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Ionization of atomic hydrogen by electrons: the role of the contributions of the pseudo-states in the second Born approximation

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Abstract
The second Born approximation is often used, particularly when we study double processes such as the ionization–excitation and the double ionization of atoms and molecules by charged particles. But when we apply this approximation, it needs the knowledge of all excited states of the target. In this study, we apply the second Born approximation by using 294 excited and pseudo-states for the ionization of atomic hydrogen by electrons. We compare the results of our model with those given by other models and to all experiments performed with an incident energy of 250 eV. We show that our new version of the second Born approximation gives better agreement than previous versions even for high values of the energy of the ejected electrons (50 eV).

(Some figures may appear in colour only in the online journal)

1. Introduction

It has been said in the literature that the ionization of atomic hydrogen by electrons can be considered as a numerically solved problem [1]. Various non-perturbative methods such as exterior complex scaling [1], convergent close coupling (CCC) [2], *R*-matrix theory [3, 4] and time-dependent close coupling [5] had demonstrated to be efficient in solving that problem. However, mostly due to limitations in the computational resources, it is necessary to apply approximated and also perturbative approaches such as the Born approximation when considering the ionization of many-electron atoms and molecules. For that reason, it is interesting to explore the capability of the Born series at different orders. The first Born order has been a great tool to obtain a first approach to many different problems and process in the collision theory. There are, however, doubts about the applicability of the second Born order when it comes from a Lippmann–Schwinger equation involving a long-range potential. There are doubts also about the class and the amount of intermediate states to be used in its calculation. In a previous paper, one of the authors showed that the Born series for the two-body Coulomb potential converge even if the interaction is of long range [6]. One of the aims of this contribution is to study the second order in the Born series for the simplest three-body problem: the ionization of hydrogen by electron impact. For this purpose, we perform a careful study of the convergence and show that it converges and also leads to very good results in comparison with other approximated models and also with *ab initio* methods.

Recently, Dal Cappello *et al* [7] have shown that the second Born approximation works very well for the ionization of atomic hydrogen for an incident energy of 250 eV and an energy of 5 eV for the ejected electron but *completely*

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fails for higher values of the energy of the ejected electrons (50 eV). This result was also found by Pathak and Srivastava [8] who only used the closure approximation. In our studies, the incident electron is described by a plane wave. It has been established that this approach works well; Chen *et al* [9] and Jones and Madison [10] have shown that a distortion of the incident electron is actually unimportant. In a previous study, Dal Cappello *et al* [7] used a first basis of intermediate states including 100 *exact* discrete states (the angular momentum varying from $L = 0$ to $L = 10$), two other bases including 31 [11] and 32 discrete and pseudo-states [12], and also the closure approximation. However, the results were far from being convincing for the case of higher values of the energy of the ejected electron. In this contribution, we continue with the study of the problem and decide to increase the size of our basis by now including 294 excited and pseudo-continuum states. In order to see the importance of the contribution of the pseudo-continuum states, 134 pseudo-states have been taken into account. We limit the value of the angular momentum to $L = 6$ because Dal Cappello *et al* [7] showed that the contributions of higher values of L give negligible contributions. Then we compare the results of our model to all experimental data for an incident energy of 250 eV.

On the experimental side, Weigold *et al* [13] have performed a set of experiments at 250 eV with a high value for the ejected electron (50 eV) leading to relative results. Lohmann *et al* [14] have made measurements with the same incident energy and provided relative results but with low energy of the ejected electron (5, 10 and 14 eV). Later, Ehrhardt *et al* [15, 16] reported absolute measurements (250 eV for the incident and 5 eV for the ejected). Jones and Madison [17] found very good agreement between their perturbative BBK approach [18] and the non-perturbative CCC theory [19, 20] and recommended us to multiply the absolute data of Ehrhardt *et al* [15, 16] by a factor of 0.88. Thus, some doubts arise from the absolute data. Then assuming that the BBK results can be considered as a good check for other perturbative calculations, we decide to compare our second Born results with this theory and with all the available sets of relative experiments at 250 eV.

We also study in greater detail the closure approximation. We have known for a long time that the closure approximation works very well for low energy for the ejected electrons [7, 9, 21, 22], but fails for higher energies [7, 8]. We decide to investigate this issue mostly in the highest possible energy regime 50 eV of the ejected electron. When applying the closure approximation, a parameter must be chosen [21]. Byron *et al* [22], Dal Cappello *et al* [7] and Sahlaoui and Bouamoud [23] have shown that the second Born approximation calculated with the closure approximation does not depend strongly on this parameter when the energy of the ejected electrons is low (5 eV). In our study, the energy can be fixed to 50 eV and we investigate the closure approximation with 40 different values of the parameter.

Atomic units are used throughout unless stated otherwise.

2. Theory

The ionization of atomic hydrogen by electrons is schematized as

$$e^- + \mathrm{H} \rightarrow 2\,e^- + \mathrm{H}^+. \tag{1}$$

If the scattered and ejected electrons are detected in coincidence, we have the well-known (e, 2e) experiments. In this case, the triple differential cross section (TDCS) is written in the Born approximation as

$$\sigma^{(3)} = \frac{d^3\sigma}{d\Omega_e\, d\Omega_s\, dE_e} = \frac{k_s k_e}{k_i}|f_{B1} + f_{B2}|^2, \tag{2}$$

where $\vec{k}_i$, $\vec{k}_s$ and $\vec{k}_e$ denote, respectively, the momenta of the incident, scattered and ejected electrons. The solid angles of the scattered and ejected electrons are $d\Omega_s$ and $d\Omega_e$. The energy interval of the ejected electron is represented by dE_e.

The conservation of the energy is written as

$$\frac{k_i^2}{2} + E_i = \frac{k_s^2}{2} + \frac{k_e^2}{2}, \tag{3}$$

where E_i is the energy of the initial state ($E_i = -0.5$ au).

The term f_{B1} is given by

$$f_{B1} = -\frac{1}{2\pi}\langle \exp(i\vec{k}_s\cdot\vec{r}_0)\Psi_C^-(\vec{k}_e,\vec{r}_1)|V(\vec{r}_0,\vec{r}_1)| \exp(i\vec{k}_i\cdot\vec{r}_0)\Phi_i(\vec{r}_1)\rangle, \tag{4}$$

where $V(\vec{r}_0,\vec{r}_1)$ represents the Coulomb interaction between the incident electron and the target, such as

$$V(\vec{r}_0,\vec{r}_1) = \frac{1}{r_{01}} - \frac{1}{r_0}. \tag{5}$$

The terms $\Phi_i(\vec{r}_1)$ and $\Psi_C^-(\vec{k}_e,\vec{r}_1)$ represent, respectively, the initial and final wavefunctions of atomic hydrogen.

The *exact* wavefunction for the continuum state of atomic hydrogen can be written as

$$\Psi_C^-(\vec{k}_e,\vec{r}_1) = \frac{1}{(2\pi)^{3/2}}\exp(i\vec{k}_e\cdot\vec{r}_1)\Gamma(1-i\alpha) \times \exp\left(-\frac{\pi}{2}\alpha\right)\,{}_1F_1(i\alpha, 1, -i(\vec{k}_e\cdot\vec{r}_1 + k_e r_1)),$$

and

$$\alpha = -Z/k_e, \quad Z = 1.$$

After the integration on $\vec{r}_0$, we obtain

$$f_{B1} = -\frac{2}{K^2}\langle\Psi_C^-(\vec{k}_e,\vec{r}_1)|\exp(i\vec{K}\cdot\vec{r}_1) - 1|\Phi_i(\vec{r}_1)\rangle. \tag{6}$$

The momentum transfer is defined by $\vec{K} = \vec{k}_i - \vec{k}_s$.

The term f_{B2} is given by

$$f_{B2} = \frac{1}{8\pi^4}\sum_n \int \frac{d\vec{q}}{q^2 - k_n^2 - i\varepsilon} \times\langle \exp(i\vec{k}_s\cdot\vec{r}_0)\Psi_C^-(\vec{k}_e,\vec{r}_1)|V|\exp(i\vec{q}\cdot\vec{r}_0)\Phi_n(\vec{r}_1)\rangle, \times\langle \exp(i\vec{q}\cdot\vec{r}_0)\Phi_n(\vec{r}_1)|V|\exp(i\vec{k}_i\cdot\vec{r}_0)\Phi_i(\vec{r}_1)\rangle \tag{7}$$

with $\varepsilon \rightarrow 0^+$, and the term $\Phi_n(\vec{r}_1)$ represents here the intermediate state (initial state, excited state or continuum state). The value of k_n is given by

$$\frac{k_n^2}{2} = \frac{k_i^2}{2} - (E_n - E_i). \tag{8}$$

After the integration on $\vec{r}_0$, we obtain

$$f_{B2} = \frac{2}{\pi^2}\sum_n \int \frac{d\vec{q}}{q^2 - k_n^2 - i\varepsilon}\frac{1}{K_i^2 K_f^2} \times \langle \Psi_C^-(\vec{k}_e, \vec{r}_1)|\exp(i\vec{K}_f\cdot\vec{r}_1) - 1|\Phi_n(\vec{r}_1)\rangle \times \langle \Phi_n(\vec{r}_1)|\exp(i\vec{K}_i\cdot\vec{r}_1) - 1|\Phi_i(\vec{r}_1)\rangle, \quad (9)$$

where $\vec{K}_i = \vec{k}_i - \vec{q}$ and $\vec{K}_f = \vec{q} - \vec{k}_s$, $\vec{K} = \vec{K}_i + \vec{K}_f$.

We have several methods to perform the last integration on $\vec{q}$ [23–25]. The general integral is

$$I = \int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon} W(q, \theta_q, \varphi_q) \quad (10)$$

with $\varepsilon \to 0^+$, and can be written as

$$I = P\int \frac{d\vec{q}}{q^2 - p^2} W(q, \theta_q, \varphi_q) + \frac{i\pi}{2} p \int d\hat{q} W(p, \theta_q, \varphi_q), \quad (11)$$

where P stands for the principal value.

We now adopt a subtraction procedure to perform the integral I:

$$I = \left(P\int_0^\infty \frac{\exp(-\alpha(q-p)^2)q^2 dq}{q^2 - p^2} + \frac{i\pi p}{2}\right) \times \int W(p,\theta_q, \varphi_q)\, d\hat{q} + \int \frac{W(q, \theta_q, \varphi_q) - \exp(-\alpha(q-p)^2) W(p, \theta_q, \varphi_q)}{q^2 - p^2} d\vec{q}. \quad (12)$$

We have introduced a parameter α in (12) and an exponential factor [25].

The principal value can be calculated numerically [23]:

$$P\int_0^\infty \frac{\exp(-\alpha(q-p)^2)q^2 dq}{q^2 - p^2} = \int_{-p}^\infty \exp(-\alpha z^2)\, dz + \frac{p}{2}\int_p^\infty \frac{\exp(-\alpha z^2)}{z} dz - \frac{p}{2}\int_{-p}^\infty \frac{\exp(-\alpha z^2)}{(z+2p)} dz. \quad (13)$$

The intermediate states correspond to the hydrogen atom wavefunctions. Analytic expressions are available for both bound and continuum states. However, the inclusion of all of them will require the integration over the whole continuum spectra and that makes the problem intractable. One way of avoiding this difficulty is using approximated states obtained by diagonalizing the hydrogen Hamiltonian H in an L^2 basis. In this way, a good representation of the bound and pseudo-continuum approximations for the continuum could be obtained. All the integrals over the *intermediate states* appearing in equation (9) are performed *analytically* and the integrations are performed assuming a particular form for $\Phi_n^{L,m}$, that is, a linear combination of $r^n e^{-ar}$. The analytic calculations allow us to have as maximum $n = 10$. For this reason, we used a particular form to calculate the hydrogen eigenstates by diagonalization. For the excited and pseudo-states corresponding to $L = 0$, we used

$$\Phi_n^{0,0}(\vec{r}) = Y_0^0 e^{-0.6r}\left(a_1^0 + a_2^0 r + a_3^0 r^2 + a_4^0 r^3 + a_5^0 r^4 + a_6^0 r^5\right), \quad (14)$$

and for $L = 1$ to $L = 6$,

$$\Phi_n^{L,m}(\vec{r}) = \left(r^L \sum_{i=1}^{i=21} a_i^L e^{-\alpha_i r}\right) Y_L^m. \quad (15)$$

All the parameters appearing in the exponential functions in equations (14) and (15) were fixed in such a way that the exact energy for the lowest energy level for each L was obtained. All the a_i^L parameters were determined by solving (H–E) $\Phi_n^{L,m} = 0$ variationally. The α_i parameters were also fixed in such a way that an equal number of bound (negative energy) and pseudo-continuum states (positive energy) were obtained after diagonalization.

Using the closure approximation, we have the following $\bar{f}_{B2}$ term:

$$\bar{f}_{B2} = \frac{2}{\pi^2}\int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon}\frac{1}{K_i^2 K_f^2} \langle \Psi_C^-(\vec{k}_e, \vec{r}_1)|\exp(i\vec{K}\cdot\vec{r}_1) - \exp(i\vec{K}_f\cdot\vec{r}_1) - \exp(i\vec{K}_i\cdot\vec{r}_1) + 1|\Phi_i(\vec{r}_1)\rangle, \quad (16)$$

with $\varepsilon \to 0^+$ and

$$\frac{p^2}{2} = \frac{k_i^2}{2} - \bar{w}, \quad (17)$$

$\bar{w}$ being the average excitation energy.

We also compute the well-known BBK model [18] where

$$\sigma^{(3)} = \frac{d^3\sigma}{d\Omega_e d\Omega_s dE_e} = \frac{k_s k_e}{k_i}|f|^2, \quad (18)$$

and

$$f = -\frac{1}{2\pi}\langle \Psi_C^-(\vec{k}_s, \vec{r}_0)\Psi_C^-(\vec{k}_e, \vec{r}_1) C(\alpha_{01}, \vec{k}_{01}, \vec{r}_{01})|V(\vec{r}_0, \vec{r}_1)| \exp(i\vec{k}_i\cdot\vec{r}_0)\Phi_i(\vec{r}_1)\rangle, \quad (19)$$

where

$$\vec{k}_{01} = \frac{1}{2}(\vec{k}_s - \vec{k}_e), \quad \alpha_{01} = -\frac{1}{2k_{01}}$$

and

$$C(\alpha_{01}, \vec{k}_{01}, \vec{r}_{01}) = \exp\left(-\frac{\pi}{4k_{01}}\right)\Gamma\left(1 - \frac{i}{2k_{01}}\right) {}_1F_1\left(\frac{i}{2k_{01}}, 1, -i(\vec{k}_{01}\cdot\vec{r}_{01} + k_{01}r_{01})\right),$$

with and without exchange, and find the results of Brauner *et al* [18] for the experiments performed by Ehrhardt *et al* [15, 16].

3. Results and discussion

We investigate the ionization of atomic hydrogen by electrons by comparing the results of our second Born approximation with all the data of Lohmann *et al* [14] (small values of the energy of the ejected electrons) and those of Weigold *et al* [13] (higher values of the energy of the ejected electrons).

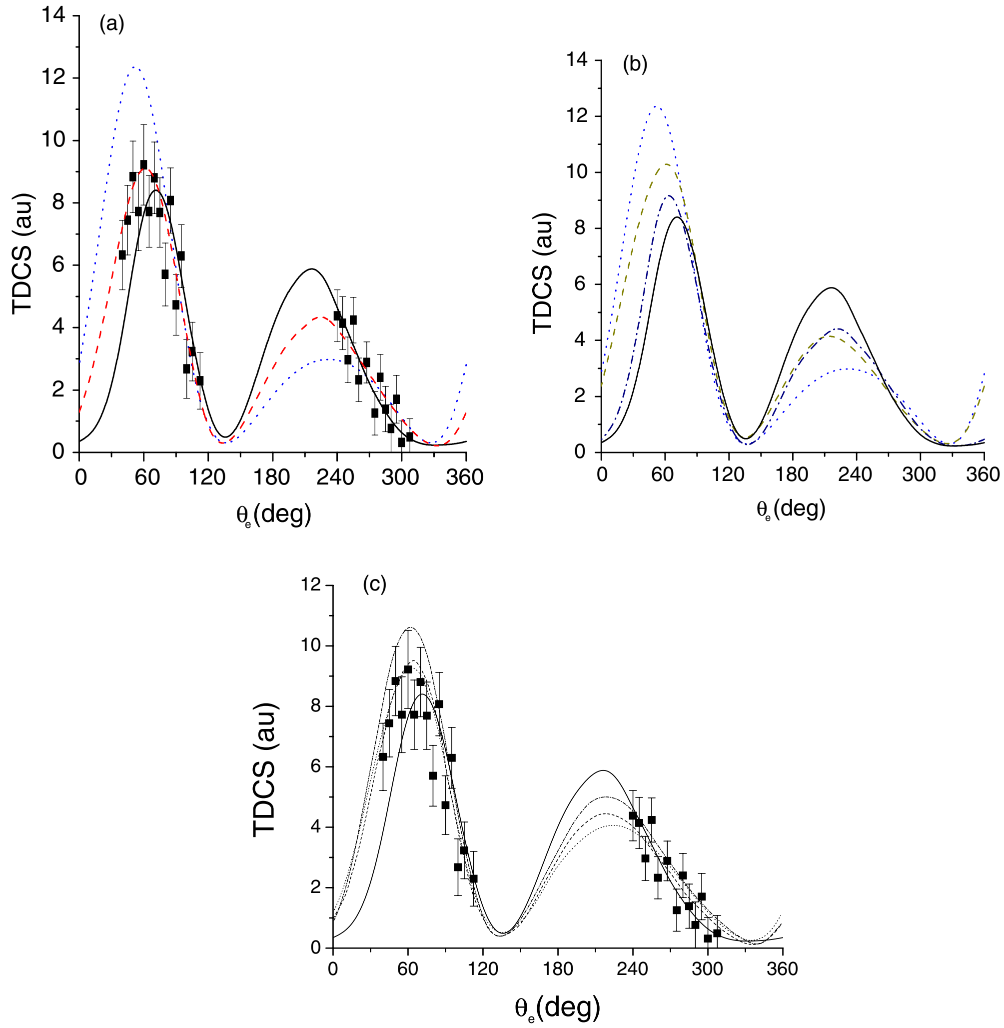

Figure 1. (a) Triple differential cross sections (TDCS) for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including only the contribution of the excited states by a dashed line, those of the second Born approximation calculated by including only the continuum states by a dash–dotted line and those of the second Born approximation calculated by including all the contributions by a full curve. (c) Same as (a) but the results of the second Born approximation calculated by including all the contributions are represented by a full curve, those of the CDW-EIS by a dotted line, those of the CCC by a dashed line, those of the DWB2 by a dash–dotted line and experiments by squares.

3.1. Small ejected energies

Figure 1 shows a comparison between our second Born approximation (with our new basis including 294 excited and pseudo-states), the BBK model, the CDW-EIS model [12], the CCC model [19, 20], the DWB2 model [11] and the data of Lohmann *et al* [14] for an incident energy of 250 eV, an ejected energy of 5 eV and a scattering angle of 3°. We notice good agreement (figure 1(a)) between experiments, the BBK model and our second Born approximation. But some small differences appear: the shift of the binary peak increases and the magnitude of the recoil lobe increases too when applying the second Born approximation. It is difficult to say if one model is better than the other. In figure 1(b), the contributions of all excited states and those of all pseudo-states have been drawn. It is clear that the contribution of the pseudo-continuum states is important. It is interesting to remember that the BBK model gives results close to those of the CDW-EIS model [12] and to the CCC approach [19, 20] (and to the absolute measurements of Ehrhardt *et al* [15, 16] with the factor of 0.88). It means that the second Born approximation calculated with the basis of Callaway [12] underestimates the recoil peak and overestimates the binary peak as the basis used by Chen *et al* [9]. These authors [9] used a pseudo-state basis set including ten s-states, nine p-states, eight d-states and seven f-states. Finally, the use of our new basis improves the agreement with the CDW-EIS [10] and the CCC [19, 20] approaches (figure 1(c)).

Figure 2 presents the same kinematical situation except for the value of the scattering angle (5°). We also observe good agreement between the BBK, our second Born approximation

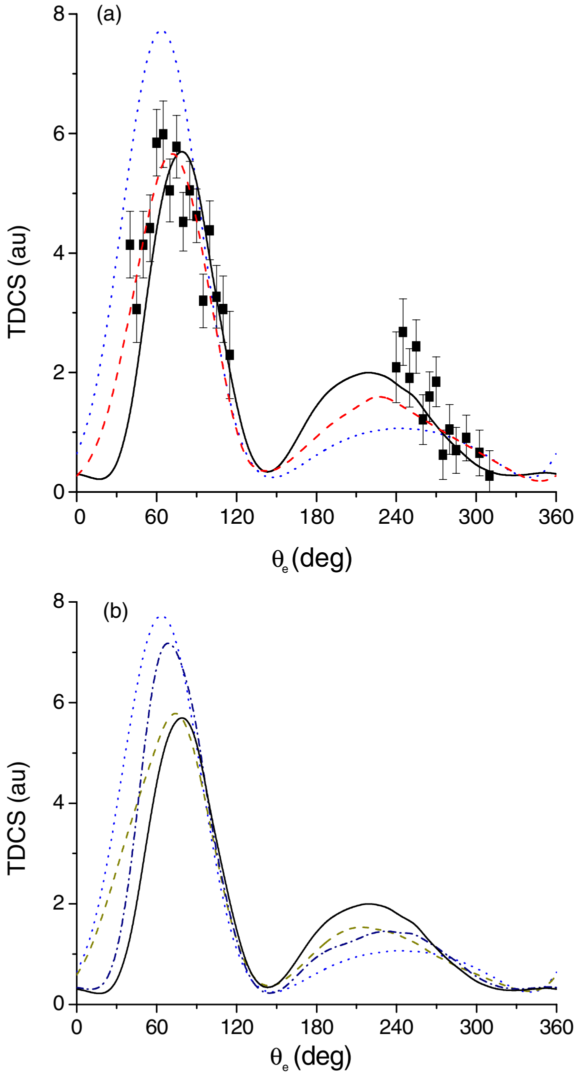

Figure 2. (a) TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 5^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including only the contribution of excited states by a dashed line, those of the second Born approximation calculated by including only the continuum states by a dash–dotted line and those of the second Born approximation calculated by including all the contributions by a full curve.

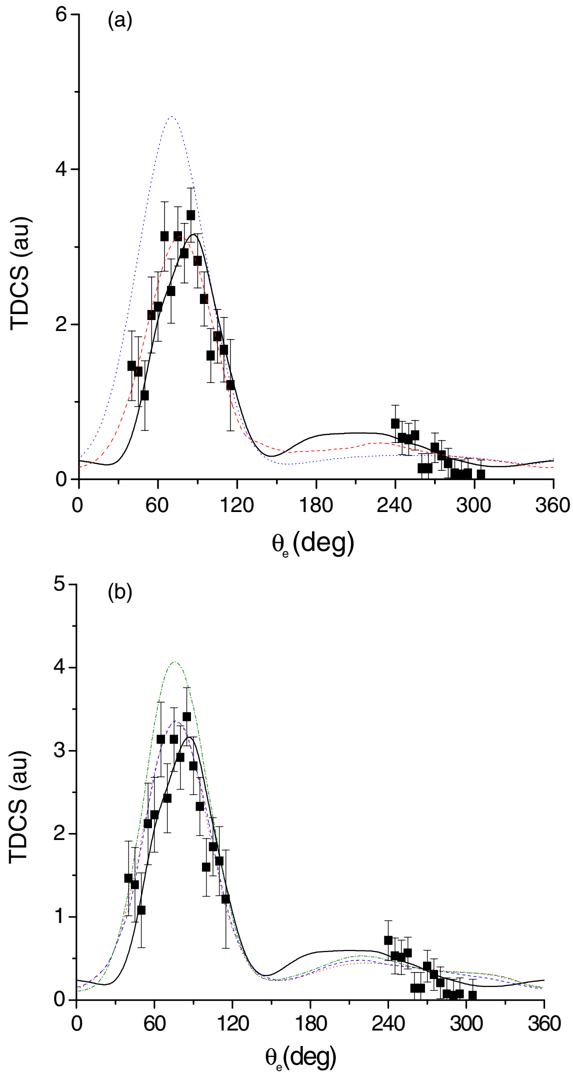

Figure 3. (a) TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 8^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the second Born approximation calculated by including all the contributions are represented by a full curve, those of the CDW-EIS by a dotted line, those of the CCC by a dashed line, those of the DWB2 by a dash–dotted line and experiments by squares.

and the experimental data (figure 2(a)). We notice smaller differences between the two models even if the shift of the binary peak and the magnitude of the recoil peak are enhanced by our model (second Born approximation). In figure 2(b), we see that the contributions of the excited states are important for the decreasing of the magnitude of the binary peak. We also find that the contribution of $L = 1$ is the most important. This result was also found by Byron *et al* [22] and Dal Cappello *et al* [7]. This result is easy to explain because it corresponds to the strong dipolar transition 1s $\rightarrow$ 2p which is important for weak momentum transfer. When studying the shift of this binary peak, we see that the most important contribution comes from the pseudo-continuum states from $L = 1$.

In figure 3, the scattering angle is fixed to 8°. We have yet good agreement between the two models (BBK and our second Born approximation) and the data (figure 3(a)), and we notice the smaller value of the magnitude of the recoil peak as expected because the value of the momentum transfer being greater. We also notice an improvement of the agreement between our second Born approximation and the CCC [19, 20] and CDW-EIS [10] approaches (figure 3(b)). As in the case of the scattering angle of 3°, the results of the second Born

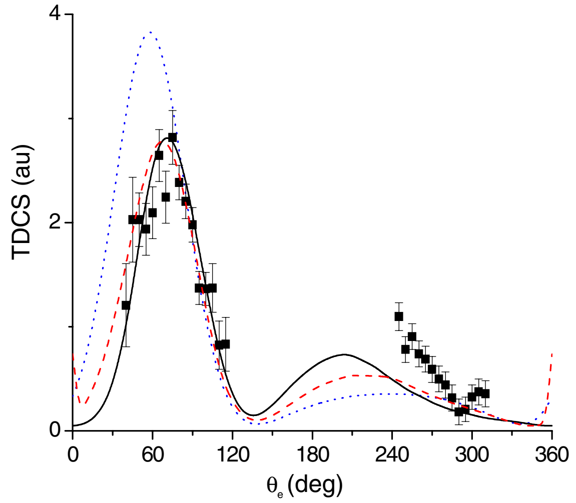

Figure 4. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 5^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 10$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

approximation obtained using the basis of Callaway [12] and Chen *et al* [9] (figure 3(b)) overestimate the magnitude of the binary peak.

Finally for this particular kinematics (250 eV for the incident and 5 eV for the ejected), we obtain excellent agreement between our model, the BBK approach and the experimental data, and only small differences for the shift of the binary peak and the magnitude of the recoil lobe are observed. Generally speaking, we notice better agreement when using our new basis.

Now we investigate the case of 250 eV for the incident and 10 eV for the ejected electron with two values of the scattering angle (5° and 8°). Figure 4 (5°) shows good agreement between our second Born approximation, the BBK model and the experimental data for the binary peak. But we notice small disagreement on the recoil peak: our second Born approximation and the BBK model are not able to reproduce the magnitude of the experimental data. In figure 5 (8°), the agreement is now excellent. For this kinematics, we notice that our second Born approximation gives results close to those given by the BBK model.

We finally study the last set of data (250 eV for the incident, 14 eV for the ejected and a scattering angle of 5° and 8°). Figure 6 (5°) shows good agreement between the two models (BBK and our second Born approximation) and the data for the binary peak. But our theories underestimate the data for the recoil lobe. It is exactly the opposite result for 8° (figure 7). The two models describe well the recoil lobe but are not able to reproduce the large shift of the binary peak.

As a first conclusion, the second Born approximation using our new basis is in the general term able to reproduce the shift and the decreasing in magnitude of the binary peak and the increasing magnitude of the recoil lobe as the BBK model does.

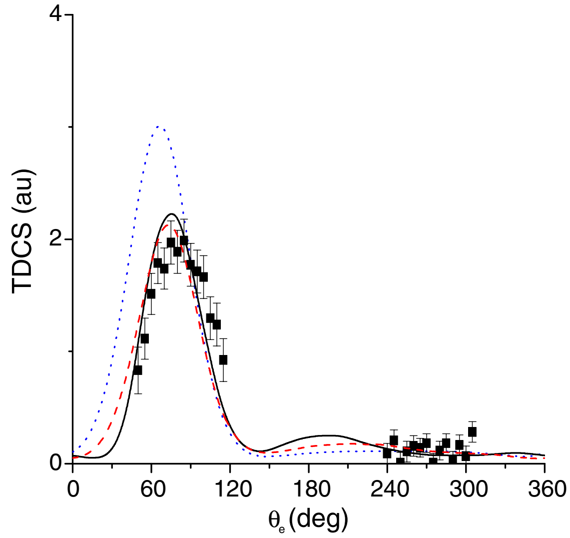

Figure 5. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 8^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 10$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

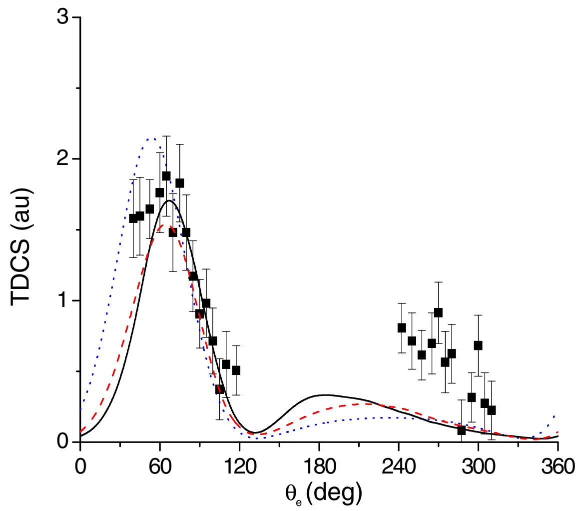

Figure 6. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 5^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 14$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

3.2. High ejected energies

We remember that until now only the BBK model [7] was able to give good agreement with experimental data provided by Weigold *et al* [13] for an ejected energy of 50 eV (250 eV for the incident energy). The second Born approximation under the closure approximation failed [7, 8] and the results obtained with a basis of 100 exact discrete states or a basis with 31 or 32 excited states and pseudo-states [7] failed as well.

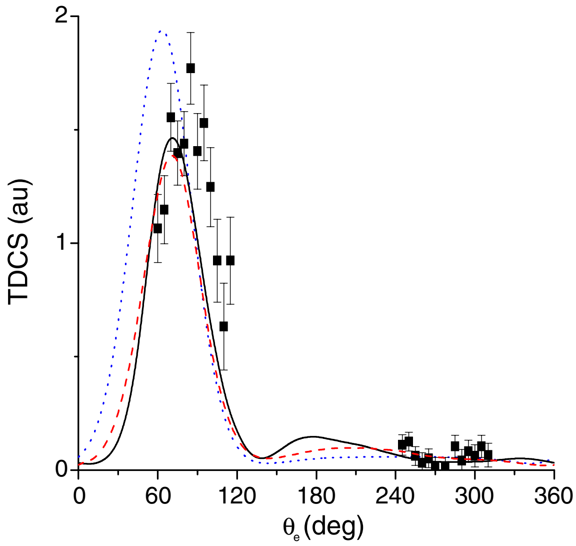

Figure 7. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 8°$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 14$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

We try to improve the agreement between the data and our model using the second Born approximation including now the contributions of 294 intermediate states.

In this study, we have normalized the relative experiments of Weigold *et al* [13] to the BBK model for a scattering angle of 25° and an ejected angle of 60°.

Figure 8 (scattering angle of 15°) shows the results of our model (second Born approximation with our new basis), those given by the first Born approximation, the second Born approximation with the basis of Callaway [12], the BBK model and the data. As previously found by Dal Cappello *et al* [7], the contributions of the excited states are small and insufficient to explain the shift of the binary peak. Now we verify that the contribution of the pseudo-continuum is strong (figure 8(b)), and when we consider all the contributions, the agreement with experiments is relatively good. We, however, notice that the agreement between the experiments and the BBK model (figure 8(a)) is a little bit better [7]. The question is now to understand why the second Born approximation is working when considering our new basis. The difference with the basis of Callaway [12] is the increasing of the number of excited and pseudo-continuum states. We study carefully each contribution and can conclude that all intermediate states must be taken into account. It is true that the most important contributions are coming from $L = 1$, but if we only consider the contribution from $L = 1$, we find no agreement with the experiments. When the energy of the ejected electrons is high (50 eV), it is important to consider a large basis with $L = 0$ to $L = 3$. This result was previously established by Popov and Benayoun [26].

In figure 9, where the scattering angle is 20°**,** we obtain good agreement between our model and the experiments, better than in the previous case. This agreement is also found by

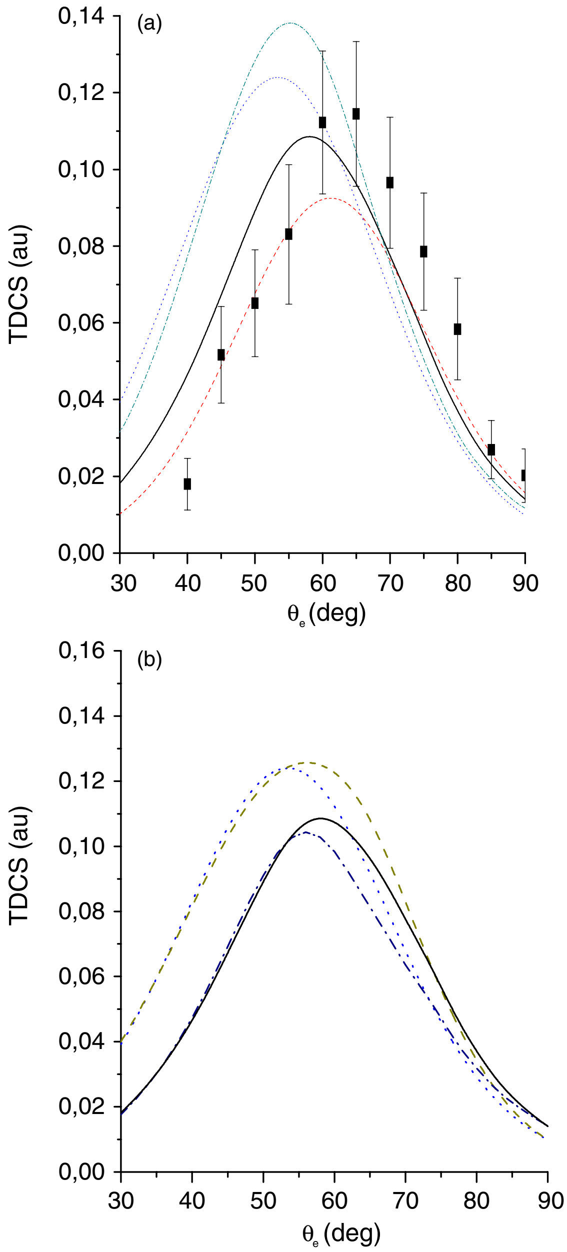

Figure 8. (a) TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 15°$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including all the contributions of our new basis by a full curve, those of the second Born approximation calculated by including all the contributions of the basis of Callaway [12] by a dash–dotted line, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including only the contribution of excited states by a dashed line, those of the second Born approximation calculated by including only the continuum states by a dash–dotted line and those of the second Born approximation calculated by including all the contributions by a full curve.

summing all the contributions (figure 9(a)). The second Born approximation calculated with the contributions of the excited

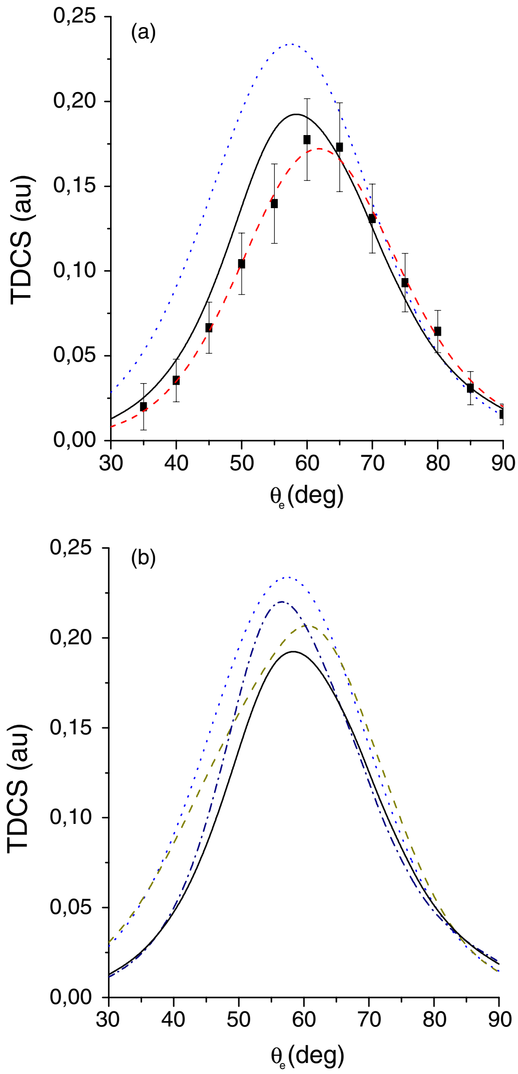

Figure 9. (a) TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 20^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including only the contribution of excited states by a dashed line, those of the second Born approximation calculated by including only the continuum states by a dash–dotted line and those of the second Born approximation calculated by including all the contributions by a full curve.

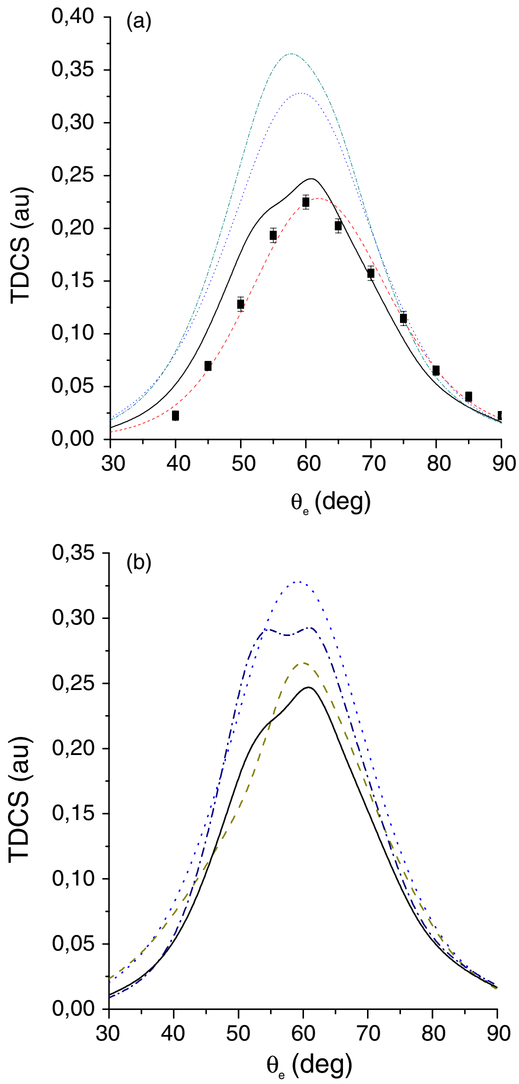

Figure 10. (a) TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 25^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including all the contributions of our new basis by a full curve, those of the second Born approximation calculated by including all the contributions of the basis of Callaway [12] by a dash–dotted line, those of the BBK model by a dashed line and experiments by squares. (b) Same as (a), but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by including only the contribution of excited states by a dashed line, those of the second Born approximation calculated by including only the continuum states by a dash–dotted line and those of the second Born approximation calculated by including all the contributions by a full curve.

states overestimates the data for small ejected angles while the second Born approximation calculated with the contributions of the pseudo-continuum states underestimates the shift of the binary peak (figure 9(b)). It is the same result for a scattering angle of 25° (figure 10). The agreement between our second Born approximation using our new basis and the data is clearly improved: the previous results given by the second Born approximation using the basis of Callaway [12] are unable to give such an agreement (figure 10(a)). We notice a double peak when the second Born approximation (using our new basis) is calculated with the contributions of the pseudo-continuum states (figure 10(b)). When the scattering angle is increasing (30°), the agreement is a little less good (figure 11). The second Born approximation improves the agreement with experiments but overestimates the data for small ejected angles. Curiously, in the previous situation (scattering angle of 35°), the agreement is better (figure 12).

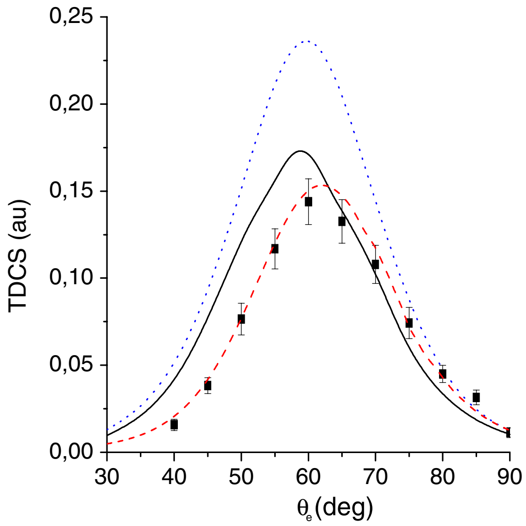

Figure 11. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 30^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

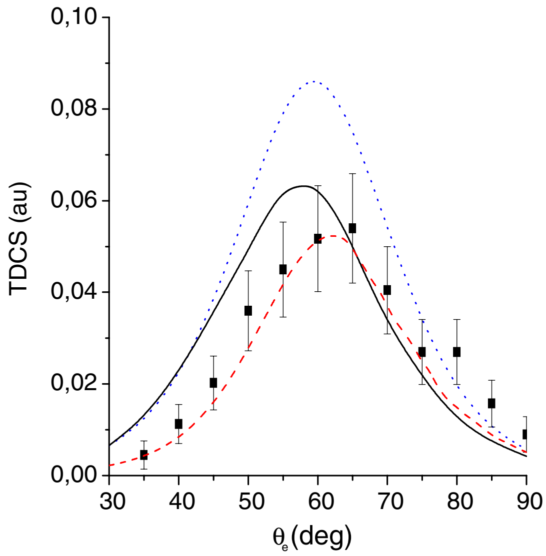

Figure 12. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 35^\circ$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a dotted line, those of the second Born approximation by a full curve, those of the BBK model by a dashed line and experiments by squares.

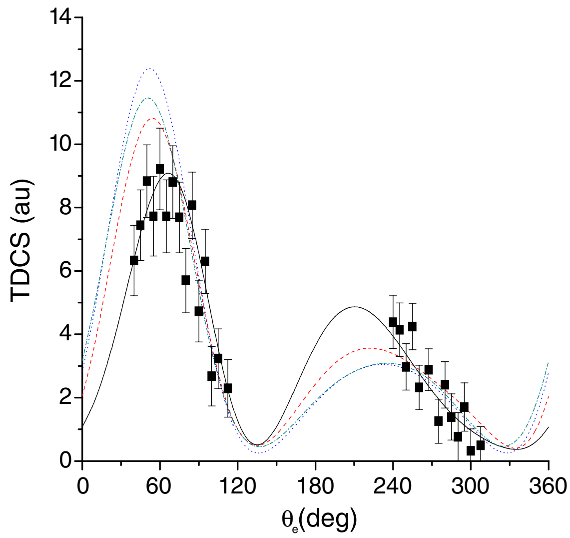

Figure 13. Same as figure 1, but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by using the closure approximation: $\bar{w} = 0$ au by a dashed line, $\bar{w} = 0.5$ au by a full curve, $\bar{w} = 2.5$ au by a dash–dotted line and experiments by squares.

Finally, we can conclude that our second Born approximation calculated with our new basis is able to give reasonable agreement with experiments even for higher ejected energy.

3.3. Closure approximation

Now, we turn to the study of the closure approximation for these two particular energy configurations (small and high ejected energies). We use 40 different values of the parameter $\bar{w}$, which is an average excitation energy, from 0 to 4.5 au. Figure 13 reproduces the results of our model for a small ejected energy (5 eV) and a small scattering angle of 3° with three different values of $\bar{w}$. We see that the value $\bar{w} = 0.5$ au gives good agreement. We remember that this value of $\bar{w}$ was used previously by Byron *et al* [27]. The agreement is not good for the two other values $\bar{w} = 0$ au (elastic collision) and $\bar{w} = 2.5$ au. When we consider the other cases (10 eV and 14 eV for the ejected energies), we also get good agreement if we use $\bar{w} = 0.5$ au. As a first conclusion for small ejected energies, we support the affirmation of Byron *et al* [27] that the closure approximation is able to reproduce the experimental data when using a *reasonable* value of the parameter $\bar{w}$ (0.3 au $< \bar{w} <$ 0.8 au). We notice that the momentum transfer is always small (from $K = 0.274$ au to $K = 0.63$ au).

Now we consider high ejected energies (50 eV) and a momentum transfer which varies from $K = 1.19$ au (scattering angle of 15°) to $K = 2.47$ au (scattering angle of 35°). We continue to use the same values of $\bar{w}$ used previously. Figure 14 (scattering angle of 15°) shows that it is impossible to find good agreement between our model (second Born approximation with the closure approximation) and the experimental data. We also used 36 other different values of $\bar{w}$ (from 0 to 4.5 au) and never find good agreement. We nevertheless notice that reasonable agreement is found for the higher value of the momentum transfer (scattering angle of 35°) when using the parameter $\bar{w} = 1.052$ au. But this result seems to be fortuitous and generally speaking it is difficult to get good agreement with the experimental data when using the second Born approximation with the closure approximation.

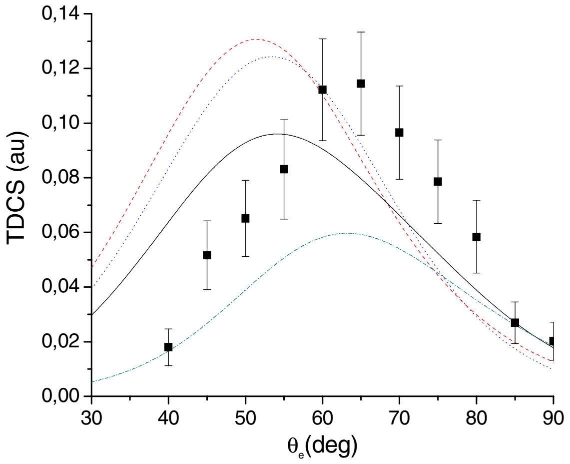

Figure 14. Same as figure 8, but the results of the first Born approximation are represented by a dotted line, those of the second Born approximation calculated by using the closure approximation: $\bar{w} = 0$ au by a dashed line, $\bar{w} = 0.5$ au by a full curve, $\bar{w} = 2.5$ au by a dash–dotted line and experiments by squares.

4. Conclusion

The second Born approximation has been applied to the study of the ionization of atomic hydrogen using a large number of intermediate discrete states; 294 basis elements, both excited and pseudo-continuum have been taken into account for different kinematics. For low ejected energy, the agreement with the BBK model and experiments is generally very good: our second Born approximation is able to explain the shift of the binary peak, the increasing of the amplitude of the recoil peak and the decreasing of the amplitude of the binary peak. The agreement is better than the one previously found using the second Born approximation with smaller [11, 12] and larger basis [9]. Our results show that the contributions of the pseudo-continuum states must be added and, as expected, that they are very important. For higher ejected energy, we show, for the first time, that the larger basis included in our second Born calculations leads to good agreement with the experimental data available. We are now approaching the perfect agreement found between the BBK model and the experiments. We are actually performing calculations trying to identify the source of the small disagreement. Even when it turns out to be numerically cumbersome, we plan to considerably increase the number of intermediate states (excited as well as pseudo-continuum states). If their contribution does not lead to better general agreement with the BBK model and the experimental data, it might result in the fact that third order Born contributions are required. This will show what the limitations of the second order are. We should mention here again that the second Born order that we are calculating is associated with a long-range Coulomb potential. No traces of problems are noticed even when the expansion associated with a long-range potential are mined by doubts. In that sense, our results are in agreement with those found in [6] where it is shown that the Born series for the two-body Coulomb potential converges.

As an additional and important conclusion, we confirm that the closure approximation is generally unable to give good agreement with experiments with high ejected energies and a high momentum transfer.

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