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Cross sections for electron–hydrogen collisions in the Born approximation to the reactance matrix

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Abstract. Born partial-wave integrals have been performed for a range of energies and total cross sections are presented for electron-hydrogen-atom excitation both in the conventional first Born approximation (Born I) and the unitarised Born approximation (Born II). Exchange effects are not included. With the exception of exact resonance-allowed transitions ($n = n'$, $\lambda = 1$) results are presented for all transitions between hydrogen-atom states whose principal quantum number is less than or equal to 4.

1. Introduction

In a recent paper (Whelan 1984a) it has been shown how one might express the Born reactance matrix of Seaton (1961) in a closed analytical form provided only that the radial atomic wavefunctions were of the form

$$\frac{P_{nl_a}}{r}(r) = \sum_{s=l_a}^{m} a_s \exp(-\beta_s r) r^s. \tag{1.1}$$

In the same paper analytic expressions were deduced for the collision strength in the conventional first Born approximation, Ω^{I}, the unitarised Born approximation, Ω^{II}, and in the simple Ochkur-Bonham approximation, $\Omega^{\mathrm{I}}(\mathrm{X})$.

In this paper excitation cross sections are presented for electron-hydrogen collisions in the two non-exchange approximations Ω^{I}, Ω^{II}, for a range of energies above the ionisation threshold.

The high-L problem is treated using the Bethe approximation to the reactance matrix (Whelan 1986). The notation of Whelan (1986) is adopted throughout.

A comparison of the results presented below and other theoretical calculations will be given elsewhere (Whelan *et al* 1986).

2. Ω^{I}(Born)

The first Born approximation to the collision strength for a transition $n, l_a \to n', l'_a$ may be written in the form (see Seaton 1961)

$$\Omega^{\mathrm{I}}(n', l'_a, n, l_a) = 8\omega_1 \sum_{\lambda=0}^{\infty} (2\lambda+1)\left(\int_{k-k'}^{k+k'} \mathrm{d}K\, K^{-3}\theta(K)\right) \tag{2.1}$$

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where

$$\theta(K)=\left(\int_0^\infty C^{l_a\,\lambda\,l'_a}_{0\,0\,0}P_{nl_a}(r)P_{n'l'_a}(r)(j_\lambda(Kr)-\delta_{\lambda 0})\,\mathrm{d}r\right)^2. \tag{2.2}$$

$\boldsymbol{K}=\boldsymbol{k}-\boldsymbol{k}'$ is the momentum transfer, ω_i is the degeneracy of the initial level, $P_{nl_a}(r)/r$ is the radial atomic wavefunction, j_λ is a spherical Bessel function and $C^{l_a\,\lambda\,l'_a}_{0\,0\,0}$ is a Clebsch-Gordan coefficient.

It is shown in Whelan (1984a)† that Ω^{I} may be written

$$\Omega^{\mathrm{I}}=8\omega_1\sum_\lambda(2\lambda+1)(C^{l_a\,0\,l'_a}_{0\,0\,0})^2\sum z(s_1,s_2,s_3,s_4,s_5,s_6)$$
$$\times(-1)^{s_5+s_6}W[2(\lambda+s_5+s_6)-3,\,s_1+s_2+s_3+s_4]/\beta^{2s_5+2s_6+s_1+s_2+s_3+s_4}. \tag{2.3}$$

The inner summation is over s_i, $1\leqslant i\leqslant 6$, and contains only a finite number of terms, z, β are defined in Whelan (1984a) (for the elastic case $n=n'$, $l_a=l'_a$, $\lambda=0$, see Whelan (1984b)) and

$$W(n,m)=\int_{k-k'}^{k+k'}\frac{K^n\,\mathrm{d}K}{(1+K^2/\beta^2)^m}=\int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}}\frac{K^n\,\mathrm{d}K}{(1+(K/\beta)^2)^m}. \tag{2.4}$$

with $n\geqslant -3$.

3. Ω^{II}(Born)

It is shown in Seaton (1961) that the Born approximation to the reactance matrix can be written in the form

$$R(n',l'_a,l';L,n,l_a,l,L)$$
$$=-2(kk')^{1/2}\sum_\lambda(2\lambda+1)\langle l'l'_aL|P_\lambda|ll_aL\rangle$$
$$\times\sum_{\mathscr{L}}\mathscr{Q}_{\lambda\mathscr{L}}(k,l,k',l')B_{\lambda\mathscr{L}}(nl_a,n'l'_a). \tag{3.1}$$

It is shown in Whelan (1984a) that

$$\beta^\lambda B_{\lambda\mathscr{L}}(nl_a,n'l'_a)$$
$$=\sum_m\sum_{s_1s_2s_3}C_m\phi(s_1,s_2,s_3)\,W(2s_3+2m-1,s_1+s_2)(kk')^{-1}$$
$$+\delta_{nn'}\delta_{\lambda 0}(kk')^{-1}\Bigg[\sum_{s_1s_2}\sum_{s_3\geqslant 1}\phi(s_1,s_2,s_3)\,W(2s_3-1,s_1+s_2)$$
$$+\sum_{s_1s_2}\tfrac{1}{2}\phi(s_1,s_2,0)\left(\frac{1}{y}+\cdots+\frac{y^{1-s_1-s_2}}{(s_1+s_2-1)}-\ln y\right)_{y=1}^{y=1+(K^2_{\mathrm{MAX}}/\beta^2)}\Bigg] \tag{3.2}$$

where the sum over m goes from 0 to $\mathscr{L}$ if $n\neq n'$, and from 1 to $\mathscr{L}$ if $n=n'$. There are a finite number of terms in each summation and ϕ is defined in Whelan (1984a). If we write $K^2=k^2+k'^2-2kk'\mu$ then C_m is given by

$$P_{\mathscr{L}}(\mu)=\sum_{m=0}^{\mathscr{L}}C_mK^{2m}$$

where $P_{\mathscr{L}}$ is a Legendre polynomial of the first kind.

† Unfortunately this paper contained a number of minor misprints, which are corrected in Whelan (1984b).

4. The inclusion of $n = 4$ states

Earlier calculations of the electron–hydrogen cross sections in the Born II approximation were performed for transitions between the states $n = 1, 2$, and $n = 1, 2, 3$ (Lawson *et al* 1961, Somerville 1963). Born II cross sections are presented below for transitions between states with $n = 1, 2, 3, 4$. The main effect of the extensions to level 4 is that the reactance matrix is now considerably larger, having 265 distinct non-zero elements compared with 65 for $n = 1, 2, 3$ and 11 for $n = 1, 2$. There are now 30 channels which we will denote by a label ν as follows:

ν	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
nl	1s	2s	2p	2p	3s	3p	3p	3d	3d	3d	4s	4p	4p	4d	4d
l	L	L	$L-1$	$L+1$	L	$L-1$	$L+1$	$L-2$	$L+2$	L	L	$L-1$	$L+1$	$L-2$	$L+2$

ν	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
nl	4d	4f	4f	4f	4f	2p	3p	3d	3d	4p	4d	4d	4f	4f	4f
l	L	$L-3$	$L-1$	$L+3$	$L+1$	L	L	$L-1$	$L+1$	L	$L-1$	$L+1$	$L-2$	$L+2$	L

The states $1 \leqslant \nu \leqslant 20$ have a different parity from those with $21 \leqslant \nu \leqslant 30$; coupling can only occur between states which have the same parity.

It will be convenient to present cross sections at an energy of k_1^2 Ryd where k_1^2 is the energy associated with level 1, i.e.

$$k_1^2 = k_2^2 + \tfrac{3}{4} = k_3^2 + \tfrac{8}{9} = k_4^2 + \tfrac{15}{16}. \tag{4.1}$$

For a transition from n to n', the energy of the colliding particle is given by $k^2 = k_n^2$ Ryd and that of the scattered particle by $k'^2 = k_{n'}^2$ Ryd.

In general, for the strong-coupling approximations, for a given k and L, a T matrix was calculated using the formula

$$\mathbf{T} = \mathbf{X} + \mathrm{i}\mathbf{Y}. \tag{4.2}$$

$$\mathbf{X} = \frac{2\mathbf{R}^2}{\mathbb{1} + \mathbf{R}^2} \qquad \mathbf{Y} = \frac{-2\mathbf{R}}{\mathbb{1} + \mathbf{R}^2} \tag{4.3}$$

which involves only one matrix inversion. The R matrix effectively breaks up into two matrices, one 20 by 20 and one 10 by 10, corresponding to the different parity groups. For large enough L all T matrices were calculated using the Bethe II approximation. When coupling became unimportant (i.e. $\mathbf{T} \simeq 2\mathrm{i}\mathbf{R}$) the Burgess sum rules were used for the dipole transitions (Burgess 1974, Whelan 1986).

5. Cancellation errors and the Born approximation

We tested for cancellation errors for the Born I approximation (equations (2.1)–(2.3)) by running our code using both REAL*8 and REAL*16 arithmetic. This had no effect on the results as presented below. We concluded from this that the weak-coupling results are not susceptible to cancellation errors.

Unfortunately the strong-coupling problem proved more difficult. When we tested the program we developed, based on equations (3.1)–(3.2), we discovered cancellation errors as L increased. For example, with $k_1 = 2$, after only 16 angular momentum states REAL*8 and REAL*16 arithmetic gave significantly different values for the partial cross section. In general for $L = 16$, $k_1 = 2$, the Born II and Bethe II partial cross sections are

not sufficiently close to justify using the latter to calculate the contributions from higher L.

Let us return to equation (3.2) for $n \neq n'$,

$$\beta^{\lambda} B_{\lambda\mathscr{L}}(nl_a, n'l'_a)$$

$$= \sum_{m=0}^{\mathscr{L}} \sum_{s_1 s_2 s_3} \frac{C_m}{kk'} \phi(s_1 s_2 s_3) \int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{K^{2s_3+2m-1}\,\mathrm{d}K}{(1+K^2/\beta^2)^{s_1+s_2}}$$

$$= \sum_{s_1 s_2 s_3} \frac{\phi(s_1 s_2 s_3)}{kk'} \int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{P_{\mathscr{L}}(\mu) K^{2s_3-1}}{(1+K^2/\beta^2)^{s_1+s_2}}\,\mathrm{d}K. \tag{5.1}$$

Similarly for $n = n'$, $\lambda \neq 0$, we have

$$\beta^{\lambda} B_{\lambda\mathscr{L}}(nl_a, n'l'_a)$$

$$= \sum_{m=1}^{\mathscr{L}} \sum_{s_1 s_2 s_3} \frac{C_m}{k^2} \phi(s_1 s_2 s_3) \int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{K^{2s_3+2m-1}}{(1+K^2/\beta^2)^{s_1+s_2}}\,\mathrm{d}K$$

$$= \sum_{s_1 s_2 s_3} \frac{\phi(s_1 s_2 s_3)}{k^2} \int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{(P_{\mathscr{L}}(\mu)-1) K^{2s_3-1}}{(1+K^2/\beta^2)^{s_1+s_2}}\,\mathrm{d}K.$$

For $n = n'$, $\lambda = 0$ we have

$$B_{0\mathscr{L}}(nl_a, n'l'_a)$$

$$= \sum_{s_1 s_2 s_3} \frac{1}{k^2} \phi(s_1 s_2 s_3) \int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{(P_{\mathscr{L}}(\mu)-1)}{(1+K^2/\beta^2)^{s_1+s_2}} K^{2s_3-1}\,\mathrm{d}K$$

$$+ k^{-2} \sum_{s_1 s_2} \sum_{s_3 \geqslant 1} \phi(s_1 s_2 s_3) W(2s_3-1, s_1+s_2)$$

$$+ \tfrac{1}{2} k^{-2} \left[\sum_{s_1 s_2} \phi(s_1 s_2 0) \left(\frac{1}{y} + \cdots + \frac{y^{1-s_1-s_2}}{s_1+s_2-1} - \ln y \right) \right]_1^{1+K_{\mathrm{MAX}}^2/\beta^2}.$$

Let us consider the integral

$$\int_{K_{\mathrm{MIN}}}^{K_{\mathrm{MAX}}} \frac{(P_{\mathscr{L}}(\mu) - \delta_{nn'}) K^{2s_3-1}}{1+K^2/\beta^{2s_1+s_2}}\,\mathrm{d}K. \tag{5.2}$$

For a given k_1, n, n', the limits of integration K_{MIN} and K_{MAX} are fixed. In the Born II code developed integrals of the type (5.2) were evaluated numerically.

$P_{\mathscr{L}}(\mu)$ was generated from the recurrence relation for increasing $\mathscr{L}$. To test for cancellation errors a program was developed which calculated $P_{\mathscr{L}}(\mu)$ at $\mathscr{L} = 78$, for one thousand points between -1 and $+1$ in REAL*8 and REAL*16 arithmetic; cancellation errors were not found to be significant.

The integral over $\mathrm{d}K$ was performed using the standard NAG routine D01AKF, a routine especially suited to oscillatory integrands. The reactance matrix elements were tested for accuracy by varying the parameters EPSREL and EPSABS (respectively user-supplied relative and absolute error tolerances). The reactance matrix elements used in the calculation of the cross sections were unaltered by decreasing EPSREL and EPSABS by a factor of 10, for all channels and for the maximum angular momentum range used in the calculation ($0 \leqslant L \leqslant 60$).

Table 1. Born I cross sections (πa_0^2, exponential notation).

	k_1							
λ	1	1.2	1.606238	2	2.711088	3	7.5	10
1s-1s(0)	0.1542+1	0.1203+1	0.7631+0	0.5227+0	0.2991+0	0.2470+0	0.4117−1	0.2323−1
1s-2s(0)	0.2483+0	0.2280+0	0.1494+0	0.1019+0	0.5776−1	0.4758−1	0.7848−2	0.4426−2
1s-2p(1)	0.1039+1	0.1307+1	0.1235+1	0.1041+1	0.7501+0	0.6626+0	0.1783+0	0.1131+0
1s-3s(0)	0.3700−1	0.4353−1	0.2957−1	0.2023−1	0.1148−1	0.9455−2	0.1559−2	0.8788−3
1s-3p(1)	0.1280+0	0.2131+0	0.2113+0	0.1784+0	0.1278+0	0.1126+0	0.2975−1	0.1879−1
1s-3d(2)	0.1369−1	0.2158−1	0.1836−1	0.1365−1	0.8249−2	0.6882−2	0.1189−2	0.6727−3
1s-4s(0)	0.1081−1	0.1588−1	0.1098−1	0.7522−2	0.4269−2	0.3516−2	0.5795−3	0.3267−3
1s-4p(1)	0.3509−1	0.7394−1	0.7503−1	0.6340−1	0.4536−1	0.3994−1	0.1048−1	0.6611−2
1s-4d(2)	0.4914−2	0.9902−2	0.8659−2	0.6463−2	0.3908−2	0.3261−2	0.5631−3	0.3187−3
1s-4f(3)	0.1206−3	0.2226−3	0.1692−3	0.1167−3	0.6561−4	0.5382−4	0.8686−5	0.4886−5
2s-2s(0)	0.1433+3	0.5544+2	0.2137+2	0.1210+2	0.5983+1	0.4790+1	0.7139+0	0.3993+0
2s-3s(0)	0.1270+2	0.6661+1	0.2760+1	0.1590+1	0.7944+0	0.6373+0	0.9563−1	0.5351−1
2s-3p(1)	0.1284+2	0.1897+2	0.1333+2	0.9644+1	0.6070+1	0.5191+1	0.1200+1	0.7443+0
2s-3d(2)	0.4497+2	0.2172+2	0.8816+1	0.5054+1	0.2517+1	0.2018+1	0.3022+0	0.1691+0
2s-4s(0)	0.1975+1	0.1282+1	0.5373+0	0.3098+0	0.1548+0	0.1242+0	0.1863−1	0.1043−1
2s-4p(1)	0.1308+1	0.3332+1	0.2411+1	0.1744+1	0.1094+1	0.9346+0	0.2142+0	0.1326+0
2s-4d(2)	0.6082+1	0.2897+1	0.1130+1	0.6409+0	0.3169+0	0.2537+0	0.3780−1	0.2114−1
2s-4f(3)	0.2906+1	0.1535+1	0.5973+0	0.3375+0	0.1664+0	0.1331+0	0.1979−1	0.1107−1
2p-2p(0)	0.9157+2	0.3695+2	0.1443+2	0.8198+1	0.4061+1	0.3252+1	0.4853+0	0.2715+0
2p-2p(2)	0.1814+2	0.6625+1	0.2498+1	0.1407+1	0.6926+0	0.5541+0	0.8237−1	0.4606−1
2p−3s(1)	0.1298+1	0.7346+0	0.4435+0	0.3126+0	0.1939+0	0.1654+0	0.3787−1	0.2346−1
2p-3p(0)	0.1273+2	0.6195+1	0.2519+1	0.1445+1	0.7197+0	0.5770+0	0.8643−1	0.4836−1
2p-3p(2)	0.2066+1	0.1236+1	0.5227+0	0.3026+0	0.1517+0	0.1217+0	0.1830−1	0.1024−1
2p-3d(1)	0.5300+2	0.4803+2	0.2870+2	0.1969+2	0.1184+2	0.1002+2	0.2177+1	0.1335+1
2p-3d(3)	0.4001+1	0.1542+1	0.5837+0	0.3288+0	0.1619+0	0.1295+0	0.1926−1	0.1077−1
2p-4s(1)	0.3183+0	0.1543+0	0.8587−1	0.5888−1	0.3567−1	0.3025−1	0.6704−2	0.4128−2
2p-4p(0)	0.2124+1	0.1192+1	0.4861+0	0.2786+0	0.1387+0	0.1112+0	0.1664−1	0.9310−2
2p-4p(2)	0.3321+0	0.2657+0	0.1119+0	0.6455−1	0.3227−1	0.2589−1	0.3885−2	0.2174−2
2p-4d(1)	0.6524+1	0.7248+1	0.4244+1	0.2867+1	0.1697+1	0.1428+1	0.3020+0	0.1841+0
2p-4d(3)	0.6562+0	0.2738+0	0.1033+0	0.5814−1	0.2863−1	0.2291−1	0.3405−2	0.1904−2
2p-4f(2)	0.1636+1	0.1546+1	0.7154+0	0.4228+0	0.2146+0	0.1727+0	0.2618−1	0.1466−1
2p-4f(4)	0.3370+0	0.1388+0	0.5244−1	0.2953−1	0.1454−1	0.1163−1	0.1729−2	0.9671−3
3s-3s(0)	0.1752+4	0.3659+3	0.1199+3	0.6529+2	0.3146+2	0.2507+2	0.3674+1	0.2052+1
3s-3d(2)	0.4267+3	0.8609+2	0.2806+2	0.1525+2	0.7343+1	0.5849+1	0.8570+0	0.4787+0
3s-4s(0)	0.1231+3	0.3823+2	0.1318+2	0.7253+1	0.3518+1	0.2806+1	0.4131+0	0.2308+0
3s-4p(1)	0.8004+2	0.1023+3	0.5818+2	0.3925+2	0.2335+2	0.1971+2	0.4268+1	0.2618+1
3s-4d(2)	0.2503+3	0.7809+2	0.2694+2	0.1482+2	0.7188+1	0.5734+1	0.8440+0	0.4716+0
3s-4f(3)	0.2053+3	0.4315+2	0.1408+2	0.7654+1	0.3686+1	0.2936+1	0.4301+0	0.2403+0
3p-3p(0)	0.1484+4	0.3114+3	0.1022+3	0.5565+2	0.2682+2	0.2137+2	0.3133+1	0.1750+1
3p-3p(2)	0.2738+3	0.5522+2	0.1799+2	0.9781+1	0.4710+1	0.3752+1	0.5497+0	0.3070+0
3p-3d(3)	0.5012+2	0.1012+2	0.3297+1	0.1792+1	0.8630+0	0.6874+0	0.1007+0	0.5626−1
3p-4s(1)	0.1469+2	0.7287+1	0.3936+1	0.2636+1	0.1562+1	0.1318+1	0.2846+0	0.1745+0
3p-4p(0)	0.1256+3	0.3730+2	0.1279+2	0.7028+1	0.3406+1	0.2717+1	0.3997+0	0.2233+0
3p-4p(2)	0.2301+2	0.8056+1	0.2824+1	0.1559+1	0.7578+0	0.6047+0	0.8913−1	0.4981−1
3p-4d(1)	0.1681+3	0.1594+3	0.8450+2	0.5576+2	0.3256+2	0.2736+2	0.5771+1	0.3522+1
3p-4d(3)	0.3042+2	0.6586+1	0.2151+1	0.1169+1	0.5631+0	0.4485+0	0.6572−1	0.3671−1
3p-4f(2)	0.3127+3	0.8443+2	0.2860+2	0.1567+2	0.7585+1	0.6048+1	0.8889+0	0.4966+0
3p-4f(4)	0.3070+2	0.6215+1	0.2026+1	0.1101+1	0.5302+0	0.4223+0	0.6187−1	0.3456−1
3d-3d(0)	0.1010+4	0.2169+3	0.7140+2	0.3890+2	0.1876+2	0.1494+2	0.2191+1	0.1224+1
3d-3d(2)	0.1346+3	0.2715+2	0.8847+1	0.4809+1	0.2316+1	0.1845+1	0.2702+0	0.1510+0
3d-3d(4)	0.1158+2	0.2413+1	0.7864+0	0.4275+0	0.2058+0	0.1640+0	0.2402−1	0.1342−1
3d-4s(2)	0.3303+1	0.9157+0	0.3141+0	0.1726+0	0.8369−1	0.6675−1	0.9823−2	0.5489−2
3d-4p(1)	0.1407+2	0.4109+1	0.1856+1	0.1176+1	0.6656+0	0.5551+0	0.1125+0	0.6814−1
3d-4p(3)	0.3561+1	0.7816+0	0.2553+0	0.1388+0	0.6684−1	0.5325−1	0.7801−2	0.4358−2
3d-4d(0)	0.1151+3	0.3141+2	0.1066+2	0.5841+1	0.2827+1	0.2254+1	0.3314+0	0.1851+0
3d-4d(2)	0.1561+2	0.4873+1	0.1682+1	0.9255+0	0.4490+0	0.3581+0	0.5272−1	0.2946−1
3d-4d(4)	0.3493+1	0.7709+0	0.2512+0	0.1366+0	0.6576−1	0.5238−1	0.7674−2	0.4287−2
3d-4f(1)	0.5793+3	0.3516+3	0.1697+3	0.1086+3	0.6174+2	0.5153+2	0.1045+2	0.6331+1
3d-4f(3)	0.2840+2	0.5904+1	0.1925+1	0.1047+1	0.5040+0	0.4015+0	0.5882−1	0.3286−1
3d-4f(5)	0.5470+1	0.1156+1	0.3768+0	0.2048+0	0.9863−1	0.7857−1	0.1151−1	0.6430−2
4s-4s(0)	0.1009+5	0.1282+4	0.3930+3	0.2109+3	0.1007+3	0.8013+2	0.1168+2	0.6523+1
4s-4d(2)	0.3348+4	0.4164+3	0.1274+3	0.6833+2	0.3263+2	0.2595+2	0.3783+1	0.2112+1
4s-4f(3)	0.4088+3	0.5087+2	0.1556+2	0.8346+1	0.3986+1	0.3170+1	0.4621+0	0.2580+0
4p-4p(0)	0.9222+4	0.1174+4	0.3601+3	0.1932+3	0.9230+2	0.7342+2	0.1070+2	0.5976+1
4p-4p(2)	0.1677+4	0.2086+3	0.6382+2	0.3423+2	0.1635+2	0.1300+2	0.1895+1	0.1058+1
4p-4d(3)	0.3806+3	0.4735+2	0.1449+2	0.7770+1	0.3711+1	0.2951+1	0.4302+0	0.2402+0

Table 1. (continued)

	k_1							
λ	1	1.2	1.606238	2	2.711088	3	7.5	10
4p-4f(2)	0.1015+4	0.1262+3	0.3861+2	0.2071+2	0.9889+1	0.7865+1	0.1146+1	0.6401+0
4p-4f(4)	0.8249+2	0.1031+2	0.3156+1	0.1692+1	0.8083+0	0.6429+0	0.9371−1	0.5232−1
4d-4d(0)	0.7588+4	0.9721+3	0.2982+3	0.1601+3	0.7646+2	0.6082+2	0.8867+1	0.4951+1
4d-4d(2)	0.9866+3	0.1227+3	0.3755+2	0.2014+2	0.9618+1	0.7650+1	0.1115+1	0.6226+0
4d-4d(4)	0.9478+2	0.1181+2	0.3612+1	0.1937+1	0.9253+0	0.7359+0	0.1073+0	0.5989−1
4d-4f(3)	0.1485+3	0.1849+2	0.5656+1	0.3033+1	0.1449+1	0.1152+1	0.1679+0	0.9377−1
4d-4f(5)	0.3169+2	0.3958+1	0.1211+1	0.6495+0	0.3102+0	0.2467+0	0.3596−1	0.2008−1
4f-4f(0)	0.5524+4	0.7149+3	0.2196+3	0.1178+3	0.5631+2	0.4479+2	0.6530+1	0.3646+1
4f-4f(2)	0.6732+3	0.8373+2	0.2562+2	0.1374+2	0.6561+1	0.5219+1	0.7607+0	0.4247+0
4f-4f(4)	0.4213+2	0.5251+1	0.1606+1	0.8615+0	0.4115+0	0.3273+0	0.4770−1	0.2663−1
4f-4f(6)	0.1244+2	0.1645+1	0.5033+0	0.2699+0	0.1289+0	0.1025+0	0.1495−1	0.8345−2

6. Results

We believe that detailed tables of these accurately checked cross sections will not only be of use in themselves, but serve as an important test case for more elaborate calculations. In table 1 cross sections are given for transitions between quantum states with $n, n' \leqslant 4$, excluding the exact resonance-allowed transitions $n = n'$, $\lambda = 1$ in the first Born approximation.

It is of interest to present partial cross sections for the different λ values separately. The value of λ is the integer given in brackets for each transition. The results are presented at $k_1^2 = 1$, 1.44, 2.58, 4, 7.35, 9, 56.25 and 100 Ryd.

In table 2 we present six-state Born II results, for transitions between states with principal quantum numbers $n = 1$, 2, 3 at the following energies: $k_1^2 = 1$, 1.44, 2.58, 4, 7.35, 9 Ryd (i.e. 13.6, 19.58, 35, 54.4, 100 and 122.4 eV respectively). These were

Table 2. Born II (six-state) cross sections (πa_0^2, exponential notation).

	k_1					
	1	1.2	1.606238	2	2.711088	3
1s-1s	0.1076+1	0.8198+0	0.5428+0	0.3925+0	0.2432+0	0.2058+0
1s-2s	0.7284−1	0.1034+0	0.9503−1	0.7508−1	0.4846−1	0.4114−1
1s-2p	0.4418+0	0.8179+0	0.9811+0	0.9058+0	0.7006+0	0.6275+0
1s-3s	0.9103−2	0.1665−1	0.1597−1	0.1301−1	0.8756−2	0.7527−2
1s-3p	0.2925−1	0.9901−1	0.1452+0	0.1426+0	0.1147+0	0.1034+0
1s-3d	0.2497−1	0.3970−1	0.3469−1	0.2333−1	0.1172−1	0.9230−2
2s-2s	0.1155+3	0.3881+2	0.1479+2	0.8826+1	0.4765+1	0.3921+1
2s-3s	0.1880+1	0.2828+1	0.1914+1	0.1255+1	0.6870+0	0.5623+0
2s-3p	0.3295+1	0.6979+1	0.8798+1	0.7681+1	0.5482+1	0.4802+1
2s-3d	0.1455+2	0.1720+2	0.8676+1	0.5058+1	0.2448+1	0.1934+1
2p-2p	0.5890+2	0.2482+2	0.1106+2	0.6858+1	0.3759+1	0.3096+1
2p-3s	0.1450+1	0.1037+1	0.4530+0	0.3011+0	0.1875+0	0.1611+0
2p-3p	0.4664+1	0.5638+1	0.2808+1	0.1648+1	0.8229+0	0.6591+0
2p-3d	0.1343+2	0.2689+2	0.2311+2	0.1760+2	0.1132+2	0.9689+1
3s-3s	0.1377+4	0.2525+3	0.8252+2	0.4769+2	0.2522+2	0.2067+2
3s-3d	0.6192+3	0.1117+3	0.3127+2	0.1573+2	0.6928+1	0.5378+1
3p-3p	0.1245+4	0.2384+3	0.8212+2	0.4779+2	0.2507+2	0.2046+2
3d-3d	0.4055+3	0.1111+3	0.4780+2	0.2986+2	0.1644+2	0.1354+2

Table 3. Born II cross sections (πa_0^2, exponential notation).

	k_1					
	1	1.2	1.606238	2	2.711088	3
1s-1s	0.1074+1	0.8167+0	0.5407+0	0.3914+0	0.2427+0	0.2054+0
1s-2s	0.7229−1	0.1010+0	0.9459−1	0.7504−1	0.4847−1	0.4114−1
1s-2p	0.4342+0	0.8103+0	0.9747+0	0.9015+0	0.6987+0	0.6262+0
1s-3s	0.9087−2	0.1844−1	0.1703−1	0.1370−1	0.9083−2	0.7773−2
1s-3p	0.2920−1	0.1084+0	0.1554+0	0.1496+0	0.1180+0	0.1059+0
1s-3d	0.2682−1	0.4466−1	0.3580−1	0.2339−1	0.1156−1	0.9099−2
1s-4s	0.1234−2	0.5252−2	0.5208−2	0.4326−2	0.2989−2	0.2592−2
1s-4p	0.6788−2	0.2786−1	0.4406−1	0.4507−1	0.3784−1	0.3451−1
1s-4d	0.4734−2	0.1533−1	0.1492−1	0.1055−1	0.5503−2	0.4360−2
1s-4f	0.5287−2	0.2818−2	0.1286−2	0.5820−3	0.1780−3	0.1210−3
2s-2s	0.1151+3	0.3929+2	0.1500+2	0.8906+1	0.4781+1	0.3930+1
2s-3s	0.1326+1	0.2298+1	0.1848+1	0.1255+1	0.6967+0	0.5706+0
2s-3p	0.2113+1	0.5795+1	0.8486+1	0.7554+1	0.5447+1	0.4782+1
2s-3d	0.1271+2	0.1527+2	0.8265+1	0.4947+1	0.2433+1	0.1927+1
2s-4s	0.2674+0	0.4409+0	0.3198+0	0.2170+0	0.1235+0	0.1022+0
2s-4p	0.8422+0	0.1400+1	0.1700+1	0.1444+1	0.1002+1	0.8700+0
2s-4d	0.1513+1	0.2034+1	0.9958+0	0.5912+0	0.2999+0	0.2405+0
2s-4f	0.1614+1	0.2216+1	0.7958+0	0.3996+0	0.1783+0	0.1401+0
2p-2p	0.5904+2	0.2535+2	0.1125+2	0.6927+1	0.3772+1	0.3103+1
2p-3s	0.1304+1	0.8736+0	0.4003+0	0.2808+0	0.1825+0	0.1580+0
2p-3p	0.4179+1	0.4801+1	0.2558+1	0.1558+1	0.8017+0	0.6463+0
2p-3d	0.1238+2	0.2441+2	0.2196+2	0.1711+2	0.1118+2	0.9605+1
2p-4s	0.2287+0	0.2873+0	0.1082+0	0.6420−1	0.3616−1	0.3031−1
2p-4p	0.8627+0	0.1241+1	0.5660+0	0.3219+0	0.1593+0	0.1277+0
2p-4d	0.1328+1	0.4289+1	0.3580+1	0.2645+1	0.1646+1	0.1397+1
2p-4f	0.1333+1	0.2320+1	0.1116+1	0.5884+0	0.2524+0	0.1931+0
3s-3s	0.1359+4	0.2643+3	0.8665+2	0.4897+2	0.2535+2	0.2068+2
3s-3d	0.5650+3	0.8863+2	0.2679+2	0.1419+2	0.6506+1	0.5058+1
3s-4s	0.2745+1	0.1535+2	0.9511+1	0.5809+1	0.3013+1	0.2460+1
3s-4p	0.6007+1	0.2828+2	0.3668+2	0.3114+2	0.2143+2	0.1862+2
3s-4d	0.1392+2	0.4390+2	0.2271+2	0.1255+2	0.5559+1	0.4270+1
3s-4f	0.5173+2	0.3667+2	0.1407+2	0.7738+1	0.3661+1	0.2900+1
3p-3p	0.1251+4	0.2475+3	0.8434+2	0.4820+2	0.2490+2	0.2024+2
3p-4s	0.3589+1	0.4397+1	0.2871+1	0.2216+1	0.1478+1	0.1284+1
3p-4p	0.1214+2	0.2394+2	0.1260+2	0.7253+1	0.3545+1	0.2848+1
3p-4d	0.1637+2	0.5905+2	0.5992+2	0.4709+2	0.3070+2	0.2634+2
3p-4f	0.6666+2	0.7112+2	0.2912+2	0.1564+2	0.7025+1	0.5437+1
3d-3d	0.4224+3	0.1338+3	0.5330+2	0.3158+2	0.1671+2	0.1366+2
3d-4s	0.4305+1	0.1523+1	0.3868+0	0.1835+0	0.7626−1	0.5945−1
3d-4p	0.1587+2	0.7343+1	0.2363+1	0.1380+1	0.7584+0	0·6353+0
3d-4d	0.3141+2	0.3341+2	0.1271+2	0.6696+1	0.3089+1	0.2449+1
3d-4f	0.7730+2	0.1864+3	0.1361+3	0.9705+2	0.5910+2	0.4996+2
4s-4s	0.7866+4	0.8948+3	0.2716+3	0.1532+3	0.8001+2	0.6548+2
4s-4d	0.3002+4	0.4080+3	0.1168+3	0.5769+2	0.2484+2	0.1986+2
4s-4f	0.8040+3	0.7119+2	0.1818+2	0.9021+1	0.4304+1	0.3779+1
4p-4p	0.7700+4	0.9187+3	0.2889+3	0.1627+3	0.8372+2	0.6841+2
4p-4f	0.1660+4	0.1634+3	0.4197+2	0.2033+2	0.8708+1	0.7039+1
4d-4d	0.5517+4	0.6540+3	0.2201+3	0.1278+3	0.6727+2	0.5524+2
4f-4f	0.1727+4	0.3445+3	0.1432+3	0.8828+2	0.4816+2	0.3967+2

calculated using Born II for $L=0$, 50, Bethe II for $L=51$, 90 and Burgess sum rules for $L\geqslant 91$. The difference between the Born II and Bethe II partial cross sections for $k_1=3$, $n=1$, 2, $n'=1$, 2, 3 for $L=36$ to 40 was better than 2% for all but three transitions and agreement was better than 4% in all cases. The Bethe I and Bethe II partial cross sections were in agreement for all dipole transitions to better than 2% over the range 70–90. In table 3 we present the full ten-state results including all 30 channels for the same energy as the six-state calculation. Born II was used for $L=0$ to 60, Bethe II for $L=61$ to 90 and Burgess sum rules for $L\geqslant 91$. It is expected that Bethe II will give results that are virtually indistinguishable from those of the Born for the range of angular momentum values, $61\leqslant L\leqslant 90$, for transitions from states with $n=1, 2, 3$ to states with $n'=1, 2, 3, 4$.

7. Discussion

This discussion is not concerned with a detailed comparison of the cross sections presented above and the results of other theoretical calculations and experiments as this will form a major part of another paper (Whelan *et al* 1986). Instead it will only be noted that, in general, when exchange is unimportant, the unitarised Born calculation tends to give results in reasonable agreement with the most accurate pseudostate calculations and experiment, indeed better than that obtained by standard close coupling in the absence of pseudostates. A comparison of tables 2 and 3 shows that the inclusion of the $n=4$ states has little effect on the $n=2$ to $n'=3$ transitions.

It is of interest to compare these results with the earlier Born calculations of Somerville (1963). For a number of energies the Born I and Born II six-state calculations afford a direct comparison with his work. There is a good agreement at all energies for the Born I case. For some dipole transitions there is a slight discrepancy at the highest energy (less than 1%).

As mentioned earlier the code developed here was tested for cancellation errors and none were found; therefore, the probable cause of the difference is the difficulty of evaluating the dipole integrals numerically at high energies.

In the Born II calculations there is a much more marked divergence. For the lowest energy $k_1^2=1$, the results presented here are in good agreement with those of Somerville, but for his highest energy, $k_1^2=4$, this is no longer the case, as seen in table 4. It is noted that the dipole results are larger than his while the non-dipole results are smaller.

Somerville lodged the reactance matrix elements he used with the archives of the Physical Society. A comparison of R and T matrix elements for the 2s–3p transition

Table 4. Born II cross sections (πa_0^2), for $k_1=2$.

Transition	Somerville	This work
2s–3p	6.46	7.68
2p–3d	17.54	17.60
2p–3s	0.2728	0.3012
2s–3s	1.40	1.26
2s–3d	5.08	5.06
2p–3p	1.74	1.65

was carried out and no significant difference was found. Only matrix elements corresponding to $L=0$, 20 are given, however. At this stage there is still a large difference between $\Omega^{\mathrm{I}}_{L=20}$ and $\Omega^{\mathrm{II}}_{L=20}$. Somerville (1985) did not generate R and T matrices for larger L because of practical difficulties in generating the reactance matrix elements. Instead he used the formula

$$\frac{Q^{L+1}}{Q^{L}}=\frac{\Omega^{L+1}}{\Omega^{L}}\simeq\left(\frac{k'}{k}\right)^{2} \qquad \text{for large } L$$

to generate the collision strengths for $L>20$. Assuming this formula to be valid for Q^{II} and Q^{I} and applying it to the cross section obtained here at $L=20$ until

$$|Q^{\mathrm{II}}_{L_0}-Q^{\mathrm{I}}_{L_0}|<10^{-2}$$

and using

$$Q^{\mathrm{II}}\simeq\sum_{L}^{L_0}(Q^{\mathrm{II}}_{L}-Q^{\mathrm{I}}_{L})+Q^{\mathrm{I}}$$

a value of $6.49\pi a_0^2$ is obtained, which is quite close to the value of $6.46\pi a_0^2$ given by Somerville. It may therefore be assumed that the differences between the results presented here and those of Somerville are due in their entirety to the difficulty of calculating the high-L contribution to the cross section accurately.

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