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Addresses for correspondence: The Chief Editor, East African Journal of Physical Sciences, School of Pure and Applied Sciences, Kenyatta University, P.O. Box 43844, Nairobi, Kenya. *E-mail*: scchhabra@avu.org

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A study of angular correlation parameters using a distorted wave model

C. S. Singh

Department of Physics, Kenyatta University, P. O. Box 43844, Nairobi, Kenya

We have used a distorted wave model suggested by Singh in calculating the angular correlation parameters λ and R for electron–hydrogen collision. In this model the initial state distorted wave is generated by the static potential in the initial state and the final state distorted wave is generated by a potential taken as the sum of one-half of the initial state static potential plus one-half of the final state static potential. The results have been compared with other theoretical and experimental results.

Key words: electron impact excitation, angular correlation parameters, distorted wave method, distortion potential

INTRODUCTION

The distorted wave model suggested by Singh (Singh, 1993) was first used for 1s-2s excitation of hydrogen atom. At 54.4 eV electron impact energy it gave the best fit with the experimental differential cross section results compared with other distorted wave model results. Later it was used (Onyango, 1996) for 1s-2p excitation of hydrogen atom by electron impact and it was found that in this case the differential cross section results due to this model were not in as good agreement with the experimental results as the results due to same other distorted wave models. Looking at these two sets of results, we thought it necessary to make a study of angular correlation parameters λ and R for $e^- - H$ scattering using this model, so that definite conclusion can be made on its suitability.

THEORY

Distorted Wave Method

The distorted wave formula can be easily derived from the two-potential scattering model (Joachain, 1983). In this model the interaction potential is broken into two parts: one which is treated exactly and the other which can be solved in an approximate manner.

Let the total Hamiltonian H of the system of an electron (projectile) and an atom (target) be:

$$H = H_0 + V \quad (1)$$

where H_0 is the Hamiltonian of the target atom plus the non-interacting projectile electron and V is the interaction between the electron and the atom.

Now we divide the interaction potential into two parts

$$V = U + W \quad (2)$$

and assume that the collision problem under the potential U can be solved exactly, that is the solution of the equation

$$(H_0 + U)\chi = E\chi \quad (3)$$

is known. E is the total energy of the system. The transition matrix for the excitation of initial state i to final state f is given by

$$T = \langle \chi_f | U | \psi_i \rangle + \langle \chi_f | W | \Psi_i \rangle \quad (4)$$

Here Ψ and ψ are the solutions of the equations

$$H_0 \psi = E \psi \quad (5)$$

$$\text{and} \quad H \Psi = E \Psi \quad (6)$$

Ψ_i satisfies the outgoing wave boundary conditions.

χ_f is a solution to equation (3) with incoming wave boundary conditions. The T -matrix given by relation (4) is exact but we cannot solve equation (6) to know Ψ exactly. So, it is here that the distorted wave method is introduced when we replace Ψ in equation (4) with its approximation as χ . The wave function of the electron is distorted by the potential U . The T -matrix now takes the form

$$T = \langle \chi_f | U | \psi_i \rangle + \langle \chi_f | W | \chi_i \rangle \quad (7)$$

χ_i satisfies equation (3) with outgoing wave boundary conditions.

If we take U as the static potential of the initial or final target states or any linear combination of these, the first term in equation (7) vanishes and we get

$$T = \langle \chi_f | W | \chi_i \rangle \quad (8)$$

While applying the distorted wave method (expression 8) we first determine the distortion potential U . There are numerous forms of it. But the most natural form is the static potential of the target atom. Many calculations (Itikawa, 1986), using the static potential of the atom as the distortion potential, have been performed with the following variations:

- (i) initial state distorted wave is generated by the static potential in the initial state and final state distorted wave is generated by the static potential in the final state,
- (ii) both initial- and final-state distorted waves are generated by the static potential in the initial state, and
- (iii) both initial and final state distorted waves are generated by the static potential in the final state.

In our model (Onyango & Singh 1997) the initial state distorted wave is generated by the static potential in the initial state and the final state distorted wave is generated by a potential taken as the sum of the one-half of the initial state static potential and one-half of the final state static potential. This is based on the following reasoning:

When the electron is in the initial state, for all the time it is in the field of the initial state of the target. Hence the distortion potential for the projectile electron in the initial state should be taken as the static potential of the target atom in its initial state.

When the energy from the projectile electron is transferred to the target atom, the atom takes time (transition time) to go to its final state. That is, there is a time lag between the time of transfer of energy and the instant when the atom reaches its final state. Thus the projectile electron in its final state 'sees' a potential which is intermediate between the initial- and final-state static potentials. Hence the final state distortion potential has been taken as the sum of one-half of the initial state static potential and one-half of the final state static potential.

Angular Correlation Parameters

The angular correlation parameters λ and R represent a more sensitive test of any theory. They are defined as follows:

$$\lambda = \sigma_0 / \sigma$$

and

$$R = \text{Re} \langle f_0^* f_1 \rangle / \sigma$$

where the spin average $\langle \rangle$ is defined as

$$\langle f_m^* f_m \rangle = \frac{1}{4} [f_m^s f_m^s + 3f_m^T f_m^T]$$

with f_m^s the spin independent singlet amplitude (direct + exchange) and f_m^T the triplet amplitude (direct + exchange) for exciting the magnetic sublevel m , the differential cross section for exciting a magnetic sublevel is

$$\sigma_m = \langle f_m^* f_m \rangle$$

and the total differential cross section σ is the sum of σ_m over all magnetic sublevels.

RESULTS AND DISCUSSION

In this calculation we used the computer program written by Madison and Bartschat (1996) with some modifications to make it calculate the λ and R parameters. The λ and R parameters results of our calculation for the excitation of the 2p state of hydrogen atom by electron impact at 54.4 eV electron impact energy are shown in Figure 1. The results are compared with some other first order distorted wave results, a second order distorted wave results (Madison *et al.*, 1991), convergent close coupling results (Bray & Stelbovics, 1992; Bubelev *et al.*, 1995) and the experimental results of Williams (1981). In the Figure 1, II refers to the distorted wave model in which both initial- and final-state distorted waves are generated by the initial state static potential, IF refers to the distorted wave model in which the initial state distorted wave is generated by the initial state static potential and the final state distorted wave is generated by the final state static potential, and MW refers to the distorted wave model in which the initial- and final-state distorted waves are generated, as suggested by Madison and Winters (1983), by a potential which is the sum of one-

third of the initial state static potential plus two-thirds of the final state static potential. We see in the Figure 1 that at lower angles ($<60^\circ$) all the first order results are in somewhat agreement with the experimental results both for λ and R parameters. But at higher angles ($>60^\circ$ and $<150^\circ$) they are in

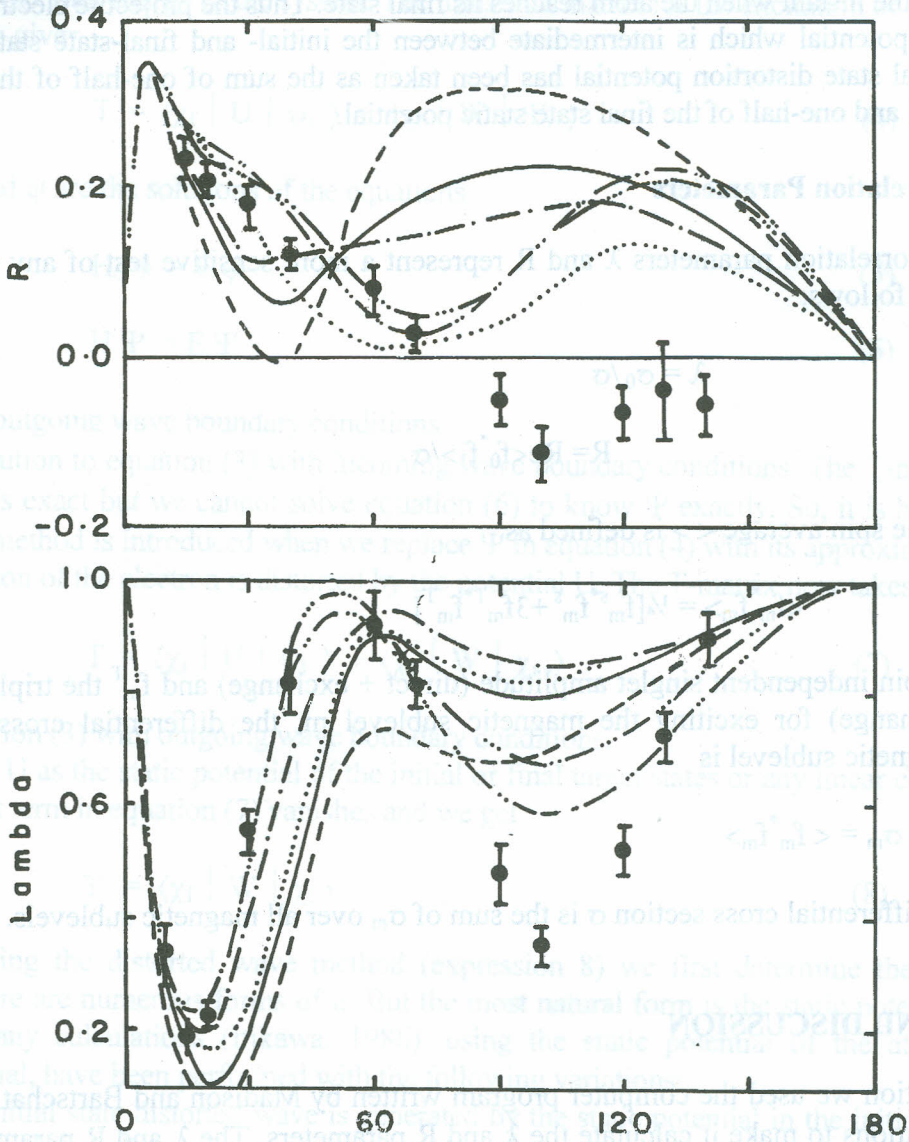


Figure 1. Lambda and R parameters for 54.4 eV excitation of 2p state of hydrogen.

— : results of the present model; : results of model II; - - - - - : results of model IF; - · - · - : results of model MW; — · — · — : second order Born results (Madison *et al.*, 1991); — ···— : convergent close coupling results (Bubelev *et al.*, 1995; Bray & Stelbovics, 1992); • : experimental results (Williams, 1981).

very poor agreement with the experimental results. The second order Born and convergent close coupling (CCC) results are in very good agreement with the experimental results for the lower ($\leq 60^\circ$) and higher ($\geq 130^\circ$) angles in case of λ parameter. But in case of R

parameter even these calculations are giving results which are poor at intermediate and higher angles. (Possibly because the R parameter depends directly upon the complex nature of the amplitude.) At lower angles the R parameter results of the CCC and second order Born results are in very good agreement with the experimental results.

In case of λ Parameter, at lower angles, the MW results are best among the first order calculations and at higher angles all the first order results are in poor agreement with the experimental results. In case of R parameter, at lower angles, up to 30° , all the first order results (except the IF results) are in good agreement with the experimental results. But in the range $30-60^\circ$ the II results are the best. At higher angles all first order results are poor.

CONCLUSION

From the above and the findings in earlier two papers (Onyango, 1996; Onyango & Singh 1997) we conclude that it cannot be said definitely which first order distorted wave method is the best one. Their performance varies depending upon the situation being considered (that is which excitation process is being considered and at what impact energy). A distorted wave method may perform well for a particular excitation at a particular energy but it may not give good results for other excitation process or for the same excitation process but at different impact energies. Also, it may be concluded that a first order distorted wave method cannot be improved to the extent that its results can match with the second order results.

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From the above and the findings in earlier two papers (Ojha *et al.* 1990, Ojha & Singh 1997) we conclude that it cannot be said definitely which first order distorted wave method is the best one. Their performance varies depending upon the situation being considered (that is which excitation process is being considered and at what impact energy). A distorted wave method may perform well for a particular excitation at a particular energy but it may not give good results for other excitation process or for the same excitation process but at different impact energies. Also, it may be concluded that a first order distorted wave method cannot be improved to the extent that its results can match with the second order results.



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