta E_{jk})+\eta}}, \tag{28}$$

whereas the collisional deexcitation rate reads

$$\tau_{kj}^{cd} = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^{+\infty} d\varepsilon'\lambda(\varepsilon')\frac{1}{1+e^{\beta_e\varepsilon'-\eta}}c\vartheta(\varepsilon')\sigma_{kj}^{cd}(\varepsilon') \times \frac{1}{1+e^{-\beta_e(\varepsilon'+\Delta E_{jk})+\eta}}. \tag{29}$$

Equations (28) and (29) are written under a relativistic form including the electron degeneracy since we integrate using Fermi-Dirac distribution functions with the Pauli blocking factor in each case. In the expression of the collisional excitation rate, the Pauli blocking factor

$$\frac{1}{1+e^{-\beta_e(\varepsilon-\Delta E_{jk})+\eta}} = 1 - \frac{1}{1+e^{\beta_e(\varepsilon-\Delta E_{jk})-\eta}} \tag{30}$$

is nothing but the available volume fraction in phase space. In the expression of the collisional deexcitation rate, the Pauli blocking factor is

$$\frac{1}{1+e^{-\beta_e(\varepsilon'+\Delta E_{jk})+\eta}} = 1 - \frac{1}{1+e^{\beta_e(\varepsilon'+\Delta E_{jk})-\eta}}. \tag{31}$$

Equations (28) and (29) need comments. These equations generalize in the relativistic regime and degeneracy domain the well-known nonrelativistic expressions when the electrons are nondegenerate. For instance, the collisional excitation rate can be written using Eqs. (16) and (19):

$$\tau_{jk}^{ce} \approx N_e \int_{\Delta E_{jk}}^{+\infty} d\varepsilon\, v(\varepsilon)\sigma_{jk}^{ce}(\varepsilon)F_{ndg}^{nr}(\varepsilon), \tag{32}$$

which sounds familiar. For the collisional deexcitation rate, we have in the same conditions

$$\tau_{jk}^{cd} \approx N_e \int_0^{+\infty} d\varepsilon\, v(\varepsilon)\sigma_{kj}^{cd}(\varepsilon)F_{ndg}^{nr}(\varepsilon). \tag{33}$$

Similar results can be obtained for the other rates in such kind of conditions.

To find the relativistic expression of the Klein-Rosseland relation, we write in Eq. (29)

$$\frac{1}{1+e^{\beta_e\varepsilon'-\eta}}\frac{1}{1+e^{-\beta_e(\varepsilon'+\Delta E_{jk})+\eta}} = e^{\beta_e\Delta E_{jk}}\frac{1}{1+e^{\beta_e(\varepsilon'+\Delta E_{jk})-\eta}}\frac{1}{1+e^{-\beta_e\varepsilon'+\eta}} \tag{34}$$

and make the change of variable $\varepsilon = \varepsilon' + \Delta E_{jk}$ in Eq. (28). We find that

$$\tau_{jk}^{ce} = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^{+\infty} d\varepsilon'\lambda(\varepsilon'+\Delta E_{jk}) \times \frac{1}{1+e^{\beta_e(\varepsilon'+\Delta E_{jk})-\eta}}c\vartheta(\varepsilon'+\Delta E_{jk})\sigma_{jk}^{ce}(\varepsilon'+\Delta E_{jk}) \times \frac{1}{1+e^{-\beta_e\varepsilon'+\eta}} \tag{35}$$

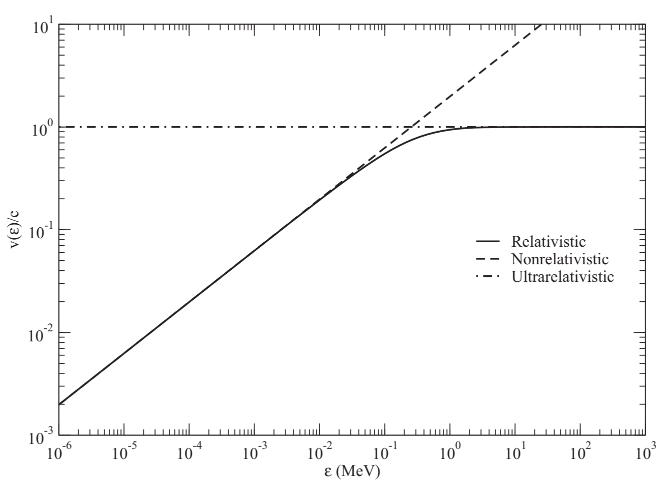

FIG. 2. $\vartheta(\varepsilon) = v(\varepsilon)/c$ as a function of ε.

and

$$\tau_{kj}^{cd} = e^{\beta_e \Delta E_{jk}} \frac{\sqrt{2} m_e^{3/2}}{\pi^2 \hbar^3} \int_0^{+\infty} d\varepsilon' \lambda(\varepsilon') \times \frac{1}{1+e^{\beta_e(\varepsilon'+\Delta E_{jk})-\eta}} c\vartheta(\varepsilon') \sigma_{kj}^{cd}(\varepsilon') \frac{1}{1+e^{-\beta_e \varepsilon'+\eta}}. \quad (36)$$

We now impose the detailed balance between τ_{jk}^{ce} and τ_{kj}^{cd}, i.e.,

$$\tau_{kj}^{cd} = \frac{g_j}{g_k} e^{\beta_e \Delta E_{jk}} \tau_{jk}^{ce}, \quad (37)$$

where g_j and g_k are the degeneracy of levels j and k, respectively. Since the obtained relation is valid for any β_e and η, we get the functional relation

$$g_j \lambda(\varepsilon + \Delta E_{jk}) \vartheta(\varepsilon + \Delta E_{jk}) \sigma_{jk}^{ce}(\varepsilon + \Delta E_{jk}) = g_k \lambda(\varepsilon) \vartheta(\varepsilon) \sigma_{kj}^{cd}(\varepsilon), \quad (38)$$

where the dummy variable ε' has been replaced by ε. The functional identity (38) is valid for any positive energy ε. This is the relativistic Klein-Rosseland formula for the microreversibility of this pair of microscopic processes. In the nonrelativistic regime, we obtain

$$g_j(\varepsilon + \Delta E_{jk}) \sigma_{jk}^{ce}(\varepsilon + \Delta E_{jk}) = g_k \varepsilon \sigma_{kj}^{cd}(\varepsilon), \quad (39)$$

whereas in the ultrarelativistic regime we have

$$g_j(\varepsilon + \Delta E_{jk})^2 \sigma_{jk}^{ce}(\varepsilon + \Delta E_{jk}) = g_k \varepsilon^2 \sigma_{kj}^{cd}(\varepsilon). \quad (40)$$

It can be checked that the relativistic Klein-Rosseland formula (38) can be obtained from the nondegenerate expressions of collisional excitation and deexcitation rates. Reciprocally, if we have this microreversibility relation between the cross sections σ_{jk}^{ce} and σ_{kj}^{cd}, the detailed balance (37) is automatically fulfilled either for degenerate or nondegenerate electrons.

B. Collisional ionization and three-body recombination

Let us consider the collisional ionization between level j to level k with differential cross section $\sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2)$ and its reverse process, i.e., the three-body recombination with cross section $\sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon)$. From Equations (5) and (25), the relativistic collisional ionization rate reads

$$I^c = \frac{\sqrt{2} m_e^{3/2}}{\pi^2 \hbar^3} \int_{\Delta E_{jk}}^{+\infty} d\varepsilon\, \lambda(\varepsilon) \frac{1}{1+e^{\beta_e \varepsilon - \eta}} \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_1 \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_2 \times c\vartheta(\varepsilon) \sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2) \delta(\varepsilon_1 + \varepsilon_2 + \Delta E_{jk} - \varepsilon) \frac{1}{(1+e^{-\beta_e \varepsilon_1 + \eta})(1+e^{-\beta_e \varepsilon_2 + \eta})} \quad (41)$$

and the relativistic three-body recombination rate reads

$$R^{3b} = \left(\frac{\sqrt{2} m_e^{3/2}}{\pi^2 \hbar^3} \right)^2 \int_{\Delta E_{jk}}^{+\infty} d\varepsilon \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_1 \lambda(\varepsilon_1) \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_2 \lambda(\varepsilon_2) c^2 \vartheta(\varepsilon_1) \vartheta(\varepsilon_2) \sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon) \times \delta(\varepsilon_1 + \varepsilon_2 + \Delta E_{jk} - \varepsilon) \frac{1}{(1+e^{\beta_e \varepsilon_1 - \eta})(1+e^{\beta_e \varepsilon_2 - \eta})} \frac{1}{1+e^{-\beta_e \varepsilon + \eta}}. \quad (42)$$

These expressions generalize the nonrelativistic expressions recently found [19,20]. To find the relativistic Fowler relation, we write

$$\frac{1}{(1+e^{\beta_e \varepsilon_1 - \eta})(1+e^{\beta_e \varepsilon_2 - \eta})} \frac{1}{1+e^{-\beta_e \varepsilon + \eta}} = e^{\beta_e(\varepsilon - \varepsilon_1 - \varepsilon_2) + \eta} \frac{1}{1+e^{\beta_e \varepsilon - \eta}} \frac{1}{(1+e^{-\beta_e \varepsilon_1 + \eta})(1+e^{-\beta_e \varepsilon_2 + \eta})} \quad (43)$$

in Eq. (42). Using the constraint $\delta(\varepsilon_1 + \varepsilon_2 + \Delta E_{jk} - \varepsilon)$, we find that

$$R^{3b} = e^{\beta_e \Delta E_{jk} + \eta} \left(\frac{\sqrt{2} m_e^{3/2}}{\pi^2 \hbar^3} \right)^2 \int_{\Delta E_{jk}}^{+\infty} d\varepsilon \frac{1}{1+e^{\beta_e \varepsilon - \eta}} \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_1 \lambda(\varepsilon_1) \int_0^{\varepsilon - \Delta E_{jk}} d\varepsilon_2 \lambda(\varepsilon_2) \times c^2 \vartheta(\varepsilon_1) \vartheta(\varepsilon_2) \sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon) \delta(\varepsilon_1 + \varepsilon_2 + \Delta E_{jk} - \varepsilon) \frac{1}{(1+e^{-\beta_e \varepsilon_1 + \eta})(1+e^{-\beta_e \varepsilon_2 + \eta})}. \quad (44)$$

We now impose the detailed balance between I^c and R^{3b}, i.e.,

$$R^{3b} = \frac{g_j}{g_k} I^c e^{\beta_e \Delta E_{jk} + \eta}. \quad (45)$$

The obtained constraint between I^c and R^{3b} is valid for any T_e and η. We find that

$$g_j \lambda(\varepsilon) \vartheta(\varepsilon) \sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2) = g_k \frac{\sqrt{2} m_e^{3/2} c}{\pi^2 \hbar^3} \lambda(\varepsilon_1) \lambda(\varepsilon_2) \vartheta(\varepsilon_1) \vartheta(\varepsilon_2) \sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon). \quad (46)$$

This is the relativistic Fowler relation. In the nonrelativistic regime, we recover the usual formula

$$g_j \varepsilon \sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2) = g_k \frac{2 m_e \varepsilon_1 \varepsilon_2}{\pi^2 \hbar^3} \sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon), \quad (47)$$

whereas in the ultrarelativistic regime, we have

$$g_j \varepsilon^2 \sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2) = g_k \frac{\varepsilon_1^2 \varepsilon_2^2}{\pi^2 \hbar^3 c^2} \sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon). \quad (48)$$

As for collisional excitation and deexcitation, the relativistic Fowler relation (46) can be derived using the nondegenerate versions of I^c and R^{3b}. Reciprocally, if we have this microreversibility relation between the cross sections $\sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2)$ and $\sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon)$, the detailed balance (45) is automatically fulfilled either for degenerate or nondegenerate electrons.

C. Dielectronic capture and autoionization

The dielectronic capture cross section and the Auger rate are related by the formula [21]

$$\sigma_{kj}^{dc}(\varepsilon) = f(\varepsilon)A_{jk}^{\mathrm{Auger}}\delta(\varepsilon - \Delta\tilde{E}_{jk}). \tag{49}$$

In this expression, $\Delta\tilde{E}_{jk} = E_j - E_k$ is the transition between level j and level k. The ionization degree of level k is one unit higher than the ionization degree of level j but since level j is autoionizing, $E_k < E_j$. The captured electron energy is equal to $\Delta\tilde{E}_{jk}$. A_{jk}^{Auger} is the autoionization rate from level j to level k. For this process, the electron is ejected with energy $\Delta\tilde{E}_{jk}$. $f(\varepsilon)$ is a generic function. The presence of the Dirac distribution makes the calculation of the dielectronic-capture rate τ_{kj}^{dc} straightforward. Using Eqs. (5), (25), and (49), we find that

$$\tau_{kj}^{dc} = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^{+\infty} d\varepsilon\, \lambda(\varepsilon)c\vartheta(\varepsilon)\sigma_{kj}^{dc}(\varepsilon)\frac{1}{1+e^{\beta_e\varepsilon-\eta}}, \tag{50}$$

i.e.,

$$\tau_{kj}^{dc} = \frac{\sqrt{2}m_e^{3/2}c}{\pi^2\hbar^3}\lambda(\Delta\tilde{E}_{jk})\vartheta(\Delta\tilde{E}_{jk})f(\Delta\tilde{E}_{jk})A_{jk}^{\mathrm{Auger}} \times \frac{1}{1+e^{\beta_e\Delta\tilde{E}_{jk}-\eta}}. \tag{51}$$

To determine $f(\varepsilon)$, we impose the detailed balance

$$\tau_{kj}^{dc} = \frac{g_j}{g_k}e^{-\beta_e\Delta\tilde{E}_{jk}+\eta}\tau_{jk}^{\mathrm{Auger}}, \tag{52}$$

where

$$\tau_{jk}^{\mathrm{Auger}} = \frac{A_{jk}^{\mathrm{Auger}}}{1+e^{-\beta_e\Delta\tilde{E}_{jk}+\eta}}. \tag{53}$$

Consequently,

$$f(\varepsilon) = \frac{g_j}{g_k}\frac{\pi^2\hbar^3}{\sqrt{2}m_e^{3/2}c\lambda(\varepsilon)\vartheta(\varepsilon)}. \tag{54}$$

This is the relativistic version of the nonrelativistic and ultrarelativistic formulas, i.e.,

$$f(\varepsilon) = \frac{g_j}{g_k}\frac{\pi^2\hbar^3}{2m_e\varepsilon} \tag{55}$$

and

$$f(\varepsilon) = \frac{g_j}{g_k}\frac{\pi^2\hbar^3c^2}{\varepsilon^2}, \tag{56}$$

respectively. These expressions are valid for any positive ε.

D. Radiative recombination and photoionization

From the photoionization and radiative recombination cross sections $\sigma_{jk}^{ri}(h\nu)$ and $\sigma_{kj}^{rr}(\varepsilon)$, the photoionization rate from level j to level k reads

$$I_{jk}^r = \frac{4\pi}{h}\int_{\Delta E_{jk}}^{+\infty} d(h\nu)\sigma_{jk}^{ri}(h\nu)\frac{I(h\nu)}{h\nu}\frac{1}{1+e^{-\beta_e(h\nu-\Delta E_{jk})+\eta}} \tag{57}$$

and the relativistic radiative recombination rate reads from Eqs. (5) and (25)

$$R_{kj}^r = \frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3}\int_0^{+\infty} d\varepsilon\, \lambda(\varepsilon)c\vartheta(\varepsilon)\sigma_{kj}^{rr}(\varepsilon) \times \frac{1}{1+e^{\beta_e\varepsilon-\eta}}I^{\mathrm{tot}}(\varepsilon+\Delta E_{jk}). \tag{58}$$

$I(h\nu)$ is the specific intensity of the radiation field and I^{tot} is equal to

$$I^{\mathrm{tot}}(h\nu) = \frac{2h\nu^3}{c^2} + I(h\nu). \tag{59}$$

To determine the relativistic Einstein-Milne relation, we suppose that the free electrons and the radiation fields are in LTE ($T_e = T_r$ where T_r is the radiation temperature) and that I_{jk}^r and R_{kj}^r obey the detailed balance

$$R_{kj}^r = \frac{g_j}{g_k}e^{\Delta E_{jk}+\eta}I_{jk}^r. \tag{60}$$

So, using

$$I(h\nu) = B_{T_r}(h\nu) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\beta_r h\nu}-1}, \tag{61}$$

where $\beta_r = 1/k_BT_r$,

$$I^{\mathrm{tot}}(h\nu) = e^{\beta_r h\nu}B_{T_r}(h\nu), \tag{62}$$

the trick

$$\frac{1}{1+e^{\beta_e\varepsilon-\eta}} = \frac{e^{-\beta_e\varepsilon+\eta}}{1+e^{-\beta_e\varepsilon+\eta}} \tag{63}$$

in Eq. (58), and making the change of variable $h\nu = \varepsilon + \Delta E_{jk}$ in Eq. (57), we find that ($T_e = T_r$)

$$\frac{g_j}{g_k}e^{\Delta E_{jk}+\eta}I_{jk}^r = \frac{g_j}{g_k}e^{\Delta E_{jk}+\eta}\frac{4\pi}{h}\int_0^{+\infty} d\varepsilon\, \sigma_{jk}^{ri}(\varepsilon+\Delta E_{jk}) \times \frac{B_{T_e}(\varepsilon+\Delta E_{jk})}{\varepsilon+\Delta E_{jk}}\frac{1}{1+e^{-\beta_e\varepsilon+\eta}} \tag{64}$$

and

$$R_{kj}^r = e^{\beta_e\Delta E_{jk}+\eta}\frac{\sqrt{2}m_e^{3/2}}{\pi^2\hbar^3} \times \int_0^{+\infty} d\varepsilon\, \lambda(\varepsilon)c\vartheta(\varepsilon)\sigma_{kj}^{rr}(\varepsilon)B_{T_e}(\varepsilon+\Delta E_{jk}) \times \frac{1}{1+e^{-\beta_e\varepsilon+\eta}}. \tag{65}$$

From the detailed balance, these two quantities are equal for any T_e and η. Consequently,

$$g_j\frac{\sigma_{jk}^{ri}(\varepsilon+\Delta E_{jk})}{\varepsilon+\Delta E_{jk}} = g_k\frac{m_e^{3/2}c}{\sqrt{2}\pi^2\hbar^2}\lambda(\varepsilon)\vartheta(\varepsilon)\sigma_{kj}^{rr}(\varepsilon). \tag{66}$$

This is the relativistic Einstein-Milne formula valid for any positive ε. In the nonrelativistic regime, we have

$$g_j \frac{\sigma_{jk}^{ri}(\varepsilon + \Delta E_{jk})}{\varepsilon + \Delta E_{jk}} = g_k \frac{m_e \varepsilon}{\pi^2 \hbar^2} \sigma_{kj}^{rr}(\varepsilon), \tag{67}$$

whereas in the ultrarelativistic regime we have

$$g_j \frac{\sigma_{jk}^{ri}(\varepsilon + \Delta E_{jk})}{\varepsilon + \Delta E_{jk}} = g_k \frac{\varepsilon^2}{2\pi^2 \hbar^2 c^2} \sigma_{kj}^{rr}(\varepsilon). \tag{68}$$

Again, these expressions are valid for any positive ε.

As for collisional excitation and deexcitation and collisional ionization and recombination, the relativistic Einstein-Milne relation (66) can be derived using the nondegenerate versions of I_{jk}^r and R_{kj}^r. Reciprocally, if we have this microreversibility relation between the cross sections $\sigma_{jk}^{ri}(h\nu)$ and $\sigma_{kj}^{rr}(\varepsilon)$, the detailed balance (60) is automatically fulfilled either for degenerate or nondegenerate electrons.

E. Photoexcitation and photodeexcitation

To be complete, we consider photoexcitation and photodeexcitation processes although they are not quite independent of the free electrons. The detailed balance matters only if $T_r = T_e$. For photoexcitation, using the cross section $\sigma_{jk}^{re}(h\nu)$ for a transition from level j to level k, one has for the rate

$$\tau_{jk}^{re} = \frac{4\pi}{h} \int_0^{+\infty} d(h\nu) \frac{\sigma_{jk}^{re}(h\nu)}{h\nu} I(h\nu), \tag{69}$$

where

$$\sigma_{jk}^{re}(h\nu) = \frac{\pi e^2 h}{m_e c} f_{jk} \Psi_{jk}(h\nu). \tag{70}$$

In this expression, f_{jk} the oscillator strength and Ψ_{jk} the line profile in absorption normalized such that

$$\int_{-\infty}^{+\infty} d(h\nu) \Psi_{jk}(h\nu) = 1. \tag{71}$$

For the photodeexcitation rate, one has

$$\tau_{kj}^{rd} = \frac{4\pi}{h} \int_0^{+\infty} d(h\nu) \frac{\sigma_{kj}^{rd}(h\nu)}{h\nu} I^{\rm tot}(h\nu), \tag{72}$$

where

$$\sigma_{kj}^{rd}(h\nu) = \frac{\pi e^2 h}{m_e c} f_{kj} \Psi_{kj}(h\nu). \tag{73}$$

$\sigma_{kj}^{rd}(h\nu)$ the cross section for photodeexcitation of level k to level j and Ψ_{kj} is the line profile in emission normalized such that

$$\int_{-\infty}^{+\infty} d(h\nu)\, \Psi_{kj}(h\nu) = 1. \tag{74}$$

The two line profiles Ψ_{jk} and Ψ_{kj} are not independent. If the free electrons are in LTE at temperature T_e, they satisfy the relation [22–24]

$$\Psi_{kj}(h\nu) = \Psi_{jk}(h\nu) e^{-\beta_e(h\nu - \Delta E_{jk})}, \tag{75}$$

where ΔE_{jk} is the excitation energy. We have also [25]

$$g_k f_{kj} = g_j f_{jk}. \tag{76}$$

From Equations (75) and (76), one has the important relation microreversibility relation

$$\sigma_{kj}^{rd}(h\nu) = \frac{g_j}{g_k} \sigma_{jk}^{re}(h\nu) e^{-\beta_e(h\nu - \Delta E_{jk})}. \tag{77}$$

The factor $e^{-\beta_e(h\nu-\Delta E_{jk})}$ is due to the difference between the line profiles in absorption or in emission. In practice, we keep this relation (77) to calculate the photoexcitation and photodeexcitation rates when $T_r \neq T_e$. It is not clear how relativistic effects can modify this fundamental identity and what to do when the free electrons are not in LTE at temperature T_e.

When the radiation field is a Planck distribution at $T_r = T_e$, Eqs. (62) and (77) lead immediately to the fact that rates (69) and (72) obey the detailed balance, i.e.,

$$\tau_{kj}^{rd} = \frac{g_j}{g_k} e^{\beta_e \Delta E_{jk}} \tau_{jk}^{re}. \tag{78}$$

Equation (77) can also be used to find another way [26] to express the photodeexcitation rate τ_{jk}^{rd} given in Eq. (72), i.e.,

$$\tau_{kj}^{rd} = \frac{g_j}{g_k} e^{\beta_e \Delta E_{jk}} \frac{4\pi}{h} \int_0^{+\infty} d(h\nu) \frac{\sigma_{jk}^{re}(h\nu)}{h\nu} I^{\rm tot}(h\nu) e^{-\beta_e h\nu}. \tag{79}$$

TABLE I. Relativistic expressions of various relations and quantities.

Symbol	Relativistic
Klein-Rosseland	$g_j \lambda(\varepsilon + \Delta E_{jk}) \vartheta(\varepsilon + \Delta E_{jk}) \sigma_{jk}^{ce}(\varepsilon + \Delta E_{jk}) = g_k \lambda(\varepsilon) \vartheta(\varepsilon) \sigma_{kj}(\varepsilon)$
Fowler	$g_j \lambda(\varepsilon) \vartheta(\varepsilon) \sigma^{ci}(\varepsilon; \varepsilon_1, \varepsilon_2) = g_k \frac{\sqrt{2} m_e^{3/2} c}{\pi^2 \hbar^3} \lambda(\varepsilon_1) \lambda(\varepsilon_2) \vartheta(\varepsilon_1) \vartheta(\varepsilon_2) \sigma^{3br}(\varepsilon_1, \varepsilon_2; \varepsilon)$
$f(\varepsilon)$	$\frac{g_j}{g_k} \frac{\pi^2 \hbar^3}{\sqrt{2} m_e^{3/2} c \lambda(\varepsilon) \vartheta(\varepsilon)}$
Einstein-Milne	$g_j \frac{\sigma_{jk}^{ri}(\varepsilon + \Delta E_{jk})}{\varepsilon + \Delta E_{jk}} = g_k \frac{m_e^{3/2} c}{\sqrt{2} \pi^2 \hbar^2} \lambda(\varepsilon) \vartheta(\varepsilon) \sigma_{kj}^{rr}(\varepsilon)$
$\lambda(\varepsilon)$	$\sqrt{\varepsilon} \sqrt{1 + \frac{\varepsilon}{2 m_e c^2}} \left(1 + \frac{\varepsilon}{m_e c^2}\right)$
$\vartheta(\varepsilon)$	$\sqrt{\frac{\frac{\varepsilon}{m_e c^2}\left(\frac{\varepsilon}{m_e c^2} + 2\right)}{\left(\frac{\varepsilon}{m_e c^2} + 1\right)^2}}$
$\varepsilon(p)$	$\varepsilon = \sqrt{p^2 c^2 + m_e^2 c^4} - m_e c^2$

TABLE II. Nonrelativistic and ultrarelativistic expressions of various relations and quantities.

Symbol	Nonrelativistic	Ultrarelativistic
Klein-Rosseland	$g_j(\varepsilon+\Delta E_{jk})\sigma_{jk}^{ce}(\varepsilon+\Delta E_{jk})=g_k\varepsilon\sigma_{kj}^{cd}(\varepsilon)$	$g_j(\varepsilon+\Delta E_{jk})^2\sigma_{jk}^{ce}(\varepsilon+\Delta E_{jk})=g_k\varepsilon^2\sigma_{kj}^{cd}(\varepsilon)$
Fowler	$g_j\varepsilon\sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2)=g_k\frac{2m_e\varepsilon_1\varepsilon_2}{\pi^2\hbar^3}\sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon)$	$g_j\varepsilon^2\sigma^{ci}(\varepsilon;\varepsilon_1,\varepsilon_2)=g_k\frac{\varepsilon_1^2\varepsilon_2^2}{\pi^2\hbar^3c^2}\sigma^{3br}(\varepsilon_1,\varepsilon_2;\varepsilon)$
$f(\varepsilon)$	$\frac{g_j}{g_k}\frac{\pi^2\hbar^3}{2m_e\varepsilon}$	$\frac{g_j}{g_k}\frac{\pi^2\hbar^3c^2}{\varepsilon^2}$
Einstein-Milne	$g_j\frac{\sigma_{jk}^{ri}(\varepsilon+\Delta E_{jk})}{\varepsilon+\Delta E_{jk}}=g_k\frac{m_e\varepsilon}{\pi^2\hbar^2}\sigma_{kj}^{rr}(\varepsilon)$	$g_j\frac{\sigma_{jk}^{ri}(\varepsilon+\Delta E_{jk})}{\varepsilon+\Delta E_{jk}}=g_k\frac{\varepsilon^2}{2\pi^2\hbar^2c^2}\sigma_{kj}^{rr}(\varepsilon)$
$\lambda(\varepsilon)$	$\sqrt{\varepsilon}$	$\frac{\varepsilon^2}{\sqrt{2}(m_ec^2)^{3/2}}$
$\vartheta(\varepsilon)$	$\sqrt{\frac{2\varepsilon}{m_ec^2}}$	1
$\varepsilon(p)$	$\frac{p^2}{2m_e}$	pc

If we use Equation (62) in this equation when the radiation field is a Planck distribution at $T_r = T_e$, one can see that the detailed balance (78) is immediately satisfied.

F. Remarks

The microreversibility relations have been written using the fundamental constants c, m_e, and $\hbar$ instead of c, m_e, and h as can be encountered in the literature for the nonrelativistic case. This is more logical since the usual fundamental constants in atomic physics are c, e, $\hbar$, and m_e where e is the elementary charge. In atomic units, $e = \hbar = m_e = 1$ and $c = 1/\alpha$ where $\alpha = e^2/\hbar c$ is the fine-structure constant. Concerning the microreversibility relations, we have seen that they can be derived from degenerate or nondegenerate electrons. This means that the relativistic effects and the degeneracy character are two independent notions, the most accurate approach being the relativistic treatment of degenerate electrons. In summary, we give in Table I the relativistic expressions of various relations and quantities and in Table II their nonrelativistic and ultrarelativistic expressions.

III. CONCLUSION

We have generalized to the relativistic regime the Klein-Rosseland, Fowler, and Einstein-Milne formulas as well as the relation between the dielectronic-capture cross section and the autoionization rate. The practical expressions have been shown to be consistent with the nonrelativistic and ultrarelativistic regimes. With the present approach, we can develop fully relativistic CRE models to describe NLTE plasmas at arbitrary degeneracy. As expected, there is a close connection between the microreversibility relations and the detailed balance between the rates of the pairs of individual microscopic processes. The treatment of degeneracy is found to be crucial.

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