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Abstract. In this work, we analytically evaluate the exact matrix element for a non-relativistic Continuum–Bound radiative transition in a Coulomb potential. We apply this result to the photoionization (and radiative recombination) process, and calculate the total cross sections giving an analytical expression for the transition from the ground state. To our best knowledge the exact solution to this problem has never been addressed even though the analytical calculation is quite simple, and the final result is not more complicated than any of its approximations. We compare our result with the well-known plane wave and Coulombian dipolar approximations, in a wide range of energies.

1. Introduction

Atomic processes that involve photons are essential for a wide range of applications. For instance, they are customarily used for the study and diagnostic of astrophysical as well as laboratory plasmas [1, 2]. At present, most studies employ the dipolar approximation [3, 4], which is customarily assumed to be a fair approximation in the non-relativistic case [5], and whose evaluation has been even numerically extended into the relativistic regime [6].

In this work, we analytically evaluate the non-relativistic total cross section including all its multipoles contributions for the ground state of a Hydrogenic system. We show that it is not more complicated than the dipolar or other usual approximations. Finally, we demonstrate that it might differ significantly from any of these standard approximations at energies within the non-relativistic regime.

2. Photoionization and Radiative Recombination

Let us consider the photoionization of a bound state ϕ of a Hydrogenic atom or ion of effective charge Z by the absorption of a photon of wave vector $\mathbf{k}$ (angular frequency $\omega = kc$) and polarization $\hat{e}$ ($\perp \mathbf{k}$), with emission of an electron of momentum $\mathbf{p}$. By energy conservation, $\omega = Z^2/2n^2 + p^2/2$, with n the principal quantum number of the bound state (Atomic units are used throughout this article). In the velocity gauge, the non-relativistic transition matrix element reads

$$T = \langle \psi_{\mathbf{p}} \mid e^{i\mathbf{k}\cdot\mathbf{r}} \, \hat{e} \cdot \nabla_{\mathbf{r}} \mid \phi \rangle , \tag{1}$$

where

$$\psi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \Gamma(1 + i\mu) \, e^{-\pi\mu/2} \, {}_1F_1\left(-i\mu, 1; i(pr + \mathbf{p}\cdot\mathbf{r})\right) e^{i\mathbf{p}\cdot\mathbf{r}}$$

represents the Coulomb continuum state of the electron emitted with momentum $\mathbf{p}$. Here we have defined the Sommerfeld parameter $\mu = Z/p$. The same transition matrix element describes the Radiative Recombination process [7], where an atom captures an electron with emission of a photon. The differential cross sections for the photoionization (PI) and radiative recombination (RR) processes read

$$\frac{d\sigma^{\mathrm{PI}}}{d\Omega_{\mathbf{p}}} = \frac{4\pi^2}{c^2}\frac{p}{k}\,|T|^2 \qquad \text{and} \qquad \frac{d\sigma^{\mathrm{RR}}}{d\Omega_{\mathbf{k}}} = \frac{4\pi^2}{c^2}\frac{k}{p}\,|T|^2 \, ,$$

By averaging on the polarization and integrating over the solid angle, the total cross sections σ^{PI} and σ^{RR} are obtained, which verify $k^2 \times \sigma^{\mathrm{PI}} = p^2 \times \sigma^{\mathrm{RR}}$.

3. Dipolar Approximation

The transition matrix element T is commonly evaluated in a dipolar approximation,

$$T_{\mathrm{D}} = \langle \psi_{\mathbf{p}} \mid \hat{e} \cdot \nabla_{\mathbf{r}} \mid \phi \rangle \, ,$$

which is valid for sufficiently low energies, namely $\omega \ll Zc/n$. For the ground state the total cross section reads [8],

$$\sigma_{\mathrm{D}} = N_{\mathrm{D}}(\mu)\,\sigma_o \tag{2}$$

where we have defined

$$N_{\mathrm{D}}(\mu) = 2\pi\mu\,\frac{1+\mu^2}{1-e^{-2\pi\mu}}\,e^{-4\mu\cot^{-1}\mu}$$

and where σ_o should be replaced by

$$\sigma_o^{\mathrm{PI}} = \frac{p}{k}\,\frac{8\pi}{3c^2}\,\frac{p^2 Z^5}{\omega^4} \qquad \text{and} \qquad \sigma_o^{\mathrm{RR}} = \frac{k}{p}\,\frac{8\pi}{3c^2}\,\frac{p^2 Z^5}{\omega^4} \, , \tag{3}$$

for the photoionization and radiative recombination processes, respectively [9]. Note that this cross section σ_o is obtained from Eq. (2) in the $\mu \to 0$ limit. The extension to arbitrary nlm states was analytically evaluated by Aaron $et\ al$ [3].

4. Plane Wave Approximation

Another commonly employed approximation replaces the exact Coulomb continuum state in (1) by a plane wave, which is valid for photon (or electron) energies much larger than that of the ground state. The transition matrix element reads

$$T_{\mathrm{PW}} = \tilde{\phi}(\mathbf{q})\,\hat{e} \cdot \mathbf{p}$$

where $\tilde{\phi}(\mathbf{q})$ is the eigenstate of the Hydrogenic atom in the momentum representation and $\mathbf{q} = \mathbf{k} - \mathbf{p}$ is the momentum transfer. These functions were evaluated by Podolsky and Pauling in 1929 [10]

$$\tilde{\phi}_{nlm}(\mathbf{q}) = 2^{2l+3}Z^{l+3}\,l!\left(\frac{(n-l-1)!}{2\pi Z\,(n+l)!}\right)^{1/2}\frac{1}{q^2}\left(\frac{nq}{(nq)^2+Z^2}\right)^{l+2}C_{n-l-1}^{l+1}\left(\frac{(nq)^2-Z^2}{(nq)^2+Z^2}\right)Y_{lm}(\hat{\mathbf{q}})$$

where $C_{\nu}^{\mu}(x)$ are the Gegenbauer polynomials. The corresponding total cross section for the ground state reads

$$\sigma_{\mathrm{PW}} = N_{\mathrm{PW}}(\mu,\nu)\,\sigma_o \, , \tag{4}$$

where

$$N_{\mathrm{PW}}(\mu,\nu) = \left[\frac{(1+\mu^2)^2}{(1+\mu^2+\mu^2\nu^2)^2 - 2\mu^2\nu^2}\right]^2 \, ,$$

with $\nu = k/Z$. Note that σ_o is recovered from Eq. (4) in the $\nu \to 0$ limit.

5. Exact non-relativistic Solution

For the ground state ϕ_{1s}, and after some simple algebra, we obtain

$$T_{\text{Exact}} = \hat{e} \cdot \nabla_{\mathbf{k}} \langle \psi_{\mathbf{p}} \mid \frac{1}{r} e^{i\mathbf{k}\cdot\mathbf{r}} \mid \phi_{1s} \rangle.$$

The matrix element can be analytically evaluated by means of Nordsieck's method [11, 12] in order to obtain

$$\langle \psi_{\mathbf{p}} \mid \frac{1}{r} e^{i\mathbf{k}\cdot\mathbf{r}} \mid \phi_{1s} \rangle = \frac{(2Z)^{1/2}}{\pi} Z^2 \, \Gamma(1 - i\mu) \, e^{-\pi\mu/2} \frac{\left(Z^2 + |\mathbf{k} - \mathbf{p}|^2\right)^{i\mu-1}}{\left((Z - ip)^2 + k^2\right)^{i\mu}} \, ,$$

so that

$$T_{\text{Exact}} = \frac{(2Z)^{5/2}}{2\pi} \frac{\Gamma(2 - i\mu) \, e^{-\pi\mu/2}}{(Z^2 + |\mathbf{k} - \mathbf{p}|^2)^2} \left(\frac{Z^2 + |\mathbf{k} - \mathbf{p}|^2}{(Z - ip)^2 + k^2} \right)^{i\mu} \hat{e} \cdot \mathbf{p} \, .$$

Finally, the corresponding total cross section reads,

$$\sigma_{\text{Exact}} = e^{4\mu\Theta} \, \frac{\sigma_D \times \sigma_{PW}}{\sigma_o} \, , \tag{5}$$

where

$$\Theta = \frac{1}{2} \cot^{-1}\left(\frac{4c^2 + Z^2 - p^2}{2pZ} \right) \, .$$

Note that in the non-relativistic regime, $\Theta \approx 0$, and therefore,

$$\sigma_{\text{Exact}} \approx \frac{\sigma_D \times \sigma_{PW}}{\sigma_o} \, . \tag{6}$$

The generalization of these results to nlm states in terms of Nordsieck's integrals is straightforward [13, 14].

In figure 1 we compare this exact solution with the plane wave σ_{PW}, dipolar σ_{D} and plane wave + dipolar σ_o approximations. We see that the plane wave approximation overestimates the total cross section on the whole energy range and, as expected, improves for increasing energies. On the contrary, the dipolar approximation fairly agrees with the exact expression but starts to fail at high but still non-relativistic energies.

6. Conclusions

We presented an analytical formula for the photoionization and radiative recombination cross sections in the non-relativistic regime which, for the ground state of a Hydrogenic atom or ion, is not more complicated than the standard Dipole or Plane Wave approximations. In fact, we show that it is given by the product of these two approximations much commonly employed in the literature.
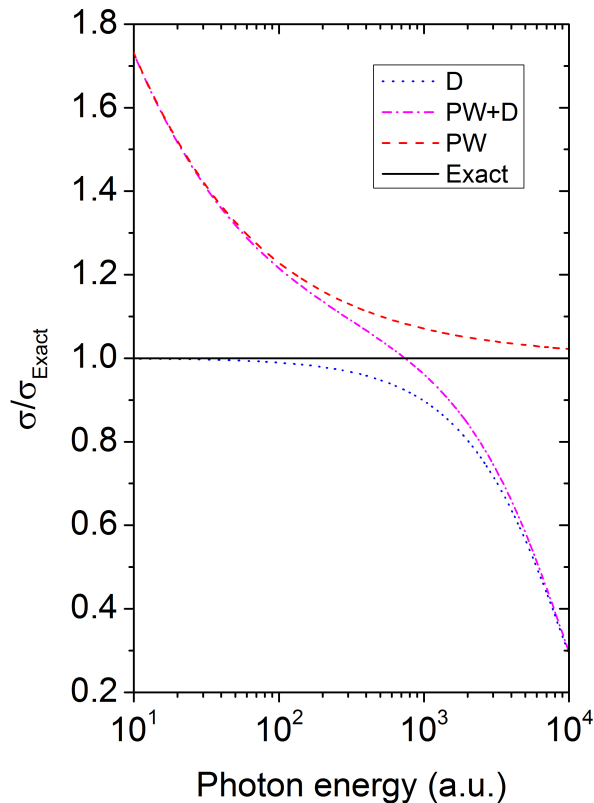
Figure 1. Non-relativistic cross section for the photoionization or radiative recombination processes (with $Z = 1$) as a function of the photon energy. The Dipolar (D), Plane Wave + Dipolar (PW+D) and Plane Wave (PW) approximations are compared with the Exact solution (Exact), as given by Eqs. (2), (3), (4) and (5), respectively.

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