

An eikonal approach for the atomic photoelectric effect on H-like atoms

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Most quantum mechanics textbooks introduce the atomic photoelectric effect expressing the final continuum state in the high energy limit as a plane wave. This approximation has shown to give clear differences between gauges though. In this work, we show that an approximation based on the asymptotic limit of the exact wave function for the final state leads to better results whether form of the interaction Hamiltonian is used as the photon energy increases. This asymptotic eikonal approximation leads to the exact result in velocity gauge for increasing photon energies, evidencing the relevance of the Coulomb potential even at large distances.

Keywords: Photoionization; Coulomb wave functions.

Gran parte de los textos de mecánica cuántica introducen el efecto fotoeléctrico expresando la función de onda para el estado final en el límite de altas energías como una onda plana. Sin embargo, esta aproximación conduce a resultados que dependen de la norma utilizada para el cálculo de la amplitud de transición. En este trabajo se muestra que una aproximación basada en el límite asintótico de la función de onda exacta para el estado final, conduce a mejores resultados independientemente de la forma del hamiltoniano de interacción utilizado a medida que se incrementa la energía del fotón. Esta aproximación asintótica eikonal conduce al resultado exacto en la norma de velocidad para altas energías del fotón incidente, evidenciando la relevancia del potencial coulombiano a grandes distancias.

Descriptores: Fotoionización; función de onda coulombiana.

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In the last few years, there has been a notorious increase of studies referring many electron ionization of atoms by radiation fields. This is mainly consequence, of a new generation of experimental devices, which now provide fully detailed information on the dynamic of the charged fragments involved in the collision of charged particles and photons with atoms [1, 2]. These advances in experimental studies have also encouraged theoreticians to improve the theoretical models regularly used in atomic collisions physics to describe the many particles continuum [3–5].

In spite of the conceptual advance achieved on complex multielectron systems, by the end of quantum mechanics courses the student generally does not realize the consequences of considering the many particles continuum under different approximations.

In this work we consider the atomic photoelectric effect of the hydrogen atom which is usually introduced within the semiclassical theory of radiation. The equivalence between the different representations of the interaction operator, *i.e.*, gauges, is usually shown using the Heisenberg equation of motion assuming that the exact wave functions for the initial and final states are being employed. Furthermore, the process is commonly presented in a non-relativistic high energy approximation [6–8] where terms in the Hamiltonian that scale as $1/c^2$ are neglected. This approximation is usually denoted as dipolar approximation and is valid for $a_0/\lambda \ll 1$ being a_0 the Bohr radius and λ the photon wavelength. Another usual approximation consists in considering the photoelectron continuum wave function as a plane wave. This approximation notably simplifies the analytical work and leaves

a clear qualitative insight of the differential cross sections. However, the cross sections for the photoelectric effect of hydrogen calculated in different gauges and using plane waves to represent the final electron wave function, lead to different results [9]. The main reason for this discrepancy is given by the fact that the plane wave is not a solution of $H_0 + V(r)$ (with $V(r) = -Z/r$) but of the free particle Hamiltonian H_0 . In other words, since the exact initial state is considered, the main reason for the lack of agreement between gauges is consequence of an approximated final state wave function which does not properly take account of the Coulomb potential.

In this work we propose the use of the asymptotic form of the Coulomb wave function in order to represent the photoelectron continuum. We show that the differential cross sections in both gauges lead to a better description of the process without incrementing the mathematical complexity. Comparison with the exact results obtained when the final state is represented with a Coulomb wave function is performed and the advantages of the here proposed approximation are summarized. Atomic units will be used throughout this paper.

We describe an initial bound electron in the ground state of an hydrogenic atom by,

$$\varphi_i = \frac{Z^{3/2}}{\sqrt{\pi}} e^{-Zr}. \quad (1)$$

We perform our analysis for H-like atoms but for practical purposes, we consider the value $Z = 1$ restricting ourselves to the H atom. The solution of the Schrödinger equation for the two body Coulomb problem in the continuum with in-

coming boundary condition,

$$[H_0 + V(r)] \Psi^{(-)} = E\Psi^{(-)} \quad (2)$$

is given by a Coulomb wave function [8, 10, 11],

$$\Psi_C^{(-)} = \frac{N_C}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} {}_1F_1[i\alpha, 1, -ikr - i\mathbf{k}\cdot\mathbf{r}] \quad (3)$$

where ${}_1F_1[a, c, z]$ is the Kummer function [12],

$$N_C = e^{-(\pi\alpha/2)} \Gamma(1 - i\alpha)$$

is the normalization constant and $\alpha = -Z\mu/k$ is the Sommerfeld parameter [8, 10, 11]. The momentum of the emitted electron is k and the reduced mass of the two particles system is μ . The usual plane wave approximation for the continuum state, could be easily recovered by taking the limit $\alpha \rightarrow 0$.

The differential cross section for the photoionization process is given by [6, 7],

$$\frac{d\sigma}{d\Omega} = \frac{4\pi^2 k}{c\omega} |M_{1s}^G|^2 \quad (4)$$

where ω is the photon energy, $c = 137$ and M_{1s}^G is the transition amplitude in gauge G . Taking into account the Heisenberg equation of motion $[H_0 + V(r), \mathbf{r}] = \mathbf{p}$ we obtain the following expressions for the transition amplitudes in the velocity and length gauges [9],

$$M_{1s}^V = \langle \Psi^{(-)} | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\boldsymbol{\epsilon}} \cdot \nabla | \varphi_i \rangle \quad (5)$$

$$M_{1s}^L = \omega \langle \Psi^{(-)} | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\boldsymbol{\epsilon}} \cdot \mathbf{r} | \varphi_i \rangle \quad (6)$$

where we have noted with \mathbf{k}_γ the momentum vector of the photon. In the following, we work within the dipolar approximation, which is equivalent to consider $\mathbf{k}_\gamma = 0$ in the above expressions. When the exact wave functions are used to represent the initial and final states, Eq. (5) and Eq. (6) lead identical results. This means that the obtained cross sections are gauge-independent. The transition amplitudes calculations are performed by using Nordsieck-like integrals when Coulomb wave functions are used. Nordsieck-like integrals are widely used in atomic physics and nowadays are tabulated in several textbooks and articles [7, 11, 13–15]. However, this could not be considered a straightforward calculation in a quantum mechanics course and could probably exceed the time deserved to the subject. The plane wave approximation mainly consist on the Fourier transform of the initial state which leads to

$$M_{PW}^V = i\hat{\boldsymbol{\epsilon}} \cdot \left(\frac{Z^{5/2}}{\sqrt{\pi}(2\pi)^{3/2}} \right) \frac{8\pi\mathbf{k}}{(k^2 + Z^2)^2}. \quad (7)$$

By the other side M_{PW}^L is exactly twice M_{PW}^V leading to a constant factor 4 of discrepancy between the velocity and length gauges for the differential cross section. We now consider the eikonal approximation which mainly concerns us.

Asymptotically (for large r), the continuum wave function Eq. (3) is given by [8, 12]

$$\Psi_r^{(-)} \rightarrow \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} \left\{ e^{-i\alpha \log(kr + \mathbf{k}\cdot\mathbf{r})} + \frac{\Gamma(1 - i\alpha)}{\Gamma(i\alpha)} \frac{e^{-i(kr + \mathbf{k}\cdot\mathbf{r})}}{(-kr - \mathbf{k}\cdot\mathbf{r})^{1 - i\alpha}} \right\}. \quad (8)$$

The first term of Eq.(8) is given by a plane wave times an eikonal distortion that explicitly shows that the Coulomb potential of the nucleus is felt by the emitted electron even at large distances. The second term is related to the scattering of the photoelectron by the nucleus [8] and clearly behaves as an spherical incoming wave.

As an approximated model we propose the eikonal approach which retains the asymptotic distortion effect of the Coulomb potential:

$$\Psi_{eik}^{(-)} = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} e^{-i\alpha \log(kr + \mathbf{k}\cdot\mathbf{r})}. \quad (9)$$

The transition amplitude in velocity gauge for the eikonal approximation is given by

$$M_{eik}^V = \frac{-Z^{5/2}\hat{\boldsymbol{\epsilon}}}{\sqrt{\pi}(2\pi)^{3/2}} \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r} - Zr\hat{\mathbf{r}}(kr + \mathbf{k}\cdot\mathbf{r})^{i\alpha}}. \quad (10)$$

In order to simplify calculations, we now rewrite this expression as follows:

$$M_{eik}^V = - \lim_{k' \rightarrow k} \hat{\boldsymbol{\epsilon}} \cdot \left(\frac{Z^{5/2}}{\sqrt{\pi}(2\pi)^{3/2}} \right) k^{i\alpha} i \times \nabla_{\mathbf{k}'} \left[\int d\mathbf{r} e^{-i\mathbf{k}'\cdot\mathbf{r} - Zr\hat{\mathbf{r}}(r + \hat{\mathbf{k}}\cdot\mathbf{r})^{i\alpha}} \right], \quad (11)$$

where we have considered $\mathbf{k}' = k'\hat{\mathbf{k}}$. Introducing the parabolic coordinates commonly used for the two body problem [8]:

$$\begin{aligned} \xi &= r + \hat{\mathbf{k}}\cdot\mathbf{r}, \\ \eta &= r - \hat{\mathbf{k}}\cdot\mathbf{r}, \\ \phi &= \arctan(y/x), \end{aligned}$$

where z is defined along the \mathbf{k} axis. Taking into account that the volume element in these coordinates is given by

$$d\mathbf{r} = \frac{(\xi + \eta)}{4} d\xi d\eta d\phi, \quad (12)$$

the integral between brackets in Eq. (11) turns separable:

$$I = \pi \int_0^\infty \int_0^\infty d\xi d\eta e^{-(ik' + Z)\frac{\xi}{2}} \xi^{i\alpha} e^{(ik' - Z)\frac{\eta}{2}}. \quad (13)$$

The integrals can be easily performed and they give

$$I = \frac{4\pi\Gamma(1 + i\alpha)}{(k'^2 + Z^2)} \left(\frac{ik' + Z}{2} \right)^{-i\alpha}. \quad (14)$$

Finally, the transition amplitude in velocity gauge for the eikonal approximation is obtained:

$$M_{eik}^V = (\hat{\varepsilon} \cdot \hat{\mathbf{k}}) \sqrt{\frac{2}{\pi}} Z^{5/2} k^{-i\frac{Z}{k}} \Gamma\left(1 - i\frac{Z}{k}\right) \left(\frac{ik+Z}{2}\right)^{i\frac{Z}{k}} \times \left(\frac{2k^2(ik+Z) + Z(k^2+Z^2)}{k(k^2+Z^2)^2(ik+Z)}\right). \quad (15)$$

Following the same line of reasoning, it could be shown that the length gauge transition amplitude is given by,

$$M_{eik}^L = -(\hat{\varepsilon} \cdot \hat{\mathbf{k}}) \sqrt{\frac{2}{\pi}} Z^{3/2} ik^{-i\frac{Z}{k}} \Gamma\left(1 - i\frac{Z}{k}\right) \times \left(\frac{2^{-1-i\frac{Z}{k}} Z(ik+Z)^{i\frac{Z}{k}} (5k^2+Z^2)}{k^2(k-iZ)(k+iZ)^2}\right) \quad (16)$$

Since the angular factor that modulates the transition amplitude is given by $(\hat{\varepsilon} \cdot \hat{\mathbf{k}}) = \cos\theta$, we could express

$$\frac{d\sigma^G}{d\Omega} = B^G \cos^2\theta. \quad (17)$$

The factor B^G does not depend on angular coordinates. In other words, it contains all the information on the electron emission probability as a function of the photon energy. In Fig. 1 we show B as a function of the emitted electron energy for the different models considered to represent the final wave function for the photoelectron.

Both forms (velocity and length) of the interaction Hamiltonian are presented. It could be seen that the plane wave model in velocity gauge overestimates the exact result given by the Coulomb wave function of Eq. (3) for electrons emitted with more than about 5.5 eV. The length gauge prediction

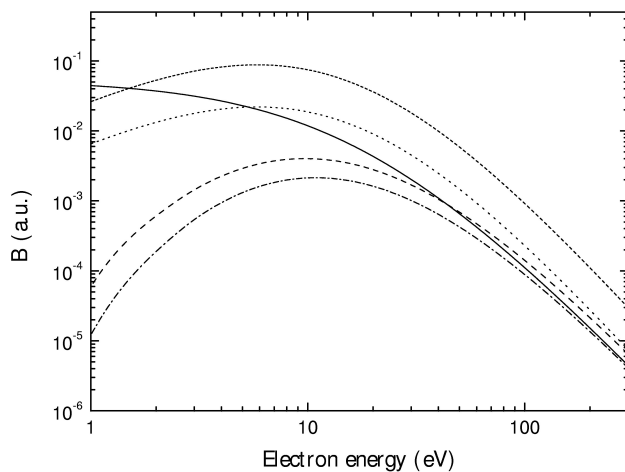


FIGURE 1. B as a function of the emitted electron energy for the different models considered. Theories are: solid-line: the Coulomb wave model; dot-dashed line: eikonal wave model in velocity gauge; dashed-line: eikonal wave model in length gauge; dotted-line: plane wave model in velocity gauge; short-dashed-line: plane wave model in length gauge.

for the same model, increases the overestimation by an exact factor 4, as already mentioned. The alternative approximated eikonal model, here suggested, shows a closer agreement between gauges compared to the plane wave model in the intermediate to high energy range. In this limit, the velocity gauge also tends to the exact result given by the Coulomb wave function as the electron energy increases. In the threshold region, both approximated models seem to fail to describe the zero energy resonance obtained with the Coulomb wave function. This explicitly shows that these approximated models could only be considered consistent in the intermediate to high energy limit.

In Fig. 2 we present the differential cross section for an electron emitted with $E = 250\text{eV}$. It could be seen that the eikonal model in both gauges is in better agreement with the Coulomb wave than the plane wave model in velocity gauge. The total cross section for the eikonal model could be easily obtained in both gauges by an angular integration of Eq. (17),

$$\sigma^{V,L} = \frac{16\pi^3 k}{3c\omega} B^{V,L}. \quad (18)$$

This total cross section represents the photoionization emission probability as a function of the photon energy.

As a conclusion, we have presented an alternative approximation in order to introduce the atomic photoelectric effect in quantum courses. We have represented the photoelectron with an asymptotically correct eikonal model. We have shown that this model reduces the gauges discrepancies typical of the plane wave approximation used so far. We have shown that in the intermediate to high energy limit this approximation in velocity gauge tends to the exact value given by the Coulomb wave. Furthermore, its implementation does not require further knowledge on special functions or integral representations. This kind of analysis, could be helpful to stimulate the student's intuition on the spurious effects inherent to the use of approximated wave functions in the description of physical processes.

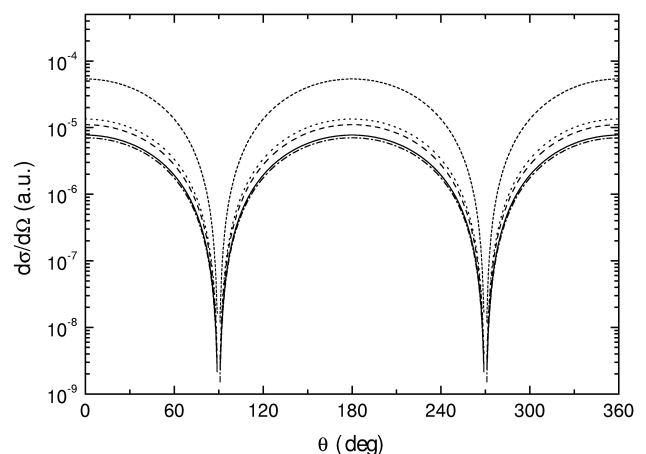


FIGURE 2. The angular distribution in atomic units for $E = 250\text{eV}$. Results obtained with the Coulomb wave function, the plane wave and the eikonal wave are shown in both length and velocity gauges. Theories as in Fig. 1.

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