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Electron-impact excitation of the $n=2$ level of atomic hydrogen at low incident energies

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Excitation ($n=2$ level) of the hydrogen atom by electron impact has been studied by using a Callaway-type variant of the polarized-orbital method. The incident wave contains the effect of exchange polarization. Two sets of differential cross sections at three incident energies near the threshold have been obtained. Our results of model II are in good agreement with measured values. The results of our model I are unsatisfactory at large scattering angles.

INTRODUCTION

There is a large number of theoretical attempts to investigate the excitation of atoms by electron impact near the threshold energies. The success is very limited. Even in the case of the hydrogen atom the situation is far from satisfactory. The failure of a few-state close-coupling approximation is well known (Kingston *et al.*[1] and Burke *et al.*[2]). Brandt and Truhlar[3] have applied a six-state close-coupling approximation to investigate the problem. Their results are reasonably good when compared with measured values.[4] Another good attempt has been made by Callaway *et al.*[5,6] who have used the hybrid pseudostate close-coupling distorted-wave model. The hydrogen atom has been represented by eleven states including four physical ($1s$, $2s$, $2p$, and $3d$) atomic states plus seven pseudostates. Instead of solving the integro-differential equation directly, they have solved the problem using the algebraic close-coupling approximation, following the method of Callaway and Wooten.[7] For partial waves $l \leq 3$ they have obtained the amplitude using the above method. The distorted-wave polarized-orbital method[8] and direct Born approximation have been used to determine the contribution of higher partial waves. Except at 13.6 eV their results are in reasonably good agreement with the measured values.[4] It may be pointed out that the methods of Brandt and Truhlar[3] and Callaway *et al.*[5,6] are laborious and time consuming. It is very difficult to apply these methods to heavier atoms. It is suggested that one should use a tractable method. In a series of papers, McDowell and his co-workers[8,10] have tried to use the polarized-orbital method to investigate this problem. The results of Scott and McDowell[10] near the threshold energies are not very satisfactory. In their study, they assumed that the polarized-orbital wave function is a good representation of the total wave function. They have followed the method of Temkin and Lamkin.[11] The potential used in this method contains excess attraction. Their elastic results[11,12] necessarily show this. Moreover, their method contains the effect of only adiabatic dipole polarization potential. The adiabatic approximation is expected to fail with the increase of energy and it overestimates the elastic cross section at high energies.

Here we reinvestigate the problem using a polarized-orbital method. We have assumed that the total incident wave is well represented by the polarized-orbital wave function. There are many variants of the polarized-orbital method. Here we have followed the method of Callaway *et al.*[13] Their formalism, apart from the adiabatic polarization potential, gives rise to a first-order correction term and to an adiabatic correction term. Callaway *et al.*[13] have not included the effect of an exchange polarization potential in their calculations. Daskhan *et al.*[14] have included this effect to study elastic electron-hydrogen atom scattering. Their potential contains the first three multipole comments ($l=0$, 1, and 2) of adiabatic polarization potential and the first two ($l=0$ and 1) components of the nonadiabatic one. It has been found that their effective potential is slightly less attractive than the desired one.

In our earlier investigation[15] we have applied this method to investigate the problem where we have neglected the matrix elements that arise from the distorted wave function. Our results are encouraging. Here, in this paper, we have included all the matrix elements. The motivation of the paper is to find the suitability of the polarized-orbital method to investigate the excitation processes.

THEORY

The total polarized wave function for the electron-hydrogen system may be given as

$$\Psi^{\pm}(\vec{r}_1,\vec{r}_2)=(1\pm P_{12})\chi(\vec{r}_1,\vec{r}_2)F^{\pm}(\vec{r}_1) \qquad (1)$$

with

$$\chi(\vec{r}_1,\vec{r}_2)=\Phi_0(\vec{r}_2)+\Phi_d(\vec{r}_1,\vec{r}_2)\ . \qquad (2)$$

Here, P_{12} permutes $\vec{r}_1$ and $\vec{r}_2$ and the upper and lower signs represent the spin states. $\Phi_0(\vec{r}_2)$ is the wave function of the hydrogen atom in its ground state and $\Phi_d(\vec{r}_1,\vec{r}_2)$ is the first-order perturbed wave function induced in the target by the presence of an incident electron.

Total wave function Ψ satisfies the Schrödinger equation

$$(H-E)\Psi^{\pm}(\vec{r}_1,\vec{r}_2)=0\ . \qquad (3)$$

Projecting onto $\chi(\vec{r}_1,\vec{r}_2)$ one can obtain the following integrodifferential equation:

$$[\nabla^2_{r_1}+k_1^2+V_s(r_1)-V_d(r_1)]F^{\pm}(\vec{r}_1)=\int d\vec{r}_2\chi^*(\vec{r}_1,\vec{r}_2)(H-E)\chi(\vec{r}_2,\vec{r}_1)F^{\pm}(\vec{r}_2) \qquad (4)$$

subject to the normalization condition

$$\int |\chi(\vec{r}_1,\vec{r}_2)|^2 d\vec{r}_2=1 \qquad (5)$$

for all values of the incident electron coordinates r_1. Here V_s is the static potential and V_d is the distortion potential in the sense of Callaway *et al.*[9] (Here V_d consists of the sum of the monopole, dipole, and quadrupole components of the adiabatic polarization potential plus the monopole and dipole component of the nonadiabatic distortion potential.)

Equation (4) with the normalization constraint (5) is variationally consistent. The solution of Eq. (4) is not an easy task. It is also not true that the solution of Eq. (4) necessarily gives reliable results (Callaway[16] and Oberoi and Callaway[17]), because the choice of our trial function may not be good enough. Instead of solving Eq. (4) we have solved the following integrodifferential equation (Daskhan *et al.*[14]):

$$[\nabla^2_{r_1}+k_1^2+V_s(r_1)-V_d(r_1)]F^{\pm}(\vec{r}_1)=\int d\vec{r}_2\Phi_0^*(\vec{r}_2)(H-E)\chi(\vec{r}_2,\vec{r}_1)F^{\pm}(\vec{r}_2)\ . \qquad (6)$$

We have performed the partial-wave analysis of Eq. (6) following Daskhan *et al.*[14] It may be mentioned that in calculating the exchange terms, the normalization constraint of Temkin and Lamkin[11] has been employed.

We have followed the method of Scott and McDowell[10] in calculating T-matrix elements

$$T^{\pm}_{\text{if}}=\langle\Phi_f(\vec{r}_2)\chi_{k_f}(\vec{r}_1)\,|\,V_f\,|\,\Psi_i^{\pm}(\vec{r}_1,\vec{r}_2)\rangle\ , \qquad (7)$$

where $\Psi_i^{\pm}(\vec{r}_1,\vec{r}_2)$ is given by Eq. (1). Here, $\chi_{k_f}(\vec{r}_1)$ is the outgoing plane wave and $\Phi_f(\vec{r}_2)$ stands for the final-state target wave function. The direct channel interaction potential is taken in the present calculations.

Here, the T-matrix element can be expressed in terms of its four components

$$T^{\pm}_{\text{if}}=(T^{D}_{\text{if}}+T^{PD}_{\text{if}})\pm(T^{E}_{\text{if}}+T^{PE}_{\text{if}}) \qquad (8)$$

we have followed the method of McDowell and his collaborators[9,10] in calculating the four matrix elements.

RESULTS AND DISCUSSIONS

The differential cross sections at three incident electron energies are plotted in Figs. 1–3 and tabulated in Table I (model I). We have presented two sets of results that have been obtained from the following relations: model I,

$$T^{\pm}_{\text{if}}=(T^{D}_{\text{if}}+T^{PD}_{\text{if}})\pm(T^{E}_{\text{if}}+T^{PE}_{\text{if}})\ ,$$

model II,

$$T^{\pm}_{\text{if}}=(T^{D}_{\text{if}}+T^{PD}_{\text{if}})\pm T^{E}_{\text{if}}\ .$$

In other words, our model II neglects the contribu-

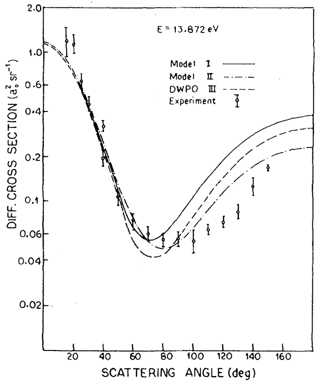

FIG. 1. Differential cross section for electron-impact excitation of H ($n=2$).

tion of the matrix element that arises from the exchange distorted wave function.

At all the incident energies given here, our two models and the distorted-wave polarized orbital (DWPO III) (Scott and McDowell)[10] predict a reliable cross section up to the scattering angle 50°. At 13.872 eV, the results of model I are in good agreement with the measured values[4] up to the scattering angle 80°. Above this scattering angle, model I overestimates the cross section appreciably. In this angular region, our values differ from that of DWPO III by about 20%, our values being higher. On the other hand, results of model II lie below the prediction of Scott and McDowell[10] above the scattering angle 85° and are in better agreement with the experimental values. Out of the three theoretical results plotted here, our model II results are in best agreement with the observed findings.

At the incident energy 16.456 eV, the agreement between the observed data and theoretical values are in better agreement than those at 13.872 eV. As in the previous case, the results of model I overestimate the cross section at large scattering angles. In this angular range, our results differ from those of Scott and McDowell[10] by about 16%, our values being higher. The results of model II are in very good agreement at all scattering angles. It may be mentioned that at these two energies, the results of our earlier paper,[15] in which the contributions of T_{if}^{D} and T_{if}^{E} have been included, are also in good agreement with measured values.

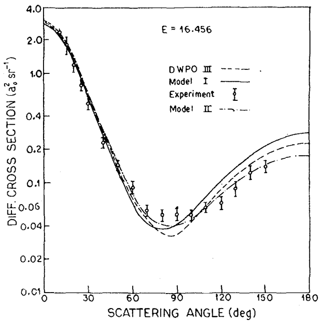

FIG. 2. Differential cross section for electron-impact excitation of H ($n=2$).

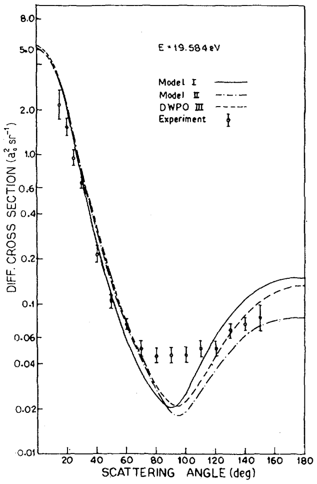

FIG. 3. Differential cross section for electron-impact excitation of H ($n=2$).

At the incident energy 19.584 eV, agreements between the theoretical values and experimental findings are not good above the scattering angle 70°. Three theoretical curves maintain the same features as shown at lower energies.

Our two models necessarily suggest that the large-angle behavior of the cross section is appreciably influenced by the exchange polarization term. This has also been noticed by Scott and McDowell.[10] Incident wave functions contain also the effect of the exchange polarization. This might be responsible for the large-angle behavior of our model II. Although theoretically inconsistent, our model II may be the suitable method for obtaining excitation cross section.

One of the probable reasons for this large-angle behavior is due to the fact that in the exchange channel in the present method, as well as in DWPO III, adiabatic assumption has been made. In this said energy range, the effect of continuum is expected to influence the cross section appreciably. This form of the polarized-orbital wave function has not taken the effect of continuum adequately.

TABLE I. Differential cross section in units of $a_0^2\,\mathrm{sr}^{-1}$ for electron-impact excitation of the $n=2$ level of atomic hydrogen computed in model I at incident energies of 1.02, 1.21, and 1.44 Ry.

θ		$E=1.02$ Ry			$E=1.21$ Ry			$E=1.44$ Ry	
(deg)	2s	2p	Total	2s	2p	Total	2s	2p	Total
0	6.07−2	1.15	1.21	9.97−2	2.93	3.03	2.07−1	5.64	5.84
10	5.47−2	1.01	1.06	8.64−2	2.38	2.46	1.75−1	4.06	4.23
20	4.06−2	6.90−1	7.31−1	5.53−2	1.34	1.39	1.04−1	1.83	1.93
30	2.69−2	3.90−1	4.17−1	2.46−2	6.14−1	6.39−1	4.01−2	6.91−1	7.31−1
40	1.99−2	1.96−1	2.16−1	7.30−3	2.70−1	2.77−1	8.80−3	2.62−1	2.71−1
50	2.06−2	9.16−2	1.12−1	4.40−3	1.19−1	1.24−1	3.70−3	1.09−1	1.13−1
60	2.58−2	4.17−2	6.75−2	9.60−3	5.37−2	6.33−2	7.80−3	5.01−2	5.79−2
70	3.17−2	2.26−2	5.43−2	1.63−2	2.63−2	4.26−2	1.08−2	2.55−2	3.57−2
80	3.65−2	2.23−2	5.88−2	2.13−2	1.67−2	3.80−2	1.13−2	1.31−2	4.40−2
90	4.03−2	3.59−2	7.62−2	2.42−2	1.68−2	4.10−2	1.14−2	9.02−3	2.06−2
100	4.04−2	6.10−2	1.05−1	2.58−2	2.73−2	5.31−2	1.21−2	1.40−2	2.61−2
110	4.75−2	9.54−2	1.43−1	2.75−2	4.99−2	7.74−2	1.47−2	2.67−2	4.14−2
120	5.13−2	1.36−1	1.87−1	2.99−2	8.06−2	1.11−1	1.83−2	4.38−2	6.21−2
130	5.49−2	1.79−1	2.34−1	3.33−2	1.12−1	1.45−1	2.21−2	6.29−2	8.50−2
140	5.79−2	2.21−1	2.79−1	3.73−2	1.40−1	1.78−1	2.49−2	8.42−2	1.09−1
150	6.01−2	2.58−1	3.18−1	4.14−2	1.70−1	2.12−1	2.66−2	1.05−1	1.32−1
160	6.14−2	2.87−1	3.48−1	4.50−2	2.04−1	2.49−1	2.75−2	1.18−1	1.37−1
170	6.20−2	3.05−1	3.67−1	4.76−2	2.32−1	2.80−1	2.79−2	1.26−1	1.54−1
180	6.22−2	3.11−1	3.73−1	4.85−2	2.43−1	2.91−1	2.80−2	1.27−1	1.55−1

We conclude that the representation of the total incident wave by the polarized-orbital method of Temkin and Lamkin[11] or that of Callaway[13] may not be suitable.[16] There are two ways of improving this result in the framework of the polarized-orbital method. One can use a distorted-wave method in which the final channel wave function is replaced by a distorted one. This suggestion has also been made by Bransden and McDowell.[18] One may also use a two-function polarized-orbital method to represent the total wave function of the incident channel.[19]

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