The scattering of electrons by hydrogen atoms

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Abstract. The scattering of an electron by a hydrogen atom is considered with particular reference to the errors implicit in the Born and Born–Oppenheimer approximations. A new approximation to the scattering amplitudes is proposed with a view to minimizing these errors. Results of calculations using this method are shown to be encouraging, the cases considered being the elastic scattering of an electron by a hydrogen atom in its ground state and the excitation of the 2s state from the ground state.

1. Introduction

For many years considerable effort has been devoted to the calculation of cross sections for the collision of an electron with a hydrogen atom but, as yet, with only limited success. Excepting the elaborate variational calculations which have been carried out for elastic scattering, the most sophisticated approach has been made by means of the close-coupling approximation. This work is reviewed by Burke and Smith (1962). Surprisingly this method appears to have severe limitations. Burke (1963) has shown that in the evaluation of the 1s–2s excitation cross section the close-coupling method converges only slowly and a prohibitive amount of computation is needed to yield accurate results for this case. It is therefore of interest to consider some simpler approximations, in the hope that an understanding of the reasons for their success or failure will contribute towards an understanding of the close-coupling method.

The most simple method of calculating cross sections is by means of Born’s approximation. This method is of use in some cases; for example, when properly defined (Rudge and Seaton 1965), it can give quite reasonable results for the ionization cross section. On the other hand it fails utterly except at high energies when used to calculate the elastic scattering cross section where the effect of exchange is very important. One might expect this to be the case in any transition between states of the same angular momentum.

Exchange may be taken into account by means of the Born–Oppenheimer (BO) approximation. The usefulness of this method, however, is curtailed by the fact that it frequently yields results, especially near threshold, which exceed conservation limits (Bates et al. 1950). Several modifications of this method have therefore been proposed and used with varying success (Feenberg 1932, Mittleman 1962, Bell and Moiseiwitsch 1963, Ochkur 1964).

In the present paper an attempt is made to find forms of trial functions to use in variational expressions for the scattering amplitudes which, while more refined than plane waves, are yet simple enough to yield reasonably accurate results readily. Special interest centres on the region near threshold where the failure of theoretical calculations is most marked. The cases considered are the elastic scattering of electrons by atomic hydrogen in its ground state and the excitation of the 2s state from the ground state.
2. Theory

2.1. Determination of the exchange scattering amplitude

Our approach will be to adopt certain forms of trial wave functions which offer some improvement over plane wave trial solutions in the variational principle of Kohn (1948) for the scattering amplitude. Denoting the total energy of the system by \( E \) and using atomic units we define

\[
\mathcal{L} = \nabla_1^2 + \nabla_2^2 + 2\left( \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} \right).
\]

We denote the eigenstates of hydrogen belonging to eigenvalue \( E_n \) by \( \psi_n(r) \) and define the energy relation

\[
k_n^2 = 2(E - E_n).
\]

Then if \( \Psi^1(r_1, r_2) \) is a trial solution having the asymptotic form

\[
\Psi^1(r_1, r_2) \sim \psi_0(r_1) \exp(i\mathbf{k}_0 \cdot \mathbf{r}_2) + \sum_n \psi_n(r_1) f_{0n}(\mathbf{k}_0, \mathbf{r}_2)^{-1} \exp(ik_n r_2)
\]

\[
\sim \sum_n \psi_n(r_2) g_{0n}(\mathbf{k}_0, \mathbf{r}_1)^{-1} \exp(ik_n r_1)
\]

while \( \Psi^2(r_1, r_2) \) is a trial solution having the asymptotic form

\[
\Psi^2(r_1, r_2) \sim \psi_0^*(r_1) \exp(-i\mathbf{k}_p \cdot \mathbf{r}_2) + \sum_m \psi_m^*(r_1) f_{pm}(\mathbf{k}_0, \mathbf{r}_2)^{-1} \exp(ik_m r_2)
\]

\[
\sim \sum_m \psi_m^*(r_2) g_{pm}(\mathbf{k}_0, \mathbf{r}_1)^{-1} \exp(ik_m r_1)
\]

then it is straightforward to show (Kohn 1948) that the error in the scattering amplitude is

\[
\delta f_{op}(\mathbf{k}_0, \mathbf{k}_p) = -\frac{1}{4\pi} I_1 + \text{second-order terms}
\]

where

\[
I_1 = \int \Psi^2(r_1, r_2) \mathcal{L} \Psi^1(r_1, r_2) d\mathbf{r}_1 d\mathbf{r}_2.
\]

Similarly

\[
\delta g_{op}(\mathbf{k}_0, \mathbf{k}_p) = -\frac{1}{4\pi} I_2 + \text{second-order terms}
\]

where

\[
I_2 = \int \Psi^2(r_2, r_1) \mathcal{L} \Psi^1(r_1, r_2) d\mathbf{r}_1 d\mathbf{r}_2.
\]

The Born and BO expressions for the scattering amplitudes result from using

\[
\Psi^1(r_1, r_2) = \psi_0(r_1) \exp(i\mathbf{k}_0 \cdot \mathbf{r}_2) \quad \text{and} \quad \Psi^2(r_1, r_2) = \psi_0^*(r_1) \exp(-i\mathbf{k}_p \cdot \mathbf{r}_2).
\]

The approximation of Oppenheimer fails primarily because the final state is not orthogonal to the initial state and this leads to spuriously large terms in the exchange scattering amplitude. The suggestion has been made by Ochkur (1964) that better results may obtain if, instead of using the full BO expression for the scattering amplitude, only the leading term in an expansion of powers of \( 1/k_0^2 \) is retained. This suggestion is an
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interesting but seemingly arbitrary one and has been analysed in more detail by Rudge (1965).† There it was shown that the Ochkur result is not consistent with a choice of trial functions in the variational principle (7) which satisfy the proper boundary conditions (3) and (4). On the other hand this difficulty and the ambiguities of Ochkur’s approach are removed by making the choice

\[ \Psi^1(r_1, r_2) = \psi_0(r_1) \exp(i \mathbf{k}_0 \cdot \mathbf{r}_2) \]

\[ \Psi^2(r_2, r_1) = -\frac{\psi_0^*(r_2)}{\psi_0(r_1)(k_0 - i)^2} \nabla \cdot \{ \psi_0(r_1) \exp(- i \mathbf{k}_0 \cdot \mathbf{r}_1) \}. \]

It is clear that these functions do satisfy the correct boundary conditions and that they are orthogonal. The chief defect of the BO method is therefore overcome. Further, the choice (10) will in general lead to a complex exchange scattering amplitude. This is a necessary requirement if conservation conditions are to be met since the exact exchange scattering amplitude satisfies the equation (Demkov 1963)

\[ g_{\ell n}(\mathbf{\hat{k}}_0, \mathbf{\hat{k}}_j) - g_{\ell n}^*(\mathbf{\hat{k}}_j, \mathbf{\hat{k}}_i) \]

\[ = \frac{i}{2\pi} \sum_{\ell} \frac{k_n}{\gamma_n} \int \left[ g_{\ell n}(\mathbf{\hat{k}}_0, \mathbf{\hat{r}}_2) f_{\ell n}^*(\mathbf{\hat{k}}_j, \mathbf{\hat{r}}_2) + f_{\ell n}(\mathbf{\hat{k}}_i, \mathbf{\hat{r}}_2) g_{\ell n}^*(\mathbf{\hat{k}}_j, \mathbf{\hat{r}}_2) \right] d \mathbf{\hat{r}}_2. \]

In particular, for \( \ell = j \) and \( \mathbf{\hat{k}}_i = \mathbf{\hat{k}}_j \), we have the result that

\[ 2f(g_{\ell n}(\mathbf{\hat{k}}_0, \mathbf{\hat{k}}_j)) = \frac{\gamma_n}{\pi} \sum_{\ell} \gamma_n \int \left[ g_{\ell n}(\mathbf{\hat{k}}_0, \mathbf{\hat{r}}_2) f_{\ell n}^*(\mathbf{\hat{k}}_i, \mathbf{\hat{r}}_2) \right] d \mathbf{\hat{r}}_2. \]

We may thus expect, by virtue of the choice (10), a considerable improvement over the BO method and might hope that results of calculations corresponding to this choice will remain reasonably accurate down to threshold.

Using (7) and (10) we obtain the result that for elastic scattering

\[ g_{1s,1s}(\mathbf{\hat{k}}_0, \mathbf{\hat{k}}_0') = -\frac{32}{(k_0 - i)^2(4 + t^2)^2} \]

where \( t = k_0 - k_0' \) while for the excitation of the 2s state the result is that

\[ g_{1s,2s}(\mathbf{\hat{k}}_0, \mathbf{\hat{k}}_1) = -\frac{16t^2}{\sqrt{2}(k_1 - i)^2(4 + t^2)^2} \]

where \( t = k_0 - k_1 \).

2.2. Spin change cross sections

It may be shown (e.g. Dalgarno and Rudge 1965) that, for an atom in a \(^2S\) state, if the nuclear spin is \( I \) and the initial total spin of the atom is \( F \), the cross section for the process in which \( F \) changes to \( F' \) and the atom is excited from state 0 to state \( \ell \) is given by

\[ Q_{0,n}(F, F') = \frac{2F' + 1}{2(I + 1)} Q_{0,n}^{ex} \] (in units of \( \pi a_0^2 \))

where the spin exchange cross section \( Q_{0,n}^{ex} \) is given by

\[ Q_{0,n}^{ex} = \frac{4\pi^2 k_0}{k_n} \int |g_{0n}(\mathbf{\hat{k}}_0, \mathbf{\hat{k}}_n)|^2 d\mathbf{\hat{k}}_0 d\mathbf{\hat{k}}_n. \]

† Equations (5), (6), (7) and (8) of this letter should be multiplied by -1.
For the case of elastic scattering this may be written as

\[ Q_{0,0}^{\text{ex}} = k_0^{-1} \sum_{n=0}^{\infty} (2l+1) \sin^2(\eta_l(0) - \eta_l(1)) \]  
(in units of \( \pi a_0^2 \))  
(17)

where \( \eta_l(0) \) and \( \eta_l(1) \) are phase shifts corresponding to \( S = 0 \) and \( S = 1 \) respectively \( S \) being the total spin. Using equations (13), (14) and (16) gives us the results that

\[ Q_{1s}^{1s} = 16(1 + k_0^2)^{-2} \left( 1 + \frac{k_0^2}{3} \right) \]  
(18)

\[ Q_{1s,2s}^{1s} = \frac{64}{15k_0^2(1 + k_0^2)^2} \left[ \phi((k_0 - k_1)^2) - \phi((k_0 + k_1^2)^2) \right] \]  
(19)

where

\[ \phi(x) = (x + 2.25)^{-2}(10x^2 + 11.25x + 5.0625) \]  
(20)

2.3. Determination of the direct scattering amplitude

The Born approximation to the direct scattering amplitude is certainly better than the Oppenheimer approximation for the exchange scattering amplitude. Nevertheless, one might seek to improve on the use of plane waves here also. The form of the error in Born’s approximation for \( e^{-} - H \) scattering may be obtained by similar methods to those of Klein and Zemach (1959) for potential scattering. Thus the total wave function of the system \( \Psi(r_1, r_2) \) satisfies either of the two integral equations

\[ \Psi(r_1, r_2) = \psi_0(r_1) \exp(ik_0 \cdot r_2) + \int G_0(r_1, r_2; r_1', r_2') V(r_1', r_2') \Psi(r_1', r_2') dr_1' dr_2' \]  
(21)

\[ \Psi(r_1, r_2) = \psi_0(r_1) \exp(ik_0 \cdot r_2) + \int G_1(r_1, r_2; r_1', r_2') V(r_1', r_2') \psi_0(r_1) \exp(ik_0 \cdot r_2') dr_1' dr_2' \]  
(22)

wherein

\[ V(r_1, r_2) = \frac{1}{r_2 \cdot r_2} \]  
(23)

where

\[ \mathcal{L} G(r_1, r_2; r_1', r_2') = \delta(r_1 - r_1') \delta(r_2 - r_2') \]  
(24)

and where

\[ \{ \mathcal{L} + V(r_1, r_2) \} G_0(r_1, r_2; r_1', r_2') = \delta(r_1 - r_1') \delta(r_2 - r_2') \]  
(25)

If the expression (22) is substituted on the right-hand side of (21) the form taken by \( \Psi(r_1, r_2) \) is the Born expression for \( \Psi(r_1, r_2) \) plus the exact correction to this expression.

Using explicit representations for the Green’s functions the form of this correction may then be evaluated. The algebra is lengthy, but the final result shows that Born’s approximation is in error; firstly, because the initial state is not chosen orthogonal to the bound states of the negative hydrogen ion and, secondly, because it is the terms which are ignored in the Born method which allow the exact unitary relation (Demkov 1963)

\[ i A^\dagger(i_t, i) A^\dagger(i, i_s) = -2 \frac{n}{\pi} \sum_n k_n \left[ \int f_n^i(k_t, \hat{\mathbf{r}}_2) f_n^i(\hat{\mathbf{r}}_2, \mathbf{\hat{r}}_2) + g_n^i(k_t, \mathbf{\hat{r}}_2) g_n^i(\mathbf{\hat{r}}_2, \mathbf{\hat{r}}_2) \right] d\mathbf{r}_2 \]  
(26)

to be met. For \( i = j \) and \( \hat{\mathbf{k}}_s = \mathbf{\hat{k}}_s \), (26) becomes

\[ 2 S^j f_n^i(\mathbf{\hat{k}}_s) \mathbf{\hat{k}}_s) = \frac{1}{2\pi} \sum_n k_n \int \left[ |f_n^i(\mathbf{\hat{k}}_s, \mathbf{\hat{r}}_2)|^2 + |g_n^i(\mathbf{\hat{k}}_s, \mathbf{\hat{r}}_2)|^2 \right] d\mathbf{r}_2. \]  
(27)
Both these objections to Born’s approximation may be partially met by employing for the initial state the function

$$\Psi^1(r_1, r_2) = \frac{-\psi_0(r_1) \nabla^2 \psi_0(r_2) \exp(i \mathbf{k}_0 \cdot r_2)}{(k_0 - i)^2 \psi_0(r_2)} \tag{28}$$

while the most simple choice of the second trial solution is

$$\Psi^2(r_1, r_2) = \psi_0^{(*)} r_1) \exp(-i \mathbf{k}_v \cdot r_2). \tag{29}$$

These wave functions might be expected to offer some advantage over the use of plane waves throughout. Using equations (5), (28) and (24) we find that

$$f_{1s,1s}(\mathbf{k}_0, \mathbf{k}_0') = \frac{2}{(k_0 - i)^2} \left( \frac{(1 + k_0^2)(t^2 + 8)}{(t^2 + 4)^2} - \frac{1}{t} \tan^{-1} \left( \frac{1}{2} \right) \right) \tag{30}$$

and that

$$f_{1s,2s}(\mathbf{k}_0, \mathbf{k}_1) = \frac{-16(k_0^2 - \frac{1}{2} - \frac{8}{t^2})}{\sqrt{2}(k_0 - i)^2(\frac{8}{t^2} + t^2)}. \tag{31}$$

In (30) \( t = k_0 - k_0' \) and in (31) \( t = k_0 - k_1 \). The total cross section for excitation of the \( n \)th state is now given in units of \( \pi a_0^2 \) by

$$Q_{0,n} = \frac{k_n}{4\pi^2 k_0} \int \left[ |f(\mathbf{k}_0, \mathbf{k}_n)|^2 + |g(\mathbf{k}_0, \mathbf{k}_n)|^2 - R[f(\mathbf{k}_0, \mathbf{k}_n)g^*(\mathbf{k}_0, \mathbf{k}_n)] \right] d\mathbf{k}_0 d\mathbf{k}_n. \tag{32}$$

From (12) and (27)

$$\sum_n Q_{0,n} = \frac{4}{k_0} \int \left\{ f_{00}(\mathbf{k}_0, \mathbf{k}_0) - \frac{1}{2} g_{00}(\mathbf{k}_0, \mathbf{k}_0) \right\} d\mathbf{k}_0 d\mathbf{k}_0. \tag{33}$$

3. Results

3.1. Spin change cross sections

In order to compare results for elastic scattering with accurate values the results for the phase shifts have been taken from the work of Schwartz (1961), Burke and Schey (1962) and Burke, Schey and Smith (1963). The adopted values for these phase shifts (modulo \( \pi \)) are shown in table 1. Figure 1 shows the resulting spin change cross section compared with results given by equation (18).

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† Scattering lengths in units of \( a_0 \).
The cross section $Q_{1s,2s}^{ex}$ has been measured experimentally by Lichten and Schulz (1959). They obtain a value for this cross section relative to the total cross section

![Graph showing cross sections](image1)

**Figure 1.** Results for elastic spin change cross section. Curve A, present calculation; curve B, using the phase shifts of table 1.

![Graph showing cross sections](image2)

**Figure 2.** Results for the $1s$–$2s$ spin change cross section. Curve A, Burke *et al.* 1963; curve B, present calculation; curve C, 'experimental' value.

$Q_{1s,2s}$. Their value for this latter cross section is subject to some uncertainty since it was normalized to Born's approximation at 50 ev. A second measurement of $Q_{1s,2s}$ has
been made by Stebbings et al. (1960) (and corrected by Lichten 1961). Their results differ markedly from those of Lichten and Schultz. In figure 2 there is displayed an experimental value for $Q_{1s,2s}^{ex}$ which is obtained by adopting the results of Stebbings et al. for $Q_{1s,2s}$ and the results of Lichten and Schultz for the ratio $Q_{1s,2s}^{ex}/Q_{1s,2s}$. Also shown are the results of the present calculation using equation (19) and the results of Burke, Schey and Smith (1963).

3.2. Total cross sections

Figure 3 shows the results of the present calculation for the elastic scattering cross section as compared with results obtained using the phase shifts of table 1.

![Figure 3](image)

Figure 3. Results of the total elastic scattering cross section. Curve A, present calculation; curve B, using the phase shifts of table 1; curve C, Born approximation.

Figure 4 shows results which have been obtained for the total 1s–2s cross section. The lowest curve is taken from the experimental results of Stebbings et al. (1960) (corrected for cascade from the 3p state and multiplied by 1.5 (Lichten 1961)). Also shown are the experimental results of Lichten and Schultz (1959) for energies less than 50 ev, the curve above this energy being obtained using Born’s approximation. A third curve representing the theoretical results of Burke, Schey and Smith (1963), using the 1s–2s–2p close-coupling approximation, is also shown, together with a single point at 16.5 ev obtained by Burke (1963) using the close-coupling method with 3s and 3p states also included.

Figure 5 presents the experimental results of Stebbings et al. and the results of the present calculation.

Finally, in table 2 there is presented a comparison of various theoretical calculations. The second Born 1s–2s–2p calculation is taken from results of Kingston, Moiseiwitsch
and Skinner (1960) while the second Born calculations with exchange are those of Taylor (1964, Thesis, University of Amsterdam). The Born–Oppenheimer results and the

\[ \log \varepsilon \ (\varepsilon \text{ in ev}) \]

Figure 4. Results of the total $1s-2s$ cross section. Curve A, Burke et al. 1963; curve B, Lichten and Schultz 1959; curve C, Stebbings et al. 1960; ×, Burke 1963.

\[ \log \varepsilon \ (\varepsilon \text{ in ev}) \]

Figure 5. Results for the total $1s-2s$ cross section. Curve A, present calculation; curve B, results of Stebbings et al. 1960.

first-order exchange results have been obtained by Bell and Moiseiwitsch (1963). The close-coupling results are those of Burke et al. (1963).
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Table 2. Theoretical results for the total 1s–2s cross section

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4. Concluding remarks

From figure 1 we see that the exchange scattering amplitude (13) has very nearly the correct value at threshold and that the general shape of the spin exchange cross section is well reproduced. While it is not surprising that the shallow minimum is not obtained, it is surprising that the discrepancy at higher energies should be as large as it appears to be. A comparison of close-coupling phase shifts with the Schwartz values shows that the close-coupling method underestimates the singlet s-wave phase shift. It may be that at the higher energies, where close-coupling phase shifts were adopted, the discrepancy is partially accounted for by this feature.

As far as the 1s–2s spin change cross section is concerned it would appear from figure 2 that the present method yields a very much better result than that of Burke, Schey and Smith (1963). This conclusion, however, cannot be a firm one in view of the uncertainties of the experimental results.

The position with regard to the elastic scattering cross section is moderately satisfactory. Certainly the threshold value is a reasonably good one, but as in the case of the spin change cross section the rapid fall-off from threshold is not given by the present method, and in this region the relationship (33) is violated. As in the case of the spin change cross section it is possible that the discrepancy at higher energies is not as large as it appears to be if the singlet s-wave phase shift is underestimated.

Figure 4 reveals the extent of uncertainty with regard to the total 1s–2s cross section. Since the Born approximation is grossly in error for the 1s–1s cross section, as seen in figure 3, there is little reason for believing that it should be accurate for the 1s–2s cross section. One would, therefore, expect the normalization procedure of Lichten and Schultz (1959) to be incorrect; although the 1s–2s–2p close-coupling results would appear to justify their results, the further result of Burke (1963), who included the 3s and 3p states also, modifies this conclusion. It therefore seems reasonable to accept the results of Stebbings et al. (1960) as correct, to within their experimental errors, and hence this is the curve with which the present results are compared in figure 5. If the experimental curve shown there is indeed approximately correct, then the agreement of the present calculation with it is very satisfactory.

It is of interest to compare the various theoretical predictions shown in table 2. As might be expected they tend to agree at the higher energies, but the case is far otherwise in the more interesting region near threshold. The uncertainties in the experimental results make a decision as to which is the best method very difficult. The situation can
only be clearly resolved by either a further experiment or further more elaborate calculations. Such calculations might be made either using variational methods with refined trial functions, or perhaps it would be of interest to repeat the close-coupling calculations with a form of trial solution which is explicitly orthogonal to the hydrogenic bound states and thereby approximately orthogonal to the H− bound states. The singlet solutions may then be very different. As to the method proposed here, the results give some encouragement to the view that it may still be possible to obtain reasonably accurate cross sections in a simple fashion.

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References


