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Ab initio calculation of the non-relativistic free–free Gaunt factor incorporating plasma screening

G.S.J. Armstrong*, J. Colgan, D.P. Kilcrease, N.H. Magee Jr.

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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ABSTRACT

We present calculations of Gaunt factors for free–free absorption over a wide range of temperatures and densities. The calculations employ a partial wave expansion approach, which is able to account for plasma screening within the calculation of the free–free Gaunt factor. Much of the existing Gaunt factor data pertains to hydrogenic systems, and plasma screening is often incorporated in opacity calculations using approximate methods. The use of a more accurate method allows us to determine the accuracy of such approximations in calculations of the free–free monochromatic and mean opacities.

1. Introduction

We present a method to calculate non-relativistic Gaunt factors for free–free absorption using a partial wave expansion method. Previously, the Los Alamos National Laboratory light element opacity code ATOMIC [1] and its predecessor LEDCOP [2] relied on the Gaunt factor tables of Nakagawa et al. [3] to calculate free–free opacities. These tables list thermally-averaged hydrogenic Gaunt factors for a given set of photon energies, temperatures and electron degeneracies, and are derived from a series expansion approach [4] to the Sommerfeld formula for the differential cross section for free–free absorption [5]. In ATOMIC, the table values are then corrected for plasma screening using an approximate method developed by J.M. Green [6,7] (referred to as 'the Green approximation'). In the new *ab initio* approach, the non-relativistic free–free Gaunt factor is calculated using a partial wave expansion, based on the BREM-IV code also developed by J.M. Green [8,9]. This method allows the Gaunt factor to be determined at any given temperature and for any degeneracy. The new approach also provides an improved treatment of plasma screening, by calculating the continuum electron wavefunction using a screened potential. The partial wave expansion method will provide insight into the degree to which the Green screening correction currently used in ATOMIC reproduces Gaunt factors calculated using a more rigorous treatment of plasma screening. In this paper, we make comparison between the results of the partial wave expansion and those of the Green approximation. From this comparison we may determine ranges in temperature, density and photon energy at which screening plays a major role. We then examine the effect of the new free–free treatment on the Rosseland mean opacity over a wide range of temperatures and densities for hydrogen and carbon.

In the following section we give a brief overview of the partial wave expansion method, followed by a description of the theoretical approach used in the subsequent calculation of the free–free opacity. We present the results from numerous test cases, which investigate the comparison between Gaunt factors calculated using the Green approximation with those calculated using the partial wave method incorporating screening. We then investigate the sensitivity of the Rosseland mean opacity to the free–free opacity, by comparing new calculations with previous opacity data for hydrogen and carbon [1]. We end with a short conclusion.

2. Theory

2.1. Partial wave expansion for the Gaunt factor

The non-relativistic free–free Gaunt factor for a plasma of average ionization $\overline{Z}$, an initial electron energy E_i and a photon energy $\hbar\omega$ (in Rydbergs) may be obtained through a partial wave expansion of the form [8]

$$g_\mathrm{ff}(\omega, E_\mathrm{i}) = \frac{1}{2\pi(\overline{Z})^2}\sqrt{\frac{3}{E_\mathrm{i}(E_\mathrm{i}+\hbar\omega)}}\sum_{L=1}^{\infty} L\Big\{M^2\Big(k_\mathrm{i}, L; k_\mathrm{f}, L-1\Big) + M^2\Big(k_\mathrm{i}, L-1; k_\mathrm{f}, L\Big)\Big\}, \tag{1}$$

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* Corresponding author.
E-mail address: gregorya@lanl.gov (G.S.J. Armstrong).

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where L is the orbital angular momentum of the continuum electron wavefunction $\Psi_L(r,k)$, and the dipole matrix element $M(k_i,L_i;k_f,L_f)$ is given (in the acceleration gauge) by

$$M(k_i, L_i; k_f, L_f) = \frac{1}{A_i A_f}\int_0^\infty \Psi_{L_i}(r;k_i)\frac{\mathrm{d}V}{\mathrm{d}r}\Psi_{L_f}(r;k_f)\mathrm{d}r. \tag{2}$$

Here, k_i and k_f are the electron wave numbers of the initial and final states, L_i and L_f are their respective orbital angular momenta, A_i and A_f are their amplitudes, and the continuum electron wavefunction $\Psi_L(r,k)$ is given by a Green's function solution of the Schrödinger equation [10]

$$\Psi_L(r,k) = J_L(kr) + \frac{1}{k}\left[N_L(kr)\int_0^\infty \Psi_L(r,k)V(r)J_L(kr)\mathrm{d}r - J_L(kr)\int_0^\infty \Psi_L(r,k)V(r)N_L(kr)\mathrm{d}r\right], \tag{3}$$

where $J_L(kr)/kr$ and $N_L(kr)/kr$ are the regular and irregular spherical Bessel functions, and the potential $V(r)$ is given in a Yukawa form, in terms of the average ionization $\overline{Z} = n_e/n_i$ (where n_e and n_i are the electron and ion densities), and screening length λ as

$$V(r) = \frac{\overline{Z}e^2}{r}\mathrm{e}^{-r/\lambda}, \tag{4}$$

where e is the electron charge. The screening length may be chosen to be the Wigner–Seitz radius, λ_{WS}, given by

$$\lambda_{WS} = \left(\frac{3}{4\pi n_i}\right)^{1/3} \quad [\mathrm{cm}], \tag{5}$$

or the Debye radius, λ_D, which (for any degree of electron degeneracy) is given approximately by

$$\frac{1}{\lambda_D} = \left(\frac{4\pi e^2}{kT_e}\right)^{1/2}\sqrt{\sum_j n_i^{(j)}Z_{(j)}^2 + n_e\left[1+\left(\frac{kT_F}{kT_e}\right)^2\right]^{-1/2}} \quad [\mathrm{cm}], \tag{6}$$

where $Z_{(j)}$ and $n_i^{(j)}$ are the charge and ion density of ion j, kT_e is the electron temperature, and where kT_F is the Fermi temperature, given by

$$kT_F = \frac{2}{3}\frac{\hbar^2}{2m_e}\left(3\pi^2 n_e\right)^{2/3} \quad [\mathrm{erg}], \tag{7}$$

where m_e is the electron mass. When the screening length λ becomes smaller than the Wigner–Seitz radius, the simple screening picture presented above becomes questionable. Therefore, in all calculations presented here, we take the screening length to be the larger of the Debye and Wigner–Seitz radii.

2.2. Free–free absorption opacity

The non-relativistic free–free Gaunt factor may be averaged over all electron energies using a Fermi–Dirac distribution and Pauli blocking factor. The normalized Fermi–Dirac-averaged Gaunt factor is defined as

$$\overline{g}_{ff}\left(\gamma^2, u, \eta\right) = \frac{\sqrt{\pi}}{2I_{1/2}(\eta)}\int_0^\infty \frac{g_{ff}\left(u\gamma^{-2}, x\gamma^{-2}\right)}{(1+\mathrm{e}^{x-\eta})(1+\mathrm{e}^{\eta-x-u})}\mathrm{d}x, \tag{8}$$

where

$$I_{1/2}(\eta) = \int_0^\infty \frac{x^{\frac{1}{2}}}{1+\mathrm{e}^{x-\eta}}\mathrm{d}x \tag{9}$$

is a Fermi integral, and where the dimensionless quantities x,u,γ^2 and η are related to the electron energy E_e, photon energy $\hbar\omega$, temperature kT_e, and electron chemical potential μ_e as

$$x = \frac{E_e}{kT_e}, \tag{10}$$

$$u = \frac{\hbar\omega}{kT_e}, \tag{11}$$

$$\gamma^2 = \frac{\overline{Z^2}\mathrm{Ry}}{kT_e}, \tag{12}$$

$$\eta = \frac{\mu_e}{kT_e}, \tag{13}$$

where Ry is the Rydberg unit of energy, given by $2\pi^2 e^4 m_e h^{-2} \simeq 13.6057$ eV. The quantity $\overline{Z^2}$ takes the form

$$\overline{Z^2} = \sum_j \frac{Z_{(j)}^2 n_i^{(j)}}{n_T}, \tag{14}$$

where $n_T = \sum_j n_i^{(j)}$ is the total ion density.

For a given ion number density, n_i, and mass density, ρ, the free–free absorption cross section, $\sigma_{ff}(\omega,T_e)$, is given by

$$\sigma_{ff}(\omega, T_e) = \frac{4(2\pi)^{5/2}}{3\sqrt{3}}\frac{e^6\overline{Z^2}}{\hbar c m_e^{3/2}\omega^3}\frac{n_e}{\sqrt{kT_e}}\overline{g}_{ff}\left(\gamma^2, u, \eta\right) \quad [\mathrm{cm}]^2, \tag{15}$$

where c is the speed of light, and $\overline{g}_{ff}(\gamma^2, u, \eta)$ is the Fermi–Dirac-averaged Gaunt factor, defined in Eq. (8). The classical Kramers formula for the free–free absorption cross section is given by Eq. (15) with $\overline{g}_{ff}(\gamma^2, u, \eta) = 1$. Further modifications incorporating stimulated emission and the Drude model approximation for multiple collisions lead to a monochromatic free–free opacity, $k_{ff}(\omega,T_e)$, with the form [11,12]

$$k_{ff}(\omega, T_e) = \left(1 - \mathrm{e}^{-\hbar\omega/kT_e}\right)\frac{{\omega_p}^2}{\omega^2+\nu^2(\omega)}\frac{\nu(\omega)}{n(\omega)\rho c} \quad [\mathrm{cm}]^2[\mathrm{g}]^{-1}, \tag{16}$$

where $\nu(\omega)$ is the collision frequency, given by

$$\nu(\omega) = c\frac{\omega^2}{\omega_p^2}n_i\sigma_{ff}(\omega, T_e) \quad [\mathrm{s}]^{-1}, \tag{17}$$

and the refractive index $n(\omega)$ takes the form

$$n(\omega) = \sqrt{\frac{\omega\left(\omega^2-\omega_p^2+\nu^2\right)+\sqrt{(\omega^2+\nu^2)\left[\left(\omega^2-\omega_p^2\right)^2+\omega^2\nu^2\right]}}{2\omega(\omega^2+\nu^2)}}, \tag{18}$$