Electron–hydrogen-atom collisions in the presence of a laser field: Born-Oppenheimer approximation

H. S. Brandi and Belita Koiller

Departamento de Física, Pontifícia Universidade Católica, Cx.P. 38071, Rio de Janeiro, RJ, Brazil

H. G. P. Lins de Barros

Centro Brasileiro de Pesquisas Físicas, 20000, Rio de Janeiro, RJ, Brazil
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The collision of an electron and a hydrogen atom in the presence of a laser field is studied within a previously proposed approximation (based on the space-translation approximation) for the bound states of the hydrogen atom. The Green's-function formalism is applied to derive an expression for the scattering amplitude associated to multiphoton processes. The Born-Oppenheimer approximation is obtained and numerical calculations are performed for the $1s \rightarrow 2s$ inelastic excitation. It is shown as expected that exchange effects are important only for scattering processes involving low-energy electrons.

I. INTRODUCTION

During the last decade a great interest has arisen in the study of the interaction of strong laser fields with matter. Physical processes such as plasma heating by electromagnetic radiation, gas breakdown, etc., are intrinsically related with the collision of electrons with atoms or molecules in the presence of an electromagnetic field (EMF).[1-12] It is well known that for strong EMF, multiphoton processes become relevant and an adequate theoretical treatment of this problem is necessary. Since usual perturbation techniques are not appropriate to treat multiphoton emission or absorption during the scattering process, the correct description of the bound states is one of the main difficulties.[1]

Concerning the scattering of electrons by hydrogen atoms there exist a few theoretical treatments using different approximations for the scattering amplitude such as first Born,[1-3,7-12] Glauber,[13] and close-coupling.[7-8,14] It is important to note that there exists particular interest in the study of collision processes involving low-energy electrons and in this case it is necessary to include the possibility of exchange between the incoming electrons and the atomic ones. The importance of corrections on the Born approximation is discussed by Choudhury[13] and Mittleman[14] for electron collisions with hydrogen in the presence of a moderate EMF.

An alternative approach to perturbation theory is to use an adequate unitary transformation modifying the Hamiltonian of the system, in a manner that the Green's-function formalism is easily applied and a consistent treatment of the bound states in an EMF can be carried out.[9-12]

In the present work we use the so-called space translation approximation (STA)[9,15] and the Green's-function method to study the electron scattering by a hydrogen atom in the presence of a EMF. We show that calculations are greatly simplified by introducing a symmetrized transformation. Exchange is considered within the Born-Oppenheimer approximation, and numerical calculations are performed for the specific case of $1s \rightarrow 2s$ excitation. This scheme was previously used, within a slightly different approach,[12] to obtain an expression for the scattering amplitude in the first Born approximation.

In Sec. II we present the theory for the scattering amplitudes associated with excitation processes, compare the present approach with that proposed in Ref. 12, and obtain the Born-Oppenheimer approximation. Section III is devoted to numerical calculations and conclusions.

II. THEORY

Let us consider the scattering of an electron by a hydrogen atom in the presence of an EMF. Considering the proton fixed at the origin, the Hamiltonian for this system is ($\hbar = c = 1$)

$$H = (1/2m)(\vec{p}_1 - e\vec{A})^2 + V(\vec{r}_1) + (1/2m)(\vec{p}_1 - e\vec{A})^2$$
$$+ V(\vec{r}_2) + W(\vec{r}_1, \vec{r}_2) , \tag{1}$$

where $\vec{A}$ is a vector potential of the EMF and

$$V(\vec{r}) = -e^2/|\vec{r}|, \quad W(\vec{r}_1, \vec{r}_2) = e^2/|\vec{r}_1 - \vec{r}_2|. \tag{2}$$

Note that in Eq. (1) the EMF is included only through its interactions with the particles. It is well known that the quantization of the EMF is of fundamental importance in field-resonant processes, and may not be neglected then. Therefore the present treatment is not expected to be valid when the atomic excitations are purely accounted for by the EMF. We do not attempt a solution like the rotating-wave approximation (resonant condition)

 1058

as done by Gersten and Mittleman[7] since here we are mainly interested in effects due to the collision process.

In the dipole approximation, $\vec{A}$ is time dependent and spatially homogeneous:

$$\vec{A}(t) = \vec{A}_0 \cos\omega t \tag{3}$$

so that the electric field is given by $\vec{\mathcal{E}}(t) = \vec{\mathcal{E}}_0 \sin\omega t = \vec{A}_0 \omega \sin\omega t$.

We introduce the space translation approximation[9,12,15]

$$T = \exp[i\vec{\alpha}(t)\cdot(\hat{p}_1 + \hat{p}_2) + 2i\eta(t)], \tag{4}$$

where

$$\vec{\alpha}(t) \equiv -\frac{e}{m}\int^t \vec{A}(t')\,dt' = -\frac{e\vec{A}_0}{m\omega}\sin\omega t \equiv -\vec{\alpha}_0\sin\omega t, \tag{5}$$

$$\eta(t) = \frac{e^2}{mc^2}\int^t A^2(t)\,dt', \tag{6}$$

and $\hat{p}_j$ is the momentum operator associated to the jth particle.

The transformed Schrödinger equation is

$$THT^\dagger T\psi = iT\frac{\partial\psi}{\partial t} \tag{7}$$

or

$$\left(\frac{p_1^2}{2m} + V(\vec{r}_1 + \vec{\alpha}(t)) + \frac{p_2^2}{2m}\right.$$
$$\left. + V(\vec{r}_2 + \vec{\alpha}(t)) + W(\vec{r}_1, \vec{r}_2)\right)\tilde{\phi} = i\frac{\partial\tilde{\phi}}{\partial t}, \tag{8}$$

with

$$\tilde{\phi} = T\psi. \tag{9}$$

In writing (8) we used the fact that

$$W(\vec{r}_1 + \vec{\alpha}, \vec{r}_2 + \vec{\alpha}) = W(\vec{r}_1, \vec{r}_2). \tag{10}$$

The asymptotic solution ($|\vec{r}_2| \to \infty$) of (10) is obtained from

$$\left(\frac{p_1^2}{2m} + V(\vec{r}_1 + \vec{\alpha}(t)) + \frac{p_2^2}{2m}\right)\Phi = i\frac{\partial\Phi}{\partial t}. \tag{11}$$

It is given by

$$\Phi_{\vec{k},n}(\vec{r}_1, \vec{r}_2, t) = \exp i[\vec{k}\cdot\vec{r}_2 - (k^2/2m)t]\varphi_n(\vec{r}_1, t), \tag{12}$$

where $\varphi_n(\vec{r}_1, t)$ is the solution of

$$\left(\frac{p_1^2}{2m} + V(\vec{r}_1 + \vec{\alpha}(t))\right)\varphi_n(\vec{r}_1, t) = i\frac{\partial\varphi_n(\vec{r}_1, t)}{\partial t}. \tag{13}$$

There exists no closed solution for Eq. (13), but $\varphi_n(\vec{r}_1, t)$ can be approximated in the STA by[12]

$$\varphi_n(\vec{r}, t) \simeq e^{-i\epsilon_n t}e^{-i\rho_n\cos\omega t}\varphi_n^{(0)}(\vec{r}_1), \tag{14}$$

$\varphi_n^{(0)}(\vec{r}_1)$ being an eigenfunction of the free hydrogen atom, and ρ_n determined from first-order degenerate perturbation theory.[12]

We must notice that the choice of the symmetrized unitary transformation Eq. (4) instead of the asymetrical form[12]

$$T = \exp[i\vec{\alpha}(t)\cdot\hat{p}_1 + i\eta(t)] \tag{15}$$

leads to a simpler asymptotical solution and to the two-body potential expressed by Eq. (10), meaning that such interaction is not modified by the EMF in the dipole approximation. In the development of the Green's-function formalism, calculations are greatly simplified by the use of Eqs. (10) and (12) instead of those resulting from Eq. (15). Following the same approach of Refs. 2, 3, and 12, we define the Green's function for the system as

$$G(\vec{r}_1, \vec{r}_2, t', \vec{r}_1, \vec{r}_2, t)$$
$$= \frac{i}{(2\pi)^3}\sum_{n'}\int d^3k\,\Phi^*_{\vec{k},n'}(\vec{r}_1', \vec{r}_2', t')$$
$$\times \Phi_{\vec{k},n'}(\vec{r}_1, \vec{r}_2, t)\theta(t - t') \tag{16}$$

and

$$\psi_{\vec{k}_0,n}(\vec{r}_1, \vec{r}_2, t) = \Phi_{\vec{k}_0,n}(\vec{r}_1, \vec{r}_2, t) - \int d^3r_1' d^3r_2' dt'\, G(\vec{r}_1', \vec{r}_2', t', \vec{r}_1, \vec{r}_2, t)\,[V_2(\vec{r}_2' + \vec{\alpha}(t')) + W(\vec{r}_1', \vec{r}_2')]\,\psi_{\vec{k}_0,n}(\vec{r}_1', \vec{r}_2', t'). \tag{17}$$

Following Ref. 12 it is trivial to obtain an expression for the scattering amplitude for the excitation of the hydrogen atom by electron impact in the presence of an EMF. It is

$$f^\nu_{\alpha,\alpha'}(\Omega) = -\frac{m\omega}{(2\pi)^2}\int_0^{2\pi/\omega} dt\,\langle\Phi_{\vec{k}(\nu),n'}|\,V(\vec{r}_2 + \vec{\alpha}(t))$$
$$+ W(\vec{r}_1, \vec{r}_2)\,|\Phi_{\vec{k}_0,n}\rangle, \tag{18}$$

where

$$\frac{k(\nu)^2}{2m} = \frac{k_0^2}{2m} + \epsilon_n - \epsilon_{n'} - \nu\omega, \tag{19}$$

$$\alpha = \{\vec{k}_0, n\}, \quad \alpha' = \{\vec{k}(\nu), n'\}.$$

$\vec{k}(\nu) = k(\nu)\hat{r}$, and the symbol $\langle\,||\,\rangle$ means integration over coordinates $\vec{r}_1$ and $\vec{r}_2$.

From Eq. (18), the Born-Oppenheimer approximation is readily obtained by approximating the wave function of the system by a properly symmetrized asymptotic solution, that is,

$$\psi_{\vec{k}_0,n}(\vec{r}_1, \vec{r}_2, t) = \Phi_{\vec{k}_0,n}(\vec{r}_1, \vec{r}_2, t) \pm \Phi_{\vec{k}_0,n}(\vec{r}_2, \vec{r}_1, t), \tag{20}$$

where the + (−) sign corresponds to singlet (triplet) states. As usual, we rewrite Eq. (18) as

$$f^\nu_{\alpha,\alpha'}(\Omega) = f^{d,\nu}_{\alpha,\alpha'}(\Omega) \pm g^\nu_{\alpha,\alpha'}(\Omega), \tag{21}$$

where the first term gives the direct contribution

(Born approximation) and the second one gives the exchange part of the scattering amplitude.

As previously obtained,[12] the scattering amplitude for inelastic processes in the Born approximation yields

$$f^{d,\nu}_{\alpha,\alpha'}(\Omega) = i^\nu J_\nu(\rho_{n'} - \rho_n) f^B_{\alpha,\alpha'}(\Omega) , \qquad (22)$$

where

$$g^\nu_{\alpha\alpha'}(\Omega) = \frac{m\omega}{(2\pi)^2} \int_0^{2\pi/\omega} dt \int d^3r_1 d^3r_2 \, \Phi^*_{\vec{k}(\nu),n'}(\vec{r}_1,\vec{r}_2,t)[V(\vec{r}_2 + \vec{\alpha}(t)) + W(\vec{r}_1,\vec{r}_2)]\Phi_{\vec{k}_0,n}(\vec{r}_2,\vec{r}_1,t)$$

$$= \frac{m\omega}{(2\pi)^2} \int_0^{2\pi/\omega} dt \exp\left[i\left(\frac{k_\nu^2}{2m} + \epsilon_{n'} - \frac{k_0^2}{2m} - \epsilon_n\right)t + i(\rho_{n'} - \rho_n)\cos\omega t\right]$$

$$\times \int d^3r_1 d^3r_2 e^{-i\vec{k}(\nu)\cdot\vec{r}_2} e^{i\vec{k}_0\cdot\vec{r}_1} \varphi^*_{n'}(\vec{r}_1)\varphi_n(\vec{r}_2)[V(\vec{r}_2 + \vec{\alpha}(t)) + W(\vec{r}_1,\vec{r}_2)]$$

$$\equiv \tilde{g}^\nu_{\alpha,\alpha'}(l) + \bar{g}^\nu_{\alpha,\alpha'}(\Omega). \qquad (24)$$

Using the relation

$$\exp[i(\rho_{n'} - \rho_n)\cos\omega t] = \sum_l (i)^l J_l(\rho_{n'} - \rho_n)e^{il\omega t}, \qquad (25)$$

the integration over t is immediately done for the two-particle potential $W(\vec{r}_1,\vec{r}_2)$ yielding

$$\bar{g}^\nu_{\alpha,\alpha'}(\Omega) = i^\nu J_\nu(\rho_{n'} - \rho_n)\bar{g}^B_{\alpha\alpha'}(\Omega), \qquad (26)$$

where

$$\bar{g}^B_{\alpha'\alpha}(\Omega) = \frac{m}{2\pi}\int d^3r_1 d^3r_2 e^{i\vec{k}_0\cdot\vec{r}_1}\phi^*_{n'}(\vec{r}_1)$$

$$\times W(\vec{r}_1,\vec{r}_2)e^{-i\vec{k}(\nu)\cdot\vec{r}_2}\phi_n(\vec{r}_2) \qquad (27)$$

has the same structure as the field-free corresponding term, and the analytical expression for this term is in the literature for several excitation processes.[16]

The calculation of the term corresponding to the modified Coulomb potential $V(\vec{r}_2 + \vec{\alpha}(t))$ is also trivial and yields

$$\tilde{g}^\nu_{\alpha\alpha'}(\Omega) = \frac{m}{(2\pi)^4}\phi_{n'}(-\vec{k}_0)$$

$$\int d^3K \exp[i\nu\chi(\vec{K})]$$

$$\times J_\nu[(\vec{K}\cdot\vec{\alpha}_0)^2 + (\rho_{n'} - \rho_n)^2]^{1/2}\tilde{V}(\vec{K})$$

$$\times \tilde{\phi}_n[-(\vec{k}(\nu) + \vec{K})] , \qquad (28)$$

where $\tilde{\phi}_{n'}$, $\tilde{\phi}_n$, and $\tilde{V}_2$ are the Fourier transforms of $\phi_{n'}$, ϕ_n, and V_2, respectively, and the phase is defined by the angle

$$\chi(\vec{K}) \equiv \frac{1}{2}\arccos\left(\frac{(\rho_{n'} - \rho_n)^2 - (\vec{K}\cdot\vec{\alpha}_0)^2}{(\rho_{n'} - \rho_n)^2 + (\vec{K}\cdot\vec{\alpha}_0)^2}\right). \qquad (29)$$

$$f^B_{\alpha,\alpha'}(\Omega) = \frac{m}{2\pi}\int d^3r_1 d^3r_2 e^{i[\vec{k}_0 - \vec{k}(\nu)]\cdot\vec{r}_2} W(\vec{r}_1,\vec{r}_2)$$

$$\times \varphi^*_{n'}(\vec{r}_1)\varphi_n(\vec{r}_1) \qquad (23)$$

has the same structure as for the field-free case.

An expression for the exchange part of the scattering amplitude is easily obtained using the techniques of Refs. 2, 3, and 12:

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{k(\nu)}{k_0}\left[\frac{1}{4}\left|f^{d,\nu}_{\alpha\alpha'}(\Omega) + g^\nu_{\alpha\alpha'}(\Omega)\right|^2\right.$$

$$\left. + \frac{3}{4}\left|f^{d,\nu}_{\alpha\alpha'}(\Omega) - g^\nu_{\alpha\alpha'}(\Omega)\right|^2\right]. \qquad (30)$$

III. RESULTS AND CONCLUSIONS

From expression (22) and (26), we see that the direct term in the scattering amplitude and the contribution to the exchange due to the two-particle part of the potential, $W(\vec{r}_1,\vec{r}_2)$, are simply related to the corresponding field-free expressions. The basic effect of the EMF is to modulate them by the factor $i^\nu J_\nu(\rho_{n'} - \rho_n)$. The other exchange contribution, Eq. (28), is not easily evaluated from
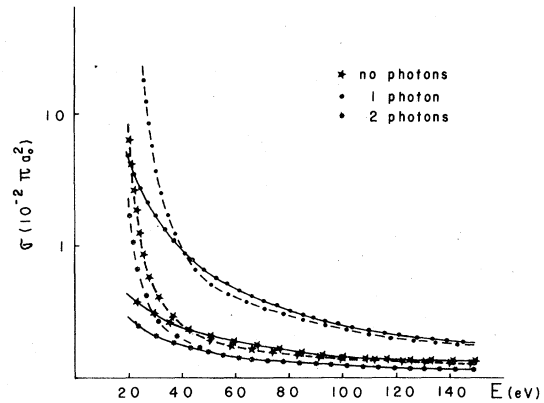

FIG. 1. Total cross section as a function of the collision energy for multiphoton processes. Field strength, $\mathcal{E}_0 = 5 \times 10^6$ V/cm; frequency, $\omega = 1.78$ eV. Full curves, Born approximation; dashed curves, Born-Oppenheimer approximation.

the corresponding expression in the zero-field case, however, its contribution may be neglected for the region of collision energies we are interested in here, namely, $E_0 = k_0^2/2m \geqslant 2Ry$. Notice that in this region the dependence in the incident momentum is dominated by $\tilde{\phi}_{n'}(-\vec{k}_0)$. For the $2s$ excitation, $\tilde{\phi}_{2s}(-\vec{k}_0) \sim 1/k_0^6$ and for other excited states, the dependence in $1/k_0$ is of even higher order. Still in this region, expression (27) behaves as $1/k_0^2$, therefore this is the only term to be considered here and no distinction appears between post and prior interactions. In the field-free case, it can be shown that in the high collision energy region the nuclear potential V does not contribute to the exchange scattering amplitude.[17]

The total cross section is obtained by angular integration of Eq. (30); when exchange effects are neglected, we get the total Born cross section. In Fig. 1, we compare the calculated total cross section for the $1s \rightarrow 2s$ excitation process as a function of the incoming electron energy for multiphoton processes in the Born and Born-Oppenheimer approximation. These results correspond to typical values of a ruby laser, i.e., $\omega = 1.78$ eV and EMF strength $\mathcal{E}_0 = 5 \times 10^6$ V/cm, yielding $\Delta\rho = \rho_{2s} - \rho_{1s} \sim 1.74$; this is within the region of validity of first-order perturbation theory developed in the STA approximation[12] $(\Delta\rho \ll Ry/\hbar\omega)$.

Notice that, for a given number of photons, the behavior of the cross section as a function of the collision energy is similar to the field-free case: the main effect of the field is to modulate the corresponding scattering amplitude by a Bessel function. Therefore, as usual, the effect of exchange is dominant in the low-energy region, and the Born approximation describes the high-energy region adequately. For the ruby laser parameters used here, the relevant processes are those involving up to two photons, the one-photon process being always the most probable one.

We have also performed calculations for a field strength $\mathcal{E}_0 = 10^7$ V/cm; for this laser intensity two- and three-photon processes are the most probable. Although in this case, the use of first-order perturbation theory for the hydrogen-atom bound states is not fully justified, there is clear indication that for high field strengths and also for low frequencies, processes involving a large number of photons tend to occur with higher probabilities.

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