Angular correlation and differential cross sections in $e^- - H(1\,^2S - 3\,^2P)$ excitation

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Differential cross sections and angular correlation parameters are calculated for electron-impact excitation of the $3\,^2P$ state in hydrogen from the ground 1^2S state using a distorted-wave approximation. The calculations are compared with the recently reported experimental and close-coupling theoretical results of J. F. Williams, A. T. Stelbovics, and I. Bray [J. Phys. B **26**, 4599 (1993)]. Present results show reasonably good agreement with both of their theoretical and experimental results.

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Electron-impact excitation of the $n=2$ states in hydrogen is fairly well studied, both theoretically and experimentally, but not much attention is paid to $n=3$ excitations in hydrogen. For example, if we consider the differential cross sections (DCS) for $3\,^2P$ excitation as well as the angular correlations resulting from its decay to the ground $1\,^2S$ state, we find that hardly any detailed studies exist [1]. The previous studies on $3\,^2P-1\,^2S$ decay are from Chwirot and Slevin [2] who performed in-plane angular correlation measurements only at 20° and 25° scattering angles for incident electron energies of 54.4 and 100 eV and the distorted-wave calculations of Katiyar and Srivastava [3]. The comparison of these experimental and theoretical results showed good qualitative agreement. Although detailed comparison was then not possible due to the lack of more experimental data.

Very recently, Williams, Stelbovics, and Bray [4] have reported detailed measurements of angular correlation parameters (ACP) λ, R, the circular polarization parameter I and the differential cross sections for the electron-impact excitation of hydrogen atoms to the $3\,^2P_j$ states. They presented their experimental results at an incident electron energy of 54.42 eV and for electron-scattering angles up to 35°. In this paper, they have also reported their converged close-coupling approximation (CCCA) calculations [5] and compared these with the experimental data. They obtained good agreement between their theory and experiment.

Over the years we have seen that a distorted-wave approximation (DWA) is quite suitable for the calculation of cross sections and angular correlation parameters for electron-impact excitation of atoms at intermediate and high incident energies and unlike close-coupling type calculations it does not suffer from the convergence problem at such energies [1,6]. The motivation therefore in this paper is to see whether a suitable DWA calculation can be performed which can provide a meaningful comparison with the recently reported results of Williams, Stelbovics, and Bray [4].

The present paper addresses the first-order form of the DWA. In fact, of all the possible theoretical approaches the first-order form of DWA has been very attractive and most widely used since it generally yields reasonably reliable results for a minimum of effort. Madison, Bray, and McCarthy [7] have performed exact second-order DWA calculations for elastic and inelastic ($n=2$) excitations in hydrogen at 54-eV incident electron energy (and have shown its superiority over first-order DWA term). These calculations are again difficult to adopt in general terms, i.e., for various transitions in hydrogen as well as in their extension to heavier atoms [6–8]. However, one could easily incorporate some of the second-order DWA features, e.g., polarization effect, through the first-order DWA using appropriate polarization potentials in the distortion potentials [9–11].

Further, the choice of the distorting potentials is one of the open questions in general for application of a DWA method. Let us say U_i and U_f are, respectively, the distortion potentials used to obtain initial and final channel projectile electron distorted waves. It should be noted that their choices are, in principle, arbitrary from a theoretical viewpoint and can be taken to be any mathematical form [6,12,13]. It has been, therefore, a practice to choose a physically meaningful distortion potential which can help in understanding the collision dynamics of the problem and can explain the experimental results closely. This aspect of flexibility in the choice of the distortion potential is basically one of the attractions of the DWA.

From an intuitive point of view, one would assume that the U_i be represented by the initial ground-state potential of the atom and the U_f by the final excited-state potential of the atom. This choice has been frequently adopted and is the traditional distorted-wave approach as described by Mott and Massey [14] (let us call this version of DWA the MM model). However, there are a number of DWA calculations [13] on hydrogen, helium, and other atoms which suggest, that the use of the same potential in both the channels, i.e., $U_i=U_f=U$ in the DWA theory, explains the experimental data in a better way. Also, the use of the same potential in both the channels ensures the orthogonality between the incident and scattered electron distorted waves [6,15]. In such calculations the choice of U is taken as either the initial ground-state atomic potential (U_g) or the excited final-state atomic potential (U_e). We refer a DWA calculation with $U=U_g$ as the GP model and when $U=U_e$ as the EP model.

In terms of the agreement with experiment, the picture has emerged that out of the MM, GP, and EP models, the EP model is the most suited for heavier atoms [13,16,17], while for lighter atoms, viz., hydrogen and helium, the situation is not as clear, as none of the above three models can be said to completely model the experimental data [13]. It looks like for better results, one would need to go for a second-order DWA calculation or improve the first-order DWA calculation by using some appropriate alternative choice for the distorting potentials [13,18,19]. From this point of view Srivastava, Katiyar, and Rai [18] proposed an alternative form of distorting the potential based on Slater's concept of transitions state. According to which, during an excitation process the projectile electron should not be described in the field of either the initial ground-state atomic potential as in the GP model or in the excited final-state atomic potential as in the EP model but by a hybrid potential in between. Srivastava, Katiyar, and Rai [18] therefore took the best in between potential as the average of both the potentials, i.e., $U=(U_g+U_e)/2$ to be the distortion potential in both the channels. They had applied their method to electron-impact $1\,^1S-2\,^1P$ excitation in helium and calculated DCS and ACP results which showed excellent agreement with the experimental data.

Our earlier DWA calculations [20] in the GP model as well as the MM- and EP-model test calculations that we carried out recently do not agree well with the experimental results of Williams, Stelbovics, and Bray [4]. In the light of the paper of Williams, Stelbovics, and Bray [4] we have therefore carried out a fresh DWA calculation for $1\,^2S-3\,^2P$ excitation in hydrogen by extending in a straightforward manner the DWA calculation of Srivastava, Katiyar, and Rai [18]. We report, in this paper, our results for DCS and ACP at 54.42 eV of incident electron energy. In our calculation, U_g and U_e are represented, respectively, by the initial and final spherically averaged atomic state static potentials plus their corresponding exchange potentials (see Srivastava [21]). In order to determine the importance of polarization effect of the target we also performed some test calculations by incorporating in our calculation the different forms of available polarization potentials [9–11]. However, the effect did not make any noticeable change in our results. Consequently the results reported here are excluding the polarization effects. This also makes us feel that for the present transition the second-order correction to DWA may not be very useful.

Before we present our results it would be desirable to explain briefly how we obtain our various ACP results from the scattering amplitudes. Let us choose the collision plane as the xz plane with the z axis along the direction of the incident electron. We denote the scattering amplitude for excitation of a magnetic sublevel m by a_m. Thus for $3p_m$ excitation of hydrogen we have a_m with $m=-1,0,1$. The three correlation parameters λ, R, and I which may be measured by the electron-photon coincidence experiment are given by

$$\lambda=\langle |a_0|^2\rangle/\sigma \ , \tag{1}$$

$$R=\mathrm{Re}\langle a_1 a_0^* \rangle/\sigma \ , \tag{2}$$

$$I=\mathrm{Im}\langle a_1 a_0^* \rangle/\sigma \tag{3}$$

with differential cross section $\sigma=\langle |a_0|^2\rangle+2\langle |a_1|^2\rangle$. Here Re and Im refer to real and imaginary parts, respectively, and $\langle\ \rangle$ means the spin average defined by

$$\langle a_m a_m^* \rangle=(a_m^s a_m^{s*}+3a_m^t a_m^{t*})/4 \ , \tag{4}$$

where superscripts s and t refer to the singlet and triplet amplitudes, respectively.

The electron-photon coincidence count rate for decay of $3\,^2P_j$ state in terms of λ and R is expressed as a function of photon detector angle θ_γ by

$$N(\theta_\gamma)=[4+3\lambda+3(1-2\lambda)\cos^2\theta_\gamma-3\sqrt{2}R\sin 2\theta_\gamma] \ . \tag{5}$$

Further, the λ, R, and I are related to the ACP defined by Andersen, Gallagher, and Hertel [22] (i.e., parameters γ, P_l, and L_y) through the relations

$$\tan 2\gamma=-2\sqrt{2}R/(2\lambda-1) \ , \tag{6}$$

$$P_l=\sqrt{8R^2+(2\lambda-1)^2} \ , \tag{7}$$

$$L_y=-2\sqrt{2}I \ . \tag{8}$$

Here γ is the "alignment angle" of the electron charge cloud of the excited state of hydrogen from the incident direction, P_l is the "linear polarization" of the charge cloud, and L_y is the "angular-momentum transferred" perpendicular to the scattering plane. Finally, we also calculate, $P^+=\sqrt{P_l^2+L_y^2}$, the measure of the degree of polarization.

We present our various calculated DWA results through Figs. 1–3. In each figure we have included for comparison the recent experimental data and the close-coupling theoretical results (viz., 70 cc calculations) of Williams, Stelbovics, and Bray [4]. Figure 1 shows the coincidence count rate [cf. Eq. (5)] with respect to the photon detection angles θ_γ ranging from 0° to 180° for scattering angles $\theta=3°$, 10°, 25°, and 35°. We see from this figure that for smaller scattering angles (viz., $\theta\le 25°$) the agreement between the two theories, i.e., CCCA and DWA, and their agreement with the experiment are excellent. In general, as the scattering angle increases the uncertainties in experiment are seen to increase with the maximum at $\theta=35°$. Also the two theories tend to differ from each other as well as with the experiment.

In Fig. 2, the DCS results (σ) along with λ, R, and I parameters are shown. For DCS, we see the DWA results are a bit higher especially in the forward direction as compared to CCCA results where no experiment exist. While at other scattering angles both the theoretical curves lie within the experimental error bar. For λ parameter, we find that the DWA results are in excellent agreement with experiment while the CCCA calculation slightly overestimates the results at angles $\ge 20°$ with respect to the experiment. For R and I parameters the CCCA can be said to be giving over all better agreement with the experiment as compared to the DWA. Further, from the present comparisons in Fig. 2 it is difficult to comment on the relative superiority between the two theories as compared to the experiment until more data

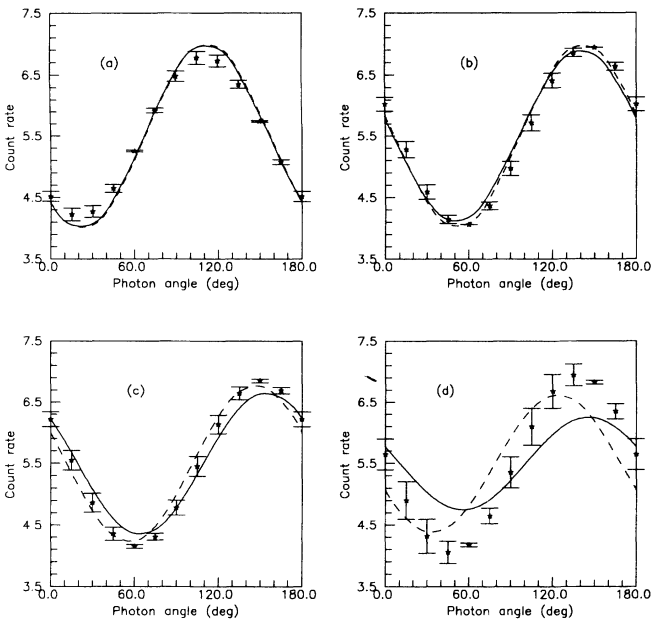

FIG. 1. The electron-photon angular correlations for the excitation to the $3\,^2P$ state in hydrogen for scattering angle θ_e = (a) 3°, (b) 10°, (c) 25°, (d) 35° at 54.42 eV of electron impact energy. CCCA results [4] (— — —); experiment [4] (* * *); present DWA results (——).

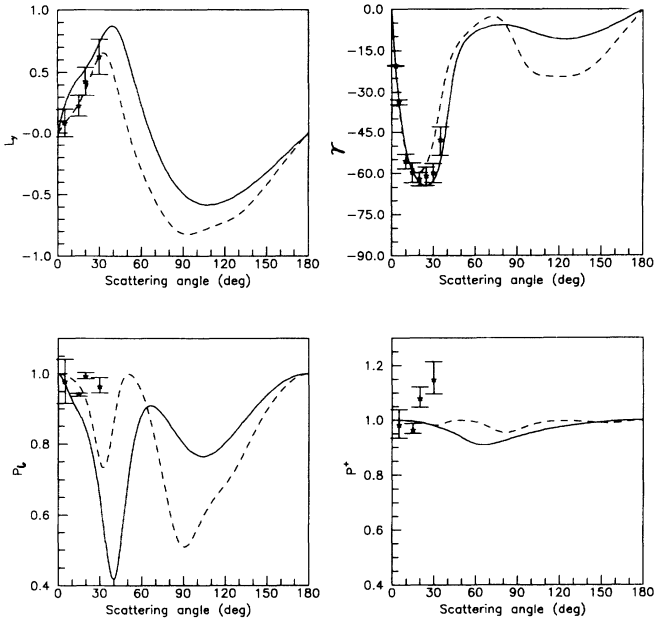

FIG. 3. The orientation parameters, Ly, alignment angle, γ, and coherence parameters, P_l and P^+, for $1\,^2S-3\,^2P$ excitation in hydrogen at incident energy of 54.42 eV. The notations for theoretical calculations and experiment are the same as in Fig. 1.

at larger scattering angles are available. In fact, the results for λ, R, and I are quite sensitive with respect to the scattering angles. Though λ is dependent only on the magnitudes of the complex amplitudes for $m=0$ and 1 magnetic substates can be said to be less sensitive as compared to R and I which depend also on the relative phases between these amplitudes [see Eqs. (1)–(3)]. Thus the better agreement of a theory with experiment for R and I along with λ would be ideal. However, it is generally seen that no single calculation accurately predicts the measured behavior of all the DCS and ACP results simultaneously for any system [1,22,23].

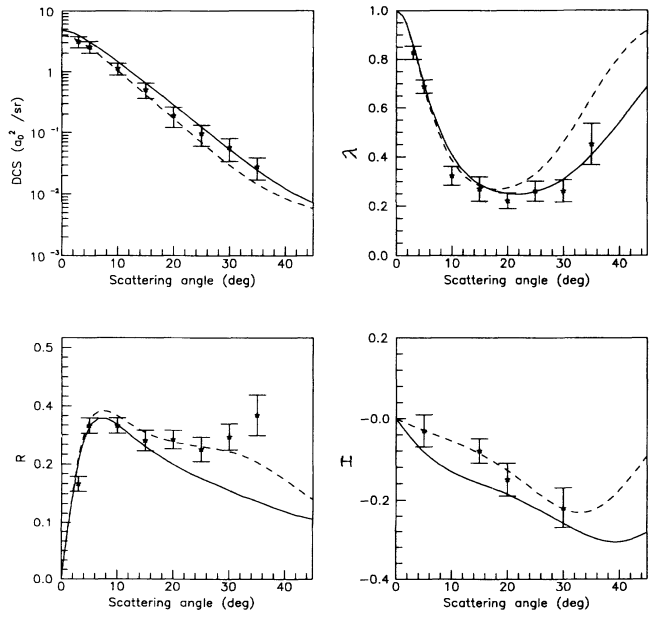

FIG. 2. Differential cross section (in units of a_0^2/sr), λ, R, and I parameters for $1\,^2S-3\,^2P$ excitation in hydrogen at incident electron energy of 54.42 eV. The notations of theoretical calculations and experiment are the same as in Fig. 1.

Finally, in Fig. 3, we compare L_y, γ, P_l, and P^+ parameters in the whole range of scattering angles (0°–180°). From this figure we see that for all the four parameters there is in general good agreement of both the theories with the experiment. However, this agreement is best for the γ and L_y parameters. For P^+ which should be ≤ 1 we see that both the theories agree quite well with the experimental data for 5° and 15° scattering angles while at higher angles, viz., 20° and 30°, the experimental results seem in error of being greater than unity. Further, it is interesting to note that though the two theories give results which resemble one another in shape they differ in magnitude especially for larger scattering angles. It would thus be interesting if more measurements were made available in the future in order to understand the differences in the two theories.

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