

A theoretical study of fast electron–atomic hydrogen scattering

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Abstract. The second order diagonalization method with a twenty states basis is used to study electron–atomic hydrogen scattering. The electron trajectory chosen makes the quantum Born approximation and the impact parameter Born approximation equivalent. Results for differential and total cross sections and for polarizations are presented and compared with experiments and other theoretical calculations.

1. Introduction

In two preceding papers, we have used the second order diagonalization method to study proton–atomic hydrogen scattering (Baye and Heenen 1973a) and proton–helium scattering (Baye and Heenen 1973b). We now extend our work to the collisions of electrons with the same atoms. Our aim is to confirm in electron collisions the very good agreement found between our theoretical results and experiments in proton–helium scattering. The large amount of experimental data in electron collisions will make this comparison particularly fruitful.

In this paper, we shall apply our theory to electron–atomic hydrogen scattering. The principal interest of collisions with hydrogen is that the wavefunctions of this atom are known exactly. In the case of the scattering with protons, there were no experimental data in the energy range studied. The situation is more favourable in the electron case, because there are experiments concerning the $n = 2$ level which allow an interesting comparison between theory and experiment.

In the next section, we briefly remind the reader of the most important features of the second order diagonalization method and we describe the form of the eikonal approximation used to determine differential cross sections with impact parameter transition amplitudes. We choose a trajectory which makes the quantum Born approximation and the eikonal form of the impact parameter Born approximation equivalent.

In § 3, we discuss various theoretical results for the $n = 2$ level and we calculate some quantities which can be compared to the experimental data. For the higher states, we compare our results for total cross sections with some other theoretical calculations. Differential cross sections for the $n > 2$ states are not presented here and are available on request.

2. Theory

The second order diagonalization method has been presented in Baye and Heenen (1973a). It is an impact parameter approximation for the collision of a structureless

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charged particle on a target whose hamiltonian is H_0 , with eigenstates $|n\rangle$. The Coulomb interaction between target and projectile is represented by H_{int} . The transition amplitude for an initial state $|o\rangle$ and a final state $|p\rangle$ is given by:

$$a_{po}(\mathbf{b}) = \langle p | e^{i\Omega} | o \rangle$$

where \mathbf{b} is the impact parameter and Ω is the following operator:

$$\Omega = -\frac{1}{\hbar} \int_{-\infty}^{+\infty} H_T(t_1) dt_1 + \frac{i}{\hbar^2} \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{t_1} dt_2 [H_T(t_1), H_T(t_2)],$$

where

$$H_T = \exp[(i/\hbar)H_0 t] H_{\text{int}} \exp[(-i/\hbar)H_0 t].$$

The matrix elements of the operator Ω are different in the electron collision from the proton or positron case. The second term of Ω is charge invariant while the first one depends on the sign of the charge of the projectile. The a_{po} are calculated by the diagonalization of the operator Ω in a restricted basis. In the following, this basis will always consist of the 20 lower states of hydrogen (1s to 4f₃) and the initial state will always be the ground state.

To calculate differential cross sections, we use the relation between semi-classical transition amplitudes and scattering amplitudes determined in the eikonal approximation (Byron 1971)

$$T_{po} = \frac{k_i}{2\pi i} \int e^{i\mathbf{q}\cdot\mathbf{b}} a_{po}(\mathbf{b}) d\mathbf{b}, \quad (1)$$

with $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$.

In this relation \mathbf{k}_i and \mathbf{k}_f are the initial and final wavevectors of the incident electron. The scattering amplitude T_{po} is related to the differential cross sections by

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} |T_{po}|^2.$$

Total cross sections are calculated by integration of $d\sigma/d\Omega$ over Ω .

As shown in Baye and Heenen (1973a), the second order diagonalization method contains the first and second orders of the impact parameter Born approximation. Hoping to enlarge the range of validity of our method at low energies and large angles (where quantum Born differs significantly from impact parameter Born approximation), we have chosen, following a suggestion of Vanderpoorten (private communication) a trajectory along the z axis which makes both forms of the Born approximation mathematically equivalent. This approximation gives the exact high energy behaviour for the cross sections.

The scattering amplitude in the quantum first Born approximation is given by:

$$T_{po}^Q = \frac{1}{2\pi i} \int e^{i\mathbf{q}\cdot\mathbf{R}} V_{po}(\mathbf{R}) d\mathbf{R}$$

with

$$\mathbf{R} = \mathbf{b} + z\hat{z}$$

and

$$V_{po} = \langle p | H_{\text{int}} | o \rangle.$$

In the eikonal impact parameter Born approximation, we have:

$$T_{p_0}^E = \frac{k_i}{2\pi i} \int e^{i\mathbf{q} \cdot \mathbf{b}} a_{p_0}(\mathbf{b}) d\mathbf{b}$$

with

$$a_{p_0}(\mathbf{b}) = \frac{1}{k_i} \int_{-\infty}^{+\infty} \exp\left(i \frac{E_p - E_o}{k_i} z\right) V_{p_0}(\mathbf{R}) dz.$$

So, we must have:

$$q_z = (\mathbf{k}_i - \mathbf{k}_f) \cdot \hat{\mathbf{z}} = \frac{E_p - E_o}{k_i} \quad (2)$$

where E_p and E_o are the energies of the final and initial states.

The relation (2) determines the angle α (see figure 1). We can see that α tends to $\frac{1}{2}\theta$ with increasing energy and with increasing θ , but is very different for small θ . Our differential cross sections are lower at small angles than those we would have obtained if we had chosen $\alpha = \frac{1}{2}\theta$, while our total cross sections are less modified. After having calculated T_{p_0} , we must perform a rotation of an angle $-\alpha$ in order to bring the z axis along \mathbf{k}_i . The dependence of $a_{p_0}(\mathbf{b})$ on the φ angle is $e^{im\varphi}$, if $|\mathbf{p}\rangle$ is a state with magnetic quantum number m . We may therefore perform the integration over φ in equation (1).

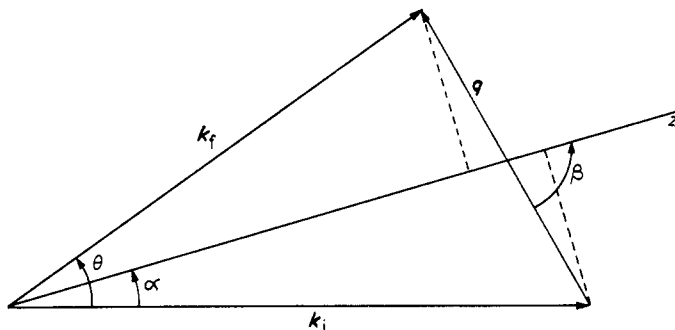


Figure 1. Choice of the z axis.

We have:

$$\mathbf{q} \cdot \mathbf{b} = qb \sin \beta \cos \varphi$$

with

$$\sin \beta = \left(1 - \frac{(E_p - E_o)^2}{q^2 k_i^2}\right)^{1/2}$$

so that we find

$$T_{p_0} = -ik_i \int_0^\infty J_m \left[qb \left(1 - \frac{(E_p - E_o)^2}{q^2 k_i^2}\right)^{1/2} \right] a_{p_0}(b) b db$$

the $a_{p_0}(b)$ being determined by use of the second order diagonalization method.

3. Results

We show in table 1 the total cross sections obtained with a twenty states basis.

Table 1. Total cross sections for the excitation of atomic hydrogen by electrons obtained with a 20 states basis

E (eV)	50	100	200	400
2s	$0.712^{-1}\dagger$	0.476^{-1}	0.268^{-1}	0.144^{-1}
2p ₀	0.426	0.242	0.131	0.663^{-1}
2p ₁	0.569	0.467	0.333	0.221
3s	0.111^{-1}	0.792^{-1}	0.475^{-2}	0.268^{-2}
3p ₀	0.802^{-1}	0.413^{-1}	0.212^{-1}	0.103^{-1}
3p ₁	0.103	0.840^{-1}	0.584^{-1}	0.381^{-1}
3d ₀	0.758^{-2}	0.250^{-2}	0.104^{-2}	0.526^{-3}
3d ₁	0.813^{-2}	0.377^{-2}	0.138^{-2}	0.388^{-3}
3d ₂	0.458^{-2}	0.372^{-2}	0.241^{-2}	0.145^{-2}
4s	0.317^{-2}	0.245^{-2}	0.155^{-2}	0.922^{-3}
4p ₀	0.260^{-1}	0.143^{-1}	0.738^{-2}	0.350^{-2}
4p ₁	0.326^{-1}	0.287^{-1}	0.205^{-1}	0.135^{-1}
4d ₀	0.260^{-2}	0.105^{-2}	0.495^{-3}	0.256^{-3}
4d ₁	0.311^{-2}	0.140^{-2}	0.524^{-3}	0.149^{-3}
4d ₂	0.212^{-2}	0.173^{-2}	0.113^{-2}	0.679^{-3}
4f ₀	0.108^{-3}	0.258^{-4}	0.620^{-5}	0.110^{-5}
4f ₁	0.123^{-3}	0.472^{-4}	0.161^{-4}	0.710^{-5}
4f ₂	0.521^{-4}	0.291^{-4}	0.101^{-4}	0.240^{-5}
4f ₃	0.255^{-4}	0.226^{-4}	0.152^{-4}	0.950^{-5}

† The superscript denotes the power of ten by which the number must be multiplied.

3.1. $n = 2$ level

3.1.1. *2s state.* We display in figure 2 the total 1s–2s cross sections.

One can see that all methods tend to the same limit above 150 eV.

The four channel results of Sullivan *et al* (1972) were close to our results in proton atomic hydrogen scattering (Baye and Heenen 1973a). In the case of electrons they turn out to be completely different. This discrepancy is difficult to understand. An important difference between both calculations is that Sullivan calculates the total cross sections by integration of the modulus square of the transition probability, which is a high energy approximation, while we integrate the differential cross sections. However, this does not seem to explain the discrepancy for 2s state. If we make the same approximation as Sullivan, our cross sections are increased by 25% at 50 eV and 5% at 100 eV (Joachain and Vanderpoorten (1973) have observed the same increase in their approximation).

Our results are very close to those obtained by Tai *et al* (1970) with the Glauber approximation, and to those of Joachain and Vanderpoorten (1973), obtained in the distorted wave approximation with the Glauber optical potential as distorted potential. However, we show in figure 3 at 100 eV, that the angular dependence of the differential

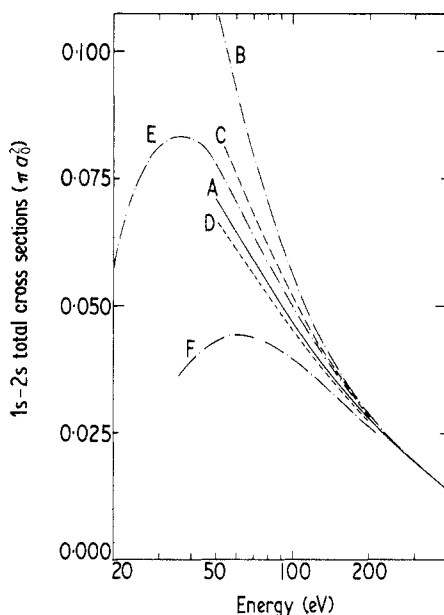


Figure 2. Total cross sections for the 1s-2s excitation of atomic hydrogen by electrons. A present work; B first Born approximation; C second Born approximation (Holt and Moiseiwitsch 1968); D distorted wave approximation of Joachain and Vanderpoorten (1973); E Glauber approximation (Tai *et al* 1970); F four channel results of Sullivan *et al* (1972).

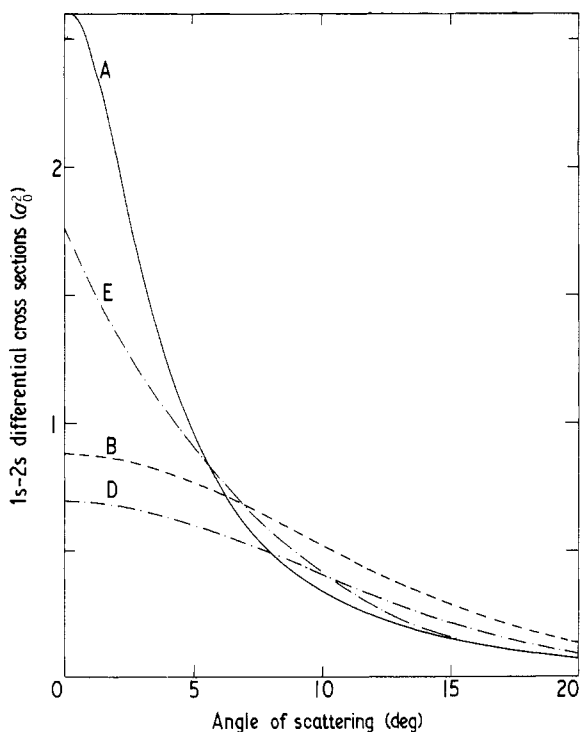


Figure 3. Differential cross sections for the 1s-2s excitation of atomic hydrogen by electrons at 100 eV. Same notations as in figure 2.

cross sections obtained by the three methods is completely different, especially at small scattering angles where our cross sections are much more peaked.

The experimental data of Kauppila *et al* (1970) have not been corrected for cascade from the higher excited states. Therefore, we follow the procedure described by Tai *et al* (1971) and compare with experiments the quantity $\sigma_{2s} + 0.23\sigma_{3p}$. The results are shown in figure 4. The first and second order Born results, calculated with the results of Holt and Moiseiwitsch (1968) and Holt (1969), greatly overestimate the cross sections. Our results are very close to those of Tai *et al* (1970) and seem to be too large at low energies. We show also the results of Sullivan *et al* (1972) which are in good agreement with the experimental data.

3.1.2. 2p states. We display in figure 5 the total 1s-2p cross sections.

We do not show the second order Born results of Holt and Moiseiwitsch (1968) and the four channel results of Sullivan *et al* (1972): they are both almost identical to ours. The difference between the calculation of the total cross sections by integration of the modulus square of the transition probability or by integration of the differential cross sections is smaller for 2p states than for 2s: only 5% at 50 eV.

In order to compare our results with experimental data we must calculate Q_{\perp} as defined by Long *et al* (1968):

$$Q_{\perp} = 0.918\sigma_{2p} + 0.246\sigma_{2p_0}.$$

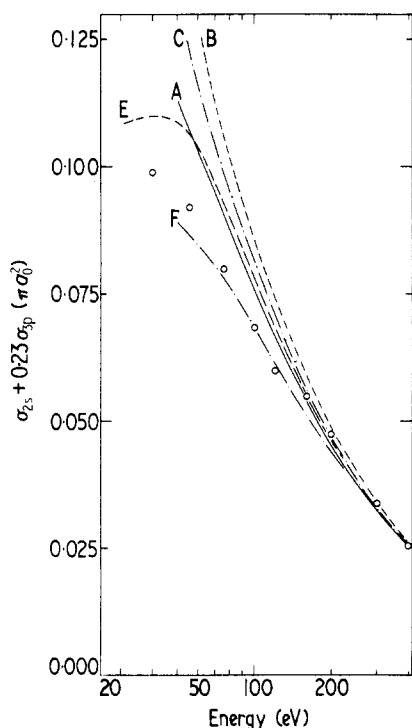


Figure 4. Total cross sections for the 1s-2s excitation of atomic hydrogen by electrons, with an estimation of cascade from the higher states. Same notations as in figure 2 with O: Experimental points of Kauppila *et al* (1970).

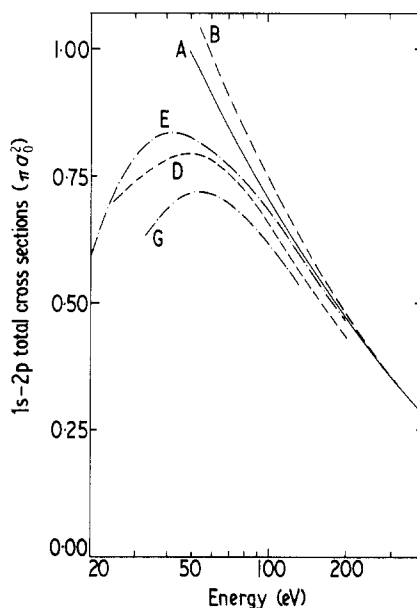


Figure 5. Total cross sections for the 1s-2p excitation of atomic hydrogen by electrons. Same notations as in figure 2 with G: Eikonal approximation of Byron (1971).

We show in figure 6 the experimental results of Long together with our theoretical results and with those of Joachain and Vanderpoorten (1973). The agreement between our theory and experiment is good for energies above 70 eV but it seems that we overestimate the cross sections at lower energies.

We show in figure 7 the polarization of the 2p–1s line. The experimental points are of Ott *et al* (1970) and are in relatively good agreement with the first Born approximation and with the results of Gerjuoy *et al* (1972). The agreement with our values is not very satisfactory.

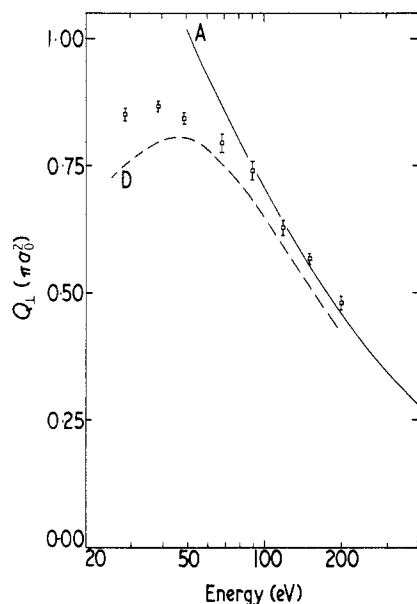


Figure 6. Relative Lyman α cross section production of atomic hydrogen excited by electrons. Same notations as in figure 2 with \square : Experimental points of Long *et al* (1969).

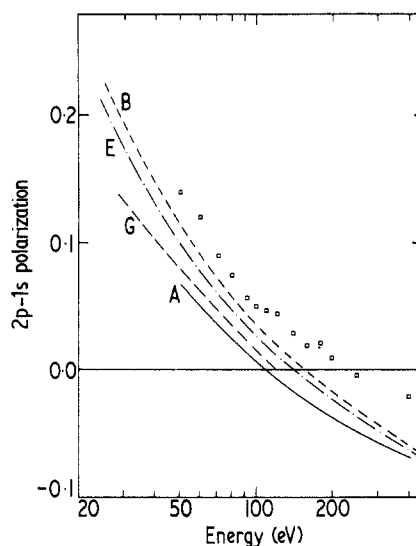


Figure 7. Polarization of the 2p–1s line of atomic hydrogen excited by electrons. Same notations as in figure 2 with E: Glauber approximation (Gerjuoy *et al* 1972) \square : Ott *et al* (1970).

We display in figure 8 our differential cross sections at 100 eV, together with Joachain and Vanderpoorten's ones. Both theoretical values are in close agreement with the other theoretical calculations.

3.2. $n > 2$ levels

There is no experiment for the $n > 2$ levels in electron–hydrogen scattering. We shall therefore only briefly compare some of our results with some other theoretical calculations.

We show in table 2 our results for the 2s, 3s, 4s cross sections at 100 and 200 eV. They are compared with the results of McDowell *et al* (1973) obtained in a polarized orbital distorted wave model. The agreement is good for the 2s state but this could be fortuitous, the shape of the differential cross sections being very different. Both methods give results smaller than the Born results.

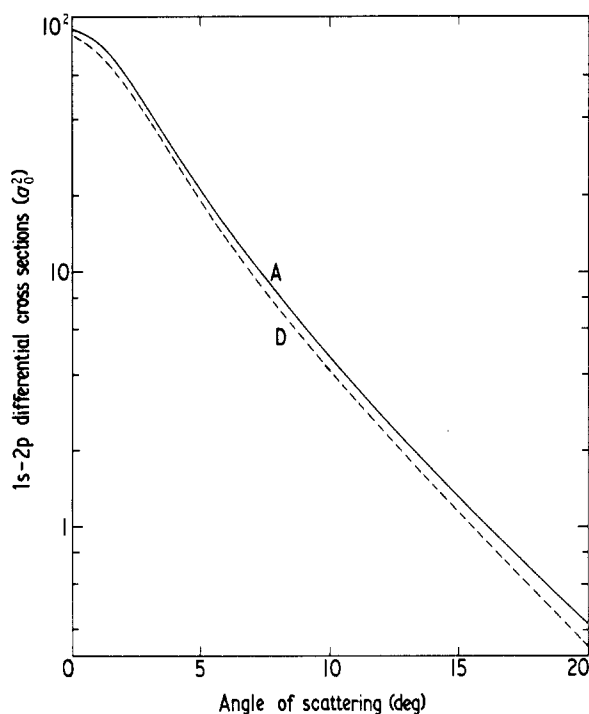


Figure 8. Differential cross sections for the 1s-2p excitation of atomic hydrogen by electrons at 100 eV. Same notations as in figure 2.

Table 2. Comparison between various theoretical results for the 1s-ns excitation of atomic hydrogen by electrons. A present work; B first Born approximation; C polarized orbital distorted wave model of McDowell *et al* (1973).

E (eV)	100			200		
	2	3	4	2	3	4
A	4.76^{-2}	7.92^{-3}	2.45^{-3}	2.68^{-2}	4.75^{-3}	1.55^{-3}
B	5.77^{-2}	1.15^{-2}	4.26^{-3}	2.95^{-2}	5.87^{-3}	2.19^{-3}
C	5.01^{-2}	9.71^{-3}	3.57^{-3}	2.75^{-2}	5.40^{-3}	2.00^{-3}

Many authors have calculated the 1s-3p cross sections. The comparison between the various results is completely identical to the one made for the 2p states. The results of Bransden (1972) and those of Holt (1969) are very close to ours while the cross sections of Tai *et al* (1970) lie lower at all energies.

It is more interesting to compare our 1s-3d cross sections with those obtained by Woollings and McDowell (1973) with various forms of the second order Born approximation. We show these results in figure 9. We can see that the cross sections obtained by Woollings and McDowell in their W McD approximation are smaller than the first order Born cross sections while our results are larger at all energies. At low energies, the difference is almost of a factor 2. This is rather puzzling because both methods take into account the important coupling with the intermediate p states. The comparison of the results obtained for the 4d states leads to the same conclusions.

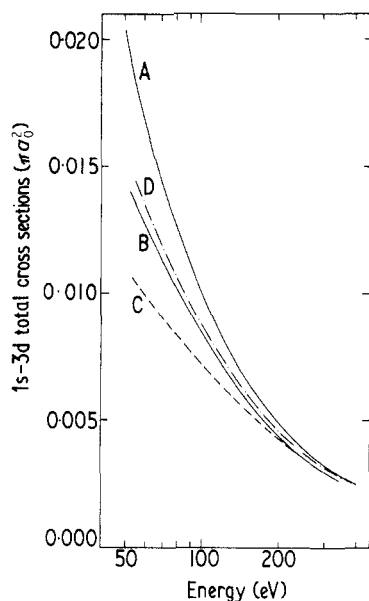


Figure 9. Total cross sections for the 1s–3d excitation of atomic hydrogen by electrons. A present work; B first Born approximation; C second Born approximation W McD (Woollings and McDowell 1973); D second Born approximation HM (Woollings and McDowell 1973).

4. Conclusion

The results given by the various theoretical methods do not show marked discrepancies like in proton–hydrogen scattering. The 2s–2p coupling which did affect mainly the 2s cross sections does not seem to have the same importance here. It is more difficult to evaluate the importance of exchange because this effect becomes important at energies where the straight line and constant velocity approximation are questionable.

The agreement with the few experimental data is good above 100 eV except for the polarization of the 2p–1s line where there is a systematic difference. Our p cross sections are probably too large below 100 eV. The disagreement between our calculations and the data of Kauppila *et al* (1970) for the 1s–2s transition in this energy range could be explained by the fact that we overestimate the correction for cascade.

Experimental data on the differential cross sections could provide much more information about the theoretical methods which give very different results in the whole angular range. The comparison between theory and experiment in electron–helium scattering will be therefore particularly interesting.

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References

- Baye D and Heenen P-H 1973a *J. Phys. B: Atom. molec. Phys.* **6** 105-13
— 1973b *J. Phys. B: Atom. molec. Phys.* **6** 1255-64
Bransden B H, Coleman J P and Sullivan J 1972 *J. Phys. B: Atom. molec. Phys.* **5** 546-58
Byron Jr F W 1971 *Phys. Rev. A* **4** 1907-17
Gerjuoy E, Thomas B K and Sheorey V B 1972 *J. Phys. B: Atom. molec. Phys.* **5** 321-33
Holt A R 1969 *J. Phys. B: Atom. molec. Phys.* **2** 1202-8
Holt A R and Moiseiwitsch B L 1968 *J. Phys. B: Atom. molec. Phys.* **1** 36-47
Joachain C J and Vanderpoorten R 1973 *J. Phys. B: Atom. molec. Phys.* **6** 622-41
Kauppila W E, Ott W R and Fite W L 1970 *Phys. Rev. A* **1**, 1099-108
Long R L, Cox D M and Smith S S 1968 *J. Res. Nat. Bur. Stand.* **72A** 521-35
McDowell M R C, Morgan L A and Myerscough V P 1973 *J. Phys. B: Atom. molec. Phys.* **6** 1435-51
Ott W R, Kauppila W E and Fite W L 1970 *Phys. Rev. A* **1**, 1089-98
Sullivan J, Coleman J P and Bransden B H 1972 *J. Phys. B: Atom. molec. Phys.* **5** 2061-5
Tai H, Bassel R H, Gerjuoy E and Franco V 1970 *Phys. Rev. A* **1** 1819-35
Woollings M J and McDowell M R C 1973 *J. Phys. B: Atom. molec. Phys.* **6** 450-61