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Two Coulomb waves theory for direct excitation

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Abstract. A theoretical model of Dewangan, in which the total scattering wave function is approximated by a distorted wave containing two Coulomb wave functions, is discussed and its relation with the Brauner–Briggs–Klar model for ionization is examined. An important feature of the theory is that it includes a second Born amplitude naturally and in addition, contains, albeit approximately, both real and imaginary parts of all higher order Born terms. The theory is applied to study the $1s \rightarrow 2s$ excitation of hydrogen by electrons in the energy range 54.4 to 400 eV. The differential and integral cross sections predicted by the theory are compared with the results of other theories and experimental data at 54.4 eV and a good agreement is found.

Keywords. Brauner–Briggs–Klar model; two-Coulomb waves.

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1. Introduction

In recent years, the Brauner–Briggs–Klar (BBK) scattering wave function [1, 2] has received considerable attention in the study of the ionization of atoms. The BBK wave function for electron/positron-hydrogen scattering essentially consists of a product of three Coulomb wave functions, and properly satisfies the boundary conditions. The origin of the three Coulomb wave functions is as follows. A product of two Coulomb wave functions is used to describe the scattered electron interacting with the two Coulomb potentials produced by the ejected electron and the target nucleus. The third Coulomb wave function is the continuum eigenfunction of the ejected electron in the field of the target nucleus. Thus, the BBK wave function describes the motion in the final channel of the ejected electron and the projectile interacting with each other and also with the target nucleus. The approximate scattering amplitude is obtained by replacing the exact scattering wave function by the BBK wave function in the prior form of the transition amplitude. An extension of the model to ionization of helium has been given by Franz and Altick [3], and Berakdar and Briggs [4]. This model has been applied recently by Berakdar *et al* [5] to study the orientation and alignment effects in ionization of H($2p$) by electron impact. The BBK wave function has also been successful in the investigation of angular distribution of electrons following double photoionization [6, 7].

In view of the current interest in the BBK theory for ionization and photoionization, it is of considerable importance to examine its applicability to direct excitation, since this would give information about its theoretical structure. In this work, we use an

approximate total scattering wave function for excitation of hydrogen proposed by Dewangan [8] and discuss its relation with the BBK wave function for ionization. We extend our preliminary study of the $1s \rightarrow 2s$ excitation of hydrogen by electron impact, performed at a single energy of 54.4 eV, to 54.4–400 eV covering a wide range in the intermediate energy region and examine the theoretical predictions by comparing them with the results of other current theories. We use atomic units, unless otherwise stated.

2. The two Coulomb wave theory for direct excitation

We consider the collision of an electron with a hydrogen atom. Let $\mathbf{r}$ and $\mathbf{r}_0$ denote the position vectors of the target electron and the incident electron with respect to the target nucleus (assumed to be infinitely heavy) respectively, and let $\mathbf{r}_{01} = \mathbf{r} - \mathbf{r}_0$ be the position vector of the incident electron with respect to the target electron. We denote the final wave vector of the incident electron by $\mathbf{k}_f$, that of the ejected electron by $\mathbf{k}$ and define $\mathbf{k}_{01} = (\mathbf{k} - \mathbf{k}_f)/2$. The BBK wave function for the final (ionization) channel is given by [1, 2]

$$\psi_f^- = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}_f\cdot\mathbf{r}_0 + i\mathbf{k}\cdot\mathbf{r}} \Gamma(1 - i\alpha_{eT}) e^{-\pi\alpha_{eT}/2} {}_1F_1(i\alpha_{eT}, 1; -ikr - i\mathbf{k}\cdot\mathbf{r})$$
$$\times \Gamma(1 - i\alpha_{PT})\, e^{-\pi\alpha_{PT}/2} {}_1F_1(i\alpha_{PT}, 1; -ik_f r_0 - i\mathbf{k}_f\cdot\mathbf{r}_0)$$
$$\times \Gamma(1 - i\alpha_{eP})\, e^{-\pi\alpha_{eP}/2} {}_1F_1(i\alpha_{eP}, 1; -ik_{01} r_{01} - i\mathbf{k}_{01}\cdot\mathbf{r}_{01}), \qquad (1)$$

where $\alpha_{eT} = -1/k$, $\alpha_{PT} = Z_P/k_f$ and $\alpha_{eP} = -Z_P/|\mathbf{k} - \mathbf{k}_f|$ in which $Z_P = -1$ is the charge of the incident electron. The BBK transition amplitude for ionization is obtained by approximating the exact total scattering wave function with the above wave function in the prior form of the transition amplitude.

One can extend the BBK model to excitation of hydrogen in a straightforward manner. The BBK scattering wave function for excitation is obtained by replacing $\Gamma(1 - i\alpha_{eT})\, e^{-\pi\alpha_{eT}/2} {}_1F_1(i\alpha_{eT}, 1; -ikr - i\mathbf{k}\cdot\mathbf{r})$, the Coulomb eigenfunction for the ejected electron, by $\phi_f(\mathbf{r})$, the bound atomic eigenfunction of the excited final state, and putting $\mathbf{k} = 0$,

$$\psi_f^- = e^{i\mathbf{k}_f\cdot\mathbf{r}_0} \phi_f(\mathbf{r}) |\Gamma(1 + i\nu_f)|^2 {}_1F_1(-i\nu_f, 1; -ik_f r_0 - i\mathbf{k}_f\cdot\mathbf{r}_0)$$
$$\times {}_1F_1(i\nu_f, 1; -ik_f r_{01}/2 + i\mathbf{k}_f\cdot\mathbf{r}_{01}/2), \qquad (2)$$

where we have defined $\nu_f = Z_P/k_f$. The BBK version of the transition amplitude for excitation is obtained by using this wave function in place of the exact wave function in the prior form of the transition amplitude.

In the context of excitation, however, it is traditional to consider the post form of the transition amplitude, rather than the prior form which is used in ionization. For the reasons that will become clear in the following, we replace $k_f/2$ by k_f in the argument of the confluent hypergeometric function appearing in (2). If we denote by $\phi_i(\mathbf{r})$ the bound atomic wave function of the initial state and by $\mathbf{k}_i$ the incident wave vector, we can immediately write the post form of scattering wave function (2) corresponding to the

entrance channel as [8]

$$\psi_i^+ = \phi_i(\mathbf{r})e^{i\mathbf{k}_i\cdot\mathbf{r}_0}|\Gamma(1+i\nu)|^2\, {}_1F_1(-i\nu, 1; ik_ir_0 - i\mathbf{k}_i\cdot\mathbf{r}_0)$$
$$\times {}_1F_1(i\nu, 1; ik_ir_{01} + i\mathbf{k}_i\cdot\mathbf{r}_{01}), \tag{3}$$

where $\nu = Z_P/k_i$. The wave function (3) contains, in essence, a product of two Coulomb wave functions which describes the continuum state of the incident electron interacting simultaneously with both the target nucleus and the bound target electron. By using the asymptotic forms of the confluent hypergeometric functions [9], we may easily see that the wave function (3) satisfies proper boundary conditions

$$\psi_i^+ \sim \phi_i(\mathbf{r})e^{i\mathbf{k}_i\cdot\mathbf{r}_0} + \text{scattered wave}. \tag{4}$$

In the T-matrix formalism, when the exact scattering wave function is approximated by (3), the post form of the transition amplitude for the $\phi_i(\mathbf{r}) \rightarrow \phi_f(\mathbf{r})$ excitation is given by

$$T_{fi} = \int d\mathbf{r}\, d\mathbf{r}_0\, e^{-i\mathbf{k}_f\cdot\mathbf{r}_0}\phi_f^*(\mathbf{r})\left(\frac{Z_P}{r_0} - \frac{Z_P}{r_{01}}\right)\psi_i^+. \tag{5}$$

Since the continuum state of the incident electron is described, in essence, by two Coulomb wave functions, the present theory, for brevity, will be called the two Coulomb waves (TCW) theory.

It should be mentioned here that the use of the wave function of the form (3) in atomic scattering calculations is not new. Vainshtein, Presnyakov and Sobelman (VPS) [10] in the context of excitation of hydrogen by electron impact, and Cheshire [11], in the context of electron capture in proton-hydrogen collisions (the CDW method), were the first to propose the use of a product of two Coulomb wave functions to describe the distortion effects on the scattering wave function. In the study of electron impact excitation of hydrogen, Vainshtein *et al* [10] used the post form of the transition amplitude (the VPS approximation). But, to evaluate the amplitude, Vainshtein *et al* [10] and subsequently other authors (see the references given in [12, 13]) applied peaking approximations to simplify the calculations. Dewangan and Bransden [12] analysed the physical content of the VPS approximation for excitation of hydrogen by proton impact and showed (see below) that the application of the peaking approximation to the VPS amplitude in essence leads to a first order amplitude that is a poor approximation to the VPS amplitude. Their analysis showed that the contribution to the VPS scattering amplitude from the incident proton-electron matrix element contains a term which is identical to a second Born amplitude for this interaction computed in a closure approximation. However, the matrix element of the incident proton-target nucleus interaction that occurs in the VPS amplitude, contains a term which is not identical to, but has a structure similar to a second Born term, for this interaction. Following this work, Dewangan [8], by modifying the VPS wave function, wrote down the TCW wave function (3) as well as the TCW transition amplitude (5) for electron hydrogen scattering and demonstrated that the transition amplitude (5) contains full closure approximation second Born terms corresponding to the incident electron-target electron and the incident electron-target nucleus interaction. Dewangan and Khadkikar [14] have developed a distorted wave expansion for the transition amplitude whose first order term is the TCW amplitude (5). It is shown in that paper that the TCW amplitude (5) contains (1) a second Born term, (2)

both real and imaginary parts of all higher (≥ 3) order Born terms in an approximate way, and that (3) the well known Glauber amplitude (for a review see [15, 16]) can be derived by introducing further approximations in the TCW amplitude. Like the TCW amplitude, the Glauber amplitude contains contributions from all orders ($n \geq 2$) of the Born terms, but in contrast to the TCW model, either all its odd-order terms are purely real and all its even-order terms are purely imaginary or vice versa. Evidently, the TCW theory includes contributions from all orders of the Born terms and goes beyond the Glauber approximation.

The TCW wave function (3) is very similar in spirit to the VPS wave function (or the wave function of the continuum distorted wave (CDW) model of Cheshire [11], see Dewangan and Eichler [17] for a discussion) but differs from the VPS (or the CDW) wave function in that the latter is based on the use of the Jacobi coordinates [18]. For an explicit expression of the VPS (or the CDW) wave functions and the transition amplitudes in both the post and prior forms for electron-hydrogen scattering, the reader is referred to Sinha *et al* [13].

One can show by following the method of Dewangan and Bransden [12] that the wave function (2), unlike (3), does not reproduce the full closure approximation second Born term and therefore we use only the wave function (3). Dewangan [8] also made a preliminary application of the TCW model to the $1s \rightarrow 2s$ excitation of hydrogen by electrons at 54.4 eV and indeed, to our knowledge, except for this application, no other calculations without further approximations for direct excitation in this method have been reported. However, as the present work based on improved numerical techniques shows, due to inaccuracies in performing numerical quadratures, the differential cross sections calculated in [8] were in error by up to about 15%, depending on scattering angles. Here it must be mentioned that Chen *et al* [19] have applied the TCW theory without any further approximation to study Ps($1s$) formation in e^+–H($1s$) collisions.

In order to perform numerical computation, we follow the method of Dewangan [8] and transform the transition amplitude (5) into momentum space. Defining the form factor,

$$G_{\rm fi}(\mathbf{p}) = \int \mathrm{d}\mathbf{r}\, \mathrm{e}^{i\mathbf{p}\cdot\mathbf{r}} \phi_{\rm f}^*(\mathbf{r}) \phi_{\rm i}(\mathbf{r}), \tag{6}$$

the transition amplitude (5) may be reduced to

$$T_{\rm fi} = T_{\rm fi}^{(1)} + T_{\rm fi}^{(2)}, \tag{7}$$

where $T_{\rm fi}^{(1)}$ is given by

$$T_{\rm fi}^{(1)} = T_{\rm fi}^{\rm B1} \left(|\Gamma(1 + i\nu)|^2 \, {}_2F_1 \left[-i\nu, i\nu; 1, \left(\frac{\mathbf{k}_i \cdot \mathbf{q}}{\omega_{\rm fi}} \right)^2 \right] \right). \tag{8}$$

Here, $\omega_{\rm fi} = \epsilon_{\rm f} - \epsilon_{\rm i}$, with $\epsilon_{\rm i}$ and $\epsilon_{\rm f}$ being the eigenenergies of the initial and final atomic states, respectively, $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is the momentum transfer and $T_{\rm fi}^{\rm B1}$ is the usual first Born transition amplitude given by

$$T_{\rm fi}^{\rm B1} = Z_P \frac{4\pi}{q^2} [G_{\rm fi}(0) - G_{\rm fi}(\mathbf{q})]. \tag{9}$$

Clearly, the amplitude $T_{\rm fi}^{(1)}$, eq. (8), is in essence a first order approximation.

The amplitude $T_{\rm fi}^{(2)}$ may be written as

$$T_{\rm fi}^{(2)} = Z_P|\Gamma(1+i\nu)|^2\left(\frac{4\nu k_i}{\pi}\right)[T^N + T^E]. \tag{10}$$

Here, the matrix element T^N is the contribution from the interaction of unit strength $(+1/r_0)$, and is given by

$$T^N = \lim_{\alpha\to 0,\,\epsilon\to 0}\int \mathrm{d}\mathbf{p}\,\frac{[G_{\rm fi}(\mathbf{k}_i-\mathbf{p})-G_{\rm fi}(0)][|\mathbf{p}-\mathbf{k}_i-\mathbf{k}_f|^2+(\alpha-ik_i)^2]^{+i\nu}}{|\mathbf{p}-\mathbf{k}_i|^{(2-2i\nu)}|\mathbf{p}-\mathbf{k}_f|^{(2+2i\nu)}(p^2-k_i^2-i\epsilon)^{(1+i\nu)}}. \tag{11}$$

The term T^E is the contribution from the interaction of unit strength $(+1/r_{01})$,

$$T^E = \lim_{\alpha\to 0,\,\epsilon\to 0}\int \mathrm{d}\mathbf{p}\,\frac{[G_{\rm fi}(\mathbf{p}-\mathbf{k}_f)-G_{\rm fi}(\mathbf{q})][|\mathbf{p}-\mathbf{k}_i-\mathbf{k}_f|^2+(\epsilon-ik_i)^2]^{-i\nu}}{|\mathbf{p}-\mathbf{k}_i|^{(2+2i\nu)}|\mathbf{p}-\mathbf{k}_f|^{(2-2i\nu)}(p^2-k_i^2-i\alpha)^{(1-i\nu)}}. \tag{12}$$

If we put $\nu = 0$, (11) and (12) reduce respectively to

$$T_{\rm B2}^N = \lim_{\epsilon\to 0}\int \mathrm{d}\mathbf{p}\,\frac{[G_{\rm fi}(\mathbf{k}_i-\mathbf{p})-G_{\rm fi}(0)]}{|\mathbf{p}-\mathbf{k}_i|^2|\mathbf{p}-\mathbf{k}_f|^2(p^2-k_i^2-i\epsilon)}, \tag{13}$$

and

$$T_{\rm B2}^E = \lim_{\alpha\to 0}\int \mathrm{d}\mathbf{p}\,\frac{[G_{\rm fi}(\mathbf{p}-\mathbf{k}_f)-G_{\rm fi}(\mathbf{q})]}{|\mathbf{p}-\mathbf{k}_i|^2|\mathbf{p}-\mathbf{k}_f|^2(p^2-k_i^2-i\alpha)}. \tag{14}$$

We may verify that, apart from a constant factor, (13) and (14) are the second Born terms for the interactions $+1/r_0$, and $+1/r_{01}$, respectively, calculated in the closure approximation in which the atomic energies of all intermediate states are taken to be ϵ_i, the energy of the initial atomic state [15, 16]. Thus, the TCW model fully includes the closure approximation second Born (CSB2) terms. It is also clear from (8), (10)–(12) that if the TCW amplitude $T_{\rm fi}$, eq. (7), is (formally) expanded in powers of ν, the term containing ν^k arises from the $(k+1)$th order Born term. Thus, we see that the (TCW) model contains contributions from both real and imaginary parts of all higher order (≥ 3) Born terms in this closure approximation.

We may note that, in earlier studies of electron impact excitation of hydrogen ([10], [13]), the first order amplitude $T_{\rm fi}^{(1)}$, eq. (8), was obtained by applying a peaking approximation to the VPS amplitude, i.e. the VPS amplitude was approximated by $T_{\rm fi}^{(1)}$. The first order (or peaking approximation) amplitude $T_{\rm fi}^{(1)}$, eq. (8), being an even function of ν, contains contributions from only odd order Born terms. Evidently, it is a poor approximation to the TCW amplitude $T_{\rm fi}$, eq. (7), since it does not include the second Born amplitude and also the effects of higher order perturbation terms contained in $T_{\rm fi}^{(2)}$, eq. (10).

Obviously, the closure approximation inherent in the TCW theory becomes more accurate when the energy difference between the initial and final atomic states is small and, in addition, there are a large number of intermediate atomic states, grouped around the initial and final atomic states, having nearly the same energy as the initial (or final)

atomic state [20]. Since this condition is encountered in transitions between excited states, the TCW model is better suited for excited-state to excited-state transitions. In this context, an appealing feature of the integral expressions (11) and (12) and hence the transition amplitude $T_{\rm fi}$ is that they depend on the initial and final atomic states only through the form factor $G_{\rm fi}(\mathbf{p})$. Since the form factor $G_{\rm fi}(\mathbf{p})$ is available in closed form for arbitrary initial and final states, the integral expression for the transition amplitude $T_{\rm fi}$ is free from parametric differentiation. We may mention that an alternative method for evaluation of the integrals containing two Coulomb wave functions used in the literature (see for example, [1, 13, 19]) depends on the technique of parametric differentiation. Although this method of parametric differentiation can be applied to excitation of $n = 2$ states, such a method, as is well known, becomes very cumbersome for higher excited atomic states. For this reason, we have preferred to develop numerical techniques for directly computing the three-dimensional integrals (11) and (12).

We have numerically evaluated the three-dimensional integrals (11) and (12) in momentum $\mathbf{p}$-space for the $1s \rightarrow 2s$ excitation of hydrogen induced by electron impact by using spherical polar coordinates $\mathbf{p} \equiv (p, \theta_p, \varphi_p)$. We have suitably divided the range $(0 \leq p \leq \infty,\ 0 \leq \theta_p \leq \pi,\ 0 \leq \varphi_p \leq 2\pi)$ of integrals into some number of intervals (depending on the incident energy) and then applied the Gaussian quadrature formulas in each of these intervals. Careful treatment was given to the regions near $\mathbf{p} = \mathbf{k}_i$ and $\mathbf{p} = \mathbf{k}_f$.

We see that the integrands in (11) and (12) contain the Coulomb distorted Green's function $1/(p^2 - k_i^2 - i\epsilon)^{(1\pm i\nu)}$, having the $i\epsilon$ prescription, i.e. the limiting $\epsilon \rightarrow 0$ procedure. A straightforward application of standard numerical quadrature formulas (e.g. the Gaussian formula [9]) to the integrals in (11) and (12) would miss the contributions originating from the $i\epsilon$ prescription. To evaluate accurately the contributions coming from the $i\epsilon$ prescription in the neighbourhood of $p = k_i$ [and also the singular region around $\mathbf{p} \rightarrow \mathbf{k}_i$], we have given special attention to the radial p-integration from $p = k_i - \Delta_1$ to $p = k_i + \Delta_1$, where Δ_1 is some small positive number and devised an auxiliary integral. The nature of the integrand becomes further involved due to the presence of the factors $[G_{\rm fi}(\mathbf{k}_i - \mathbf{p}) - G_{\rm fi}(0)]/|\mathbf{p} - \mathbf{k}_i|^{(2-2i\nu)}$ and $[G_{\rm fi}(\mathbf{p} - \mathbf{k}_f) - G_{\rm fi}(\mathbf{q})]/|\mathbf{p} - \mathbf{k}_i|^{(2+2i\nu)}$ in (11) and (12), respectively, since these terms become singular as $\mathbf{p} \rightarrow \mathbf{k}_i$. To deal with the $\mathbf{p} \sim \mathbf{k}_i$ region, we have expanded the form factors $G_{\rm fi}(\mathbf{p})$ for the $1s \rightarrow 2s$ excitation in powers of $(\mathbf{p} - \mathbf{k}_i)$ and retained the leading term. We have used the leading term to devise auxiliary integrals. In the region $\mathbf{p} \sim \mathbf{k}_i$, the integrands of the auxiliary integrals are the limiting forms of the corresponding integrands of the actual integrals (11) and (12). Moreover, the auxiliary integrals are such that they can be either evaluated analytically or accurately by numerical quadrature. Therefore, the difference of the actual integrands and the auxiliary integrands is smooth in this region and can be evaluated by numerical quadrature. The complete procedure for the $1s \rightarrow 2s$ excitation is rather lengthy and cumbersome and therefore will not be described here. It may be mentioned that the form of the auxiliary integrals depends sensitively on the form of $G_{\rm fi}(\mathbf{p})$ and hence is different for different initial and final states. The prescription for numerical integration near this region ($\mathbf{p} \sim \mathbf{k}_i$) for transitions involving non-spherical states (for example, $1s \rightarrow 2p$ excitation) becomes much more involved and we are working on this problem.

We also see that because of the factors $[|\mathbf{p} - \mathbf{k}_i - \mathbf{k}_f|^2 + (\alpha - ik_i)^2]^{+i\nu}/|\mathbf{p} - \mathbf{k}_f|^{(2+2i\nu)}$ and $[|\mathbf{p} - \mathbf{k}_i - \mathbf{k}_f|^2 + (\epsilon - ik_i)^2]^{-i\nu}/|\mathbf{p} - \mathbf{k}_f|^{(2-2i\nu)}$ in (11) and (12), respectively, the

integrands become singular as $\mathbf{p} \rightarrow \mathbf{k}_f$. However, the integrals (over $\mathbf{p}$) containing these factors in the neighbourhood of $\mathbf{p} = \mathbf{k}_f$ are well defined and can be carried out analytically. The method for performing these integrals analytically is rather cumbersome and lengthy and we shall not discuss it here. Our computer program includes these results.

We have tested the computer program by devising some test integrals which can be evaluated analytically and whose integrands in the neighbourhood of $\mathbf{p} = \mathbf{k}_i$ and $\mathbf{p} = \mathbf{k}_f$ have a very similar behaviour to those of (11) and (12). The program reproduces the analytical results to desired numerical accuracy.

3. Results and discussions

We have computed the cross sections of the TCW and closure approximation second Born (CSB2) models for the $1s \rightarrow 2s$ excitation of hydrogen by electrons in the energy range of 54.4 to 400 eV and have taken into account the exchange contributions by using the Ochkur approximation [15]. The computation of the differential cross section at one scattering angle for a single incident energy requires about 30 minutes of CPU time in the IBM 6000/R machine.

For the $n = 2$ excitation of hydrogen, a large number of sophisticated perturbative and nonperturbative theories exists [15, 16, 21–24] which include the close coupling (40CC) method based on a large basis set containing pseudostates of Wyngaarden and Walters [25], the convergent close-coupling (CCC) theory of Bray and Stelbovics [26] and Bubelev *et al* [27], the coupled-channel optical (CCO) model of Bray *et al* [28], the intermediate R-matrix method (IERM) of Scholtz *et al* [29], the exact second-order distorted wave (DWB2) theory of Madison *et al* [30] and Bubelev *et al* [27]. As stated by Bray and Stelbovics [26], among the nonperturbative theories, the results of the convergent close-coupling (CCC) theory, the coupled-channel optical (CCO) model of Bray *et al* [28], the intermediate R-matrix method (IERM) of Scholtz *et al* [29] and the close-coupling (40CC) theory of Wyngaarden and Walters [25] are in excellent agreement with each other at intermediate energies. Wyngaarden and Walters [25] have also presented the 40CC results in tabular forms. Therefore, we have compared the TCW results with the 40CC results and, for the sake of clarity, we have not included in the figures the results of the CCC, CCO, and IERM theories.

3.1 *Electron impact excitation of the* $2s$ *state at* 54.4 *eV*

For the electron impact excitation of the ground $1s$ state of the hydrogen to the $2s$ state, the incident energy 54.4 eV is special, since only at this energy, the differential cross sections have been measured by Williams in 1981 [31] (see also Williams and Wang [32] for a review of the $n = 3$ excitation of hydrogen). Figure 1 compares the differential cross sections (shown as the solid curve) of the TCW model with the experimetal data. It is seen that the TCW results (with the exchange effects included) are in very good agreement with the experimental data for scattering angles $\Theta \leq 100°$ but they are smaller than the experimental results for larger scattering angles $\Theta > 100°$. This figure also displays the results of the TCW model calculated by ignoring the exchange effects

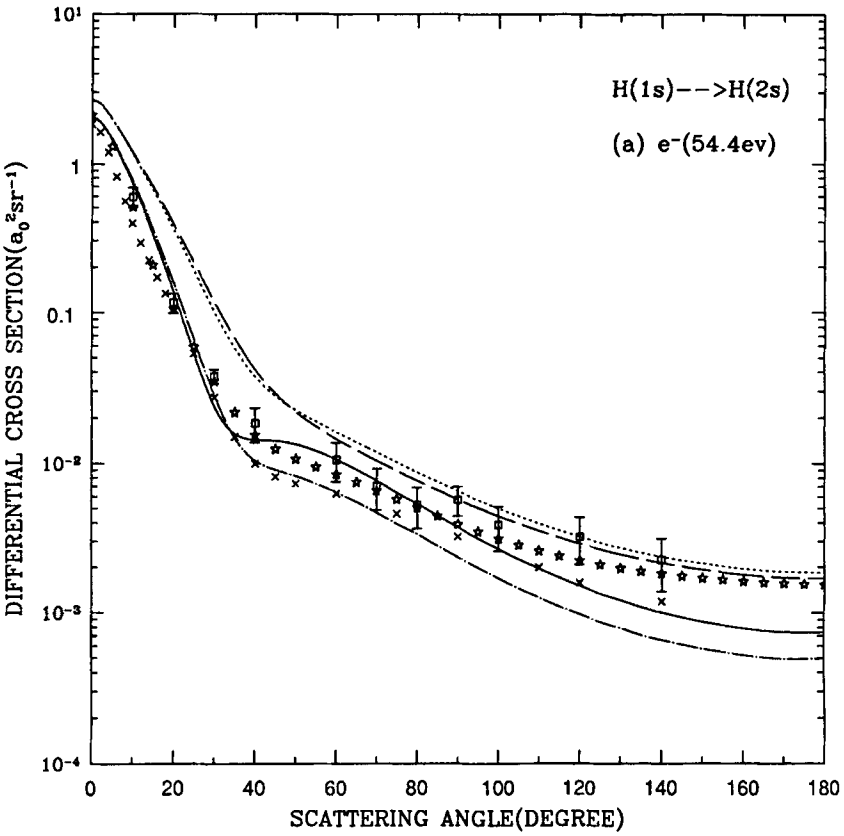

Figure 1. Differential cross sections for $e^- + \mathrm{H}(1s) \longrightarrow e^- + \mathrm{H}(2s)$ at 54.4 eV. Solid line: TCW results with exchange; dash-dot line: TCW results without exchange; dottted line: CSB2 results with exchange; dashed line: CSB2 results without exchange; stars: DWB2 results [27, 30]; crosses: 40CC results [25]; open squares with error bars: experimental results of Williams [31].

(shown as dash-dotted line). We see that the exchange effects are important at this energy. It is also seen that the CSB2 results deviate significantly from the TCW cross sections showing the importance of the higher order ($n \geq 3$) Born terms included in the TCW theory. The differential cross sections of the first Born theory, and the peaking approximation given by $T_{\mathrm{fi}}^{(1)}$, eq. (8) are not shown in the figure. The peaking approximation predicts that the differential cross sections have a shape similar to that given by the first Born theory. It is well documented in the literature (see e.g. [16]) that the first Born gives a poor description of experiment.

Figure 1 also displays the theoretical results (shown as crosses) of Wyngaarden and Walters [25] calculated by using the close coupling (40CC) method based on a large basis set consisting of s, p and d states which also includes pseudostates to account for the couplings to the continuum (and the bound states not explicitly included in the basis set). In this 40CC method, couplings to the target states of higher angular momenta ($l > 2$) are treated perturbatively in the second Born approximation. The TCW theory predicts a

slightly broader peak for smaller scattering angles in comparison to the 40CC theory of Wyngaarden and Walters [25] and gives somewhat better agreement with the experimental data in this region. Except for small scattering angles (given below), the results of the TCW model are in good overall agreement with those of 40CC method. An interesting feature of the TCW and 40CC (and also the CCC [26, 27]) theories is that they exhibit a broad shoulder around $\Theta \approx 40°$.

Madison *et al* [30] and Bubelev *et al* [27] have performed calculations of the cross sections for the $n = 2$ excitation of hydrogen by electron impact in the energy range 20–200 eV in a distorted wave second order (DWB2) theory which includes exactly the second order direct and exchange amplitudes. The DWB2 results are shown (as stars) in figure 1. We see that the TCW model (the solid curve) is in good harmony with the DWB2 theory (the stars) for scattering angles $\Theta \leq 100°$. For larger scattering angles ($\Theta > 100°$), the differential cross sections of the DWB2 theory tend towards the results of the closure approximation second Born (CSB2) model, calculated by using (13) and (14) (shown as the dotted curve). It is interesting to note that the differential cross sections of the CSB2 and DWB2 approximations agree remarkably well with the experimental data for $\Theta \geq 90°$, whereas for smaller scattering angles, the CSB2 approximation gives a poor

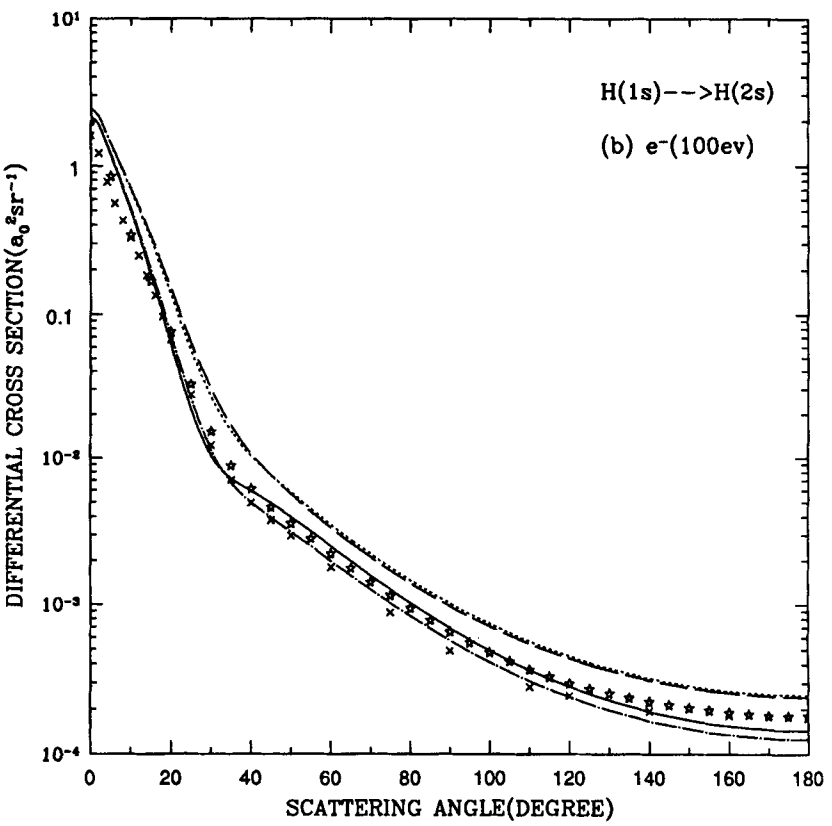

Figure 2. Differential cross sections for $e^- + \mathrm{H}(1s) \longrightarrow e^- + \mathrm{H}(2s)$ at 100 eV. The descriptions of the curves are the same as in figure 1.

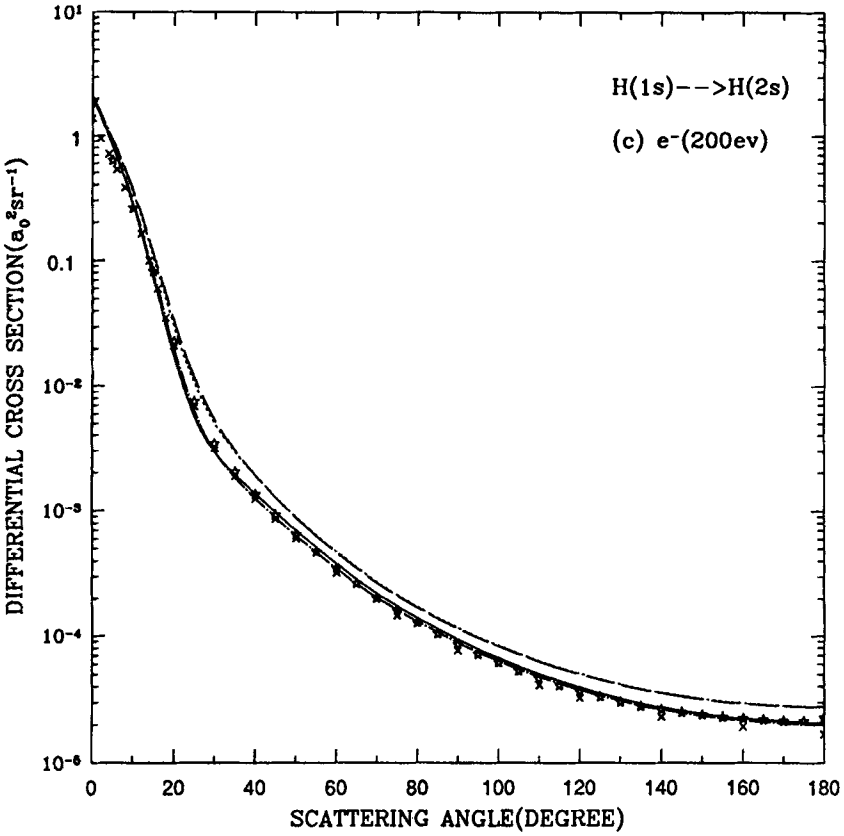

Figure 3. Differential cross sections for $e^- + \mathrm{H}(1s) \longrightarrow e^- + \mathrm{H}(2s)$ at 200 eV. The descriptions of the curves are the same as in figure 1.

description of the experimental data. Another interesting feature to note is that in contrast to the TCW, 40CC and CCC theories, the DWB2 and CSB2 models do not predict a broad shoulder around $\Theta \approx 40°$.

3.2 *Electron impact excitation of the 2s state for* 100–400 *eV*

The differential cross sections calculated in the TCW model (the solid curve) and the CSB2 approximation [both with (the long dashed curve) and without (the dotted curve) exchange contributions] are shown in figures 2–5 for incident electron energies 100–400 eV. For these energies, there are no experimental data. The results of the 40CC approximation of Wyngaarden and Walters [25] are available for 100, 200 and 300 eV which are also shown as the crosses. The stars in figures 2 and 3 represent the results of the DWB2 theory calculated by Madison *et al* [30] and Bubelev *et al* [27]. We see from these figures that for incident energy $\geq$ 200 eV, the exchange contribution is very small. The TCW model predicts somewhat larger values of the differential cross sections in the forward direction in comparison to the 40CC and the DWB2 models. This feature is due to the average excitation energy being equal to ϵ_i, the energy of the initial atomic state.

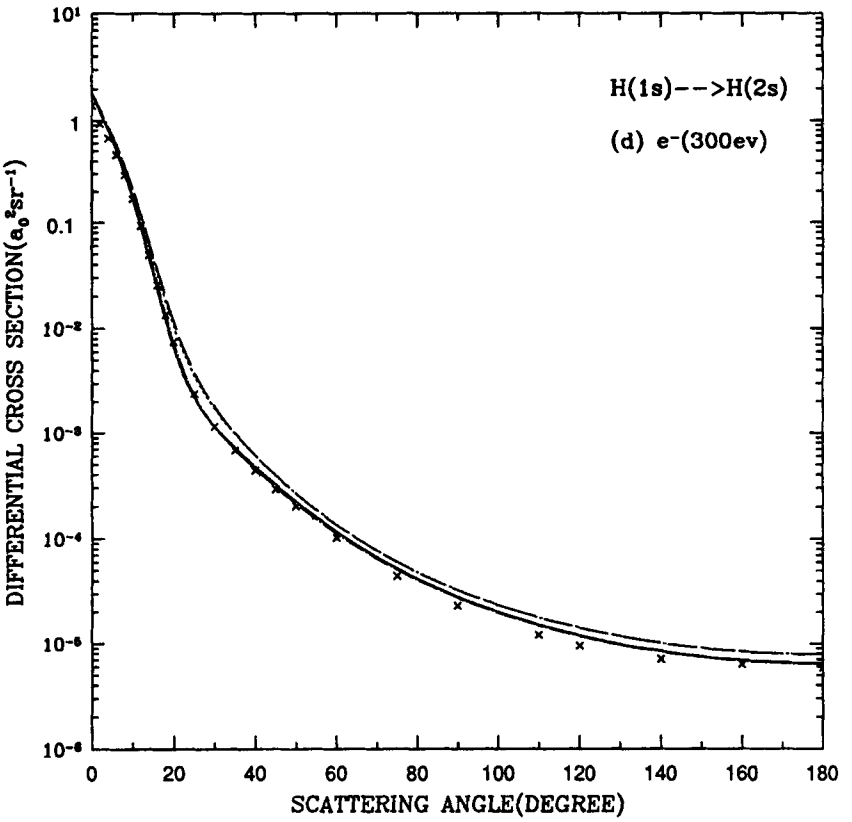

Figure 4. Differential cross sections for $e^- + \mathrm{H}(1s) \longrightarrow e^- + \mathrm{H}(2s)$ at 300 eV. The descriptions of the curves are the same as in figure 1.

We see that for the scattering angles $\Theta > 20°$, there is good overall agreement among the predictions of the TCW, 40CC and DWB2 methods.

3.3 *Integrated cross sections*

We have computed the integrated cross sections of the TCW, CSB2 and first Born theories and also of the peaking approximation given by $T_{\mathrm{fi}}^{(1)}$, eq. (8). In our calculations, we have included the exchange contribution by using the Ochkur approximation. Table 1 compares the integrated cross sections calculated in various models. The importance of the higher order Born terms included in the TCW theory once again becomes clear from the fact that the integrated CSB2 cross sections differ significantly from the integrated TCW cross sections in the energy range under consideration. Indeed, the CSB2 theory predicts the largest values of the integrated cross sections. The peaking approximation also gives larger integrated cross sections at lower energies showing the importance of the remaining terms included in the TCW theory. From the table we also see that the TCW model predicts larger values of the integrated cross section in comparison to the 40CC close coupling results of

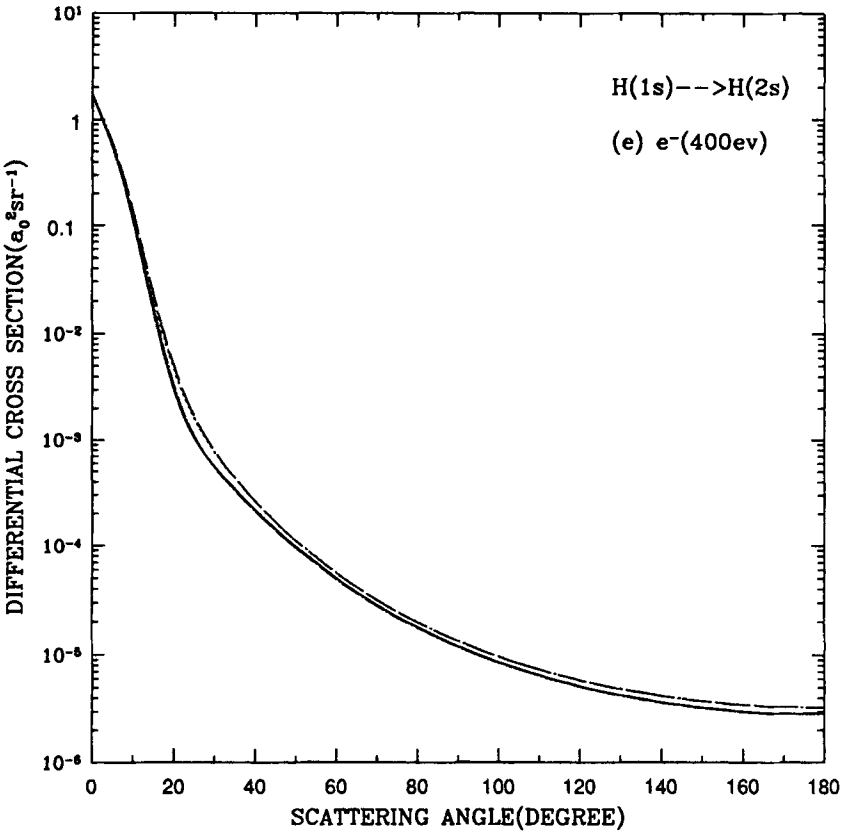

Figure 5. Differential cross sections for $e^- + \mathrm{H}(1s) \longrightarrow e^- + \mathrm{H}(2s)$ at 400 eV. The descriptions of the curves are the same as in figure 1.

Table 1. The integrated cross sections (in units of a_0^2) as a function of the incident electron energy for the $1s \longrightarrow 2s$ excitation of atomic hydrogen by electron impact. The integrated cross sections of the TCW, CSB2, peaking approximation and first Born theories include the exchange contributions through the Ochkur approximation.

Electron energy	54.4 eV	100 eV	200 eV	300 eV	400 eV
TCW	0.298	0.174	0.091	0.062	0.046
CSB2	0.568	0.261	0.114	0.072	0.052
40CC	0.204	0.126	0.079	0.057	—
Peaking approx.	0.437	0.205	0.096	0.063	0.047
First Born	0.289	0.170	0.090	0.061	0.046

Wyngaarden and Walters [25]. This is due to the larger values of the differential cross section in the forward directions (see figures 1–4) resulting from the closure approximation imbedded in the TCW model. But, as the energy increases, the integrated cross sections of both the TCW and 40CC models approach the first Born values, as one would expect.

4. Concluding remarks

In the context of recent interest in the BBK wave function for ionization, we have discussed the two Coulomb waves (TCW) model of Dewangan [8] for direct excitation. We have seen that the TCW model for excitation corresponds to the BBK model for ionization. To examine the predictions of the TCW model, we have studied the $1s \rightarrow 2s$ excitation of hydrogen by electron impact in the energy range of 54.4 to 400 eV and compared them with the results of other sophisticated perturbative and nonperturbative models. We have seen that, because of the large difference in the eigenenergies of the $1s$ and $2s$ states, the closure approximation inherent in the model may not be well justified for the $1s \rightarrow 2s$ excitation as for transitions between excited states. In spite of this limitation, the TCW results give good agreement with the experimental differential cross sections at 54.4 eV by electron impact and also compare reasonably well with the predictions of other current sophisticated theoretical models.

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