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Fivefold differential cross sections for the ionization of aligned hydrogen molecule by electron and positron impact

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ABSTRACT

We report fivefold differential cross section (5DCS) for the ionization of aligned hydrogen molecule by electron and positron impact in coplanar geometry. The calculations have been performed for an incident energy of 200 eV and ejection energies of (3.5 ± 2.5) and (16 ± 4) eV. The present calculations are based on the eikonal approximation due to Glauber, and the BBK approximation. We have included the effect of post collision interaction (PCI) in the Glauber approximation classically. A comparison is made of the present calculations with the results of other theoretical methods and the recent experiment of Senftleben et al. [28]. The present theoretical models predict that the 5DCS is maximum when the intermolecular axis is aligned along the incident beam direction. The binary to recoil peak ratios predicted by the Glauber approximation with PCI (GA-PCI) are in reasonably good agreement with the experiment. The positions of the binary peaks predicted by the BBK approximation are also in good agreement with the experiment. The positron-impact ionization cross sections obtained in the BBK and GA-PCI methods are found to be higher than the electron-impact cross sections in the binary region while the converse is true for the recoil regime. In case of positron impact, the binary peaks predicted by both the GA-PCI and BBK models shifted away from the direction of momentum transfer, and showed a trend which is opposite to the case of electron impact ionization.

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1. Introduction

Over the past two decades, the field of electron impact single ionization of one or two electron atomic target has reached a degree of maturity. Consequently, an increasing interest has grown in the study of ionization of more complex systems i.e., target as a molecule which is important for many fields such as radiation therapy, planetary atmospheres, near-stellar clouds and reactive plasmas. The fully differential cross section (FDCS) contains the complete information of an ionization process. Recently, attempts have been made both experimentally [1–4] and theoretically [3,5–17] to get the FDCS for the ionization of simple diatomic hydrogen molecule by charged particle impact. In the case of diatomic molecules, the two-center geometry of the nuclear field can give rise to interference effects. Cohen and Fano [18] were the first to predict these effects long ago in the ionization of H_2 by photon impact. Subsequently, these interference effects were also predicted by Stia et al. [19] for electron impact ionization of hydrogen molecule. But most of these attempts are devoted to non-aligned molecules. With the very recent experimental development of the fixed alignment of H_2 molecule [20–23] there has been a resurgence of theoretical study of FDCS using different models [24–27].

FDCS for the single ionization of an oriented dipolar molecule (5DCS) can be expressed as $\frac{d^5\sigma}{d\hat{\mathbf{k}}_1 d\hat{\mathbf{k}}_2 dE_2 d\phi_m d\theta_m}$, where $d\hat{\mathbf{k}}_1$ and $d\hat{\mathbf{k}}_2$ denote, respectively, elements of solid angles of the scattered projectile and the ejected electron, dE_2 represents the energy interval of the ejected electron and θ_m and ϕ_m fix the molecular alignment. Very recently, 5DCS for 200 eV electron impact ionization of hydrogen molecule has been explored experimentally as a function of molecular alignment by Senftleben et al. [23,28]. They derived the alignment of the internuclear axis from the fragmentation of the residual H_2^+ ion which was produced as a result of the ionizing collision. In fact, Senftleben et al. [23,28] considered the ground-state dissociation to study the alignment dependence of ionization into the electronic ground state of H_2^+. Moreover, they have compared their observations with the molecular three-body distorted wave model (M3DW) and the three Coulomb wave function approach. This three Coulomb wave function approach uses

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helium as a target wave function with an interference factor [19]. From now onwards, we will mention this approach as 3C–He approximation. In M3DW model, final-state Coulomb interaction between the projectile and screened nuclear charge, the Coulomb interaction between the ejected-electron and screened nuclear charge and the Coulomb interaction between projectile and ejected-electron are contained to all orders of perturbation theory. For the initial state of the above model the Coulomb interaction between the projectile and the screened nuclear charge for a neutral target is contained to all orders of perturbation theory while the initial-state non spherical projectile-active-electron interaction is the first order interaction. Senftleben et al. [23,28] have reported that M3DW reproduces most of the experimental results, although discrepancies remain. They have also mentioned that 3C–He failed to reproduce experimental FDCS at the ejection energy of (3.5 ± 2.5) eV and the scattering angle of $(16 \pm 4)^\circ$.

In the present paper we have concentrated on the calculation of the 5DCS for the ionization of hydrogen molecule by electron and positron impact. We have compared the electron impact 5DCS with the M3DW [28] approximation, the 3C–He [23] approach and experimental data [23,28]. In view of the recent demonstration of the feasibility of kinematically complete experiments for positron impact ionization of atoms using a reaction microscope [29], we have also studied 5DCS for aligned H_2 molecule. In this work we have applied the eikonal approximation due to Glauber (GA) [30] and the BBK approximation [31]. To the best of our knowledge the GA model is applied for the first time to calculate 5DCS using an interference factor. In the BBK amplitude, we have used atomic hydrogen wave function for the target and then multiply it with an interference factor given by Stia et al. [19] to obtain 5DCS. On the other hand, the Glauber approximation (GA) contains helium wave function as a target and the same interference factor. In the entrance channel, Glauber amplitude contains projectile–target correlation. In fact Glauber amplitude contains terms of all orders in V (i.e., the sum of the projectile–core and projectile–electron interactions) in its phase in an approximate way. In the exit channel we have introduced the post collision interaction (PCI) effect, i.e., projectile–ejected electron correlation in the GA (GA-PCI) following the semi-classical method used by Klar et al.[32]. On the other hand, BBK method uses an asymptotically exact scattering wave function which involves three appropriate confluent hypergeometric functions depending on the three pairwise inter-particle Coulomb interactions.

The GA has been successfully applied to a wide variety of atomic collisions [33–38]. Recently, Dey and Roy [38] applied the GA to study the role of projectile interactions in triply differential cross sections (TDCS) for excitation–ionization of helium and found that Glauber results are in reasonably good agreement with experiment for small scattering angles. The BBK method is also successfully applied to the various ionization processes [31,39–41]. In 1989, Brauner et al. [31] have derived and applied the BBK model to calculate TDCS for ionization of hydrogen atoms by electrons and positrons and found excellent agreement with measurements at electron impact energies greater than 150 eV. Since then, the BBK wave function has been used by different authors to calculate fully and partly differential cross sections for the ionization of different target atoms by different charged particles and found to be reasonably successful to predict the measured data.

2. Theory

The Glauber approximation has been described elsewhere [30,42,43], so only a brief outline will be presented here. The Glauber amplitude for the ionization of helium by an incident particle of charge z_P is given by (atomic units are used throughout, unless otherwise indicated) [35,44]

$$F(\mathbf{q},\mathbf{k_2}) = \frac{ik}{2\pi}\int d\mathbf{b}d\mathbf{r_1}d\mathbf{r_2}\phi_f^*(\mathbf{r_1},\mathbf{r_2})\Gamma(\mathbf{b},\mathbf{r_1},\mathbf{r_2})\phi_i(\mathbf{r_1},\mathbf{r_2})\exp(i\mathbf{q}.\mathbf{b}), \tag{1}$$

where

$$\Gamma(\mathbf{b},\mathbf{r_1},\mathbf{r_2}) = 1 - \left(\frac{|\mathbf{b}-\mathbf{s_1}|}{b}\right)^{2i\eta}\left(\frac{|\mathbf{b}-\mathbf{s_2}|}{b}\right)^{2i\eta}, \tag{2}$$

$\mathbf{q} = \mathbf{k} - \mathbf{k_1}$ and $\eta = -(\mu_P z_P/k)$. Here $\mathbf{k}$, $\mathbf{k_1}$ and $\mathbf{k_2}$ are the momenta of the incident particle, scattered projectile and ejected electron, respectively. μ_P represents the reduced mass of the system. $\mathbf{b}$, $\mathbf{s_1}$ and $\mathbf{s_2}$ are the respective projections of the position vectors of the incident particles and the two bound electrons onto the plane perpendicular to the direction of the Glauber path integration. In Eq. (1), $\mathbf{q}$, $\mathbf{b}$, $\mathbf{s_1}$ and $\mathbf{s_2}$ are coplanar. $\phi_i(\mathbf{r_1},\mathbf{r_2})$ and $\phi_f(\mathbf{r_1},\mathbf{r_2})$ represent the wave functions of the initial and the final states of the target, respectively. For the initial state of helium, we have chosen the analytical fit to the Hartree–Fock wavefunction given by Byron and Joachain [45]:

$$\phi_i(\mathbf{r_1},\mathbf{r_2}) = U(\mathbf{r_1})U(\mathbf{r_2}), \tag{3}$$

where

$$U(\mathbf{r}) = (4\pi)^{-1/2}(Ae^{-ar} + Be^{-br})$$
$$A = 2.60505 \quad B = 2.08144 \quad a = 1.41 \quad b = 2.61.$$

For the final-state target wave function we have used a symmetrised product of the He^+ ground state wavefunction for the bound electron times a Coulomb wave $\phi_{\mathbf{k_2}}$ orthogonalised to the ground state orbital

$$\phi_f(\mathbf{r_1},\mathbf{r_2}) = 2^{-1/2}[\phi_{\mathbf{k_2}}(\mathbf{r_1})v(\mathbf{r_2}) + v(\mathbf{r_1})\phi_{\mathbf{k_2}}(\mathbf{r_2})], \tag{4}$$

where

$$v(\mathbf{r}) = (\lambda')^{3/2}\pi^{-1/2}e^{-\lambda' r}$$
$$\phi_{\mathbf{k_2}}(\mathbf{r}) = \chi^-_{\mathbf{k_2}}(\mathbf{r}) - \langle U(\mathbf{r}')|\chi_{\mathbf{k_2}}(\mathbf{r}')\rangle U(\mathbf{r})$$
$$\chi^-_{\mathbf{k_2}}(\mathbf{r}) = (2\pi)^{-3/2}exp\left(\frac{1}{2}\gamma\pi\right)\Gamma(1+i\gamma)exp(i\mathbf{k_2}.\mathbf{r})_1F_1(-i\gamma,1,-i(k_2r+\mathbf{k_2}.\mathbf{r}))$$
$$\gamma = 1/k_2 \quad \lambda' = 2.$$

The triply differential cross section is given by

$$\frac{d^3\sigma}{d\hat{\mathbf{k}}_1 d\hat{\mathbf{k}}_2 dE_2} = \frac{k_1k_2}{k}|F(\mathbf{q},\mathbf{k_2})|^2, \tag{5}$$

where $d\hat{\mathbf{k}}_1$ and $d\hat{\mathbf{k}}_2$ denote, respectively, elements of solid angles of the scattered projectile and the ejected electron and dE_2 represents the energy interval of the ejected electron. We have introduced the two-centre picture developed by Stia et al. [19] that predicts the interference effects. Hereby, 5DCS are obtained by multiplying TDCS with the interference factor

$$I = 2[1 + \cos((\mathbf{q} - \mathbf{k_2}).\mathbf{R})], \tag{6}$$

depending on the molecular alignment $\mathbf{R}$.

Popov and coworkers [46,47] were the first to introduce a semi-classical method for the treatment of PCI in (e,2e) processes for an explanation of correct positions of binary and recoil peaks observed in triply differential cross sections. This method which described the shifts of paths of the outgoing electrons in (e,2e) experiments due to the coulomb interactions in the final state showed agreement with experiment. Later on, Popov and Erokhin [48] applied this method to (e^+, e^+e^-) process as a development of the (e,2e) method. Subsequently, Klar and coworkers [32,49] extended this method to include both trajectory and energy shifts as follows:

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