## Collisions of fast electrons with helium

# I. Various forms of the second Born approximation

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Abstract. Various forms of the second Born approximation are applied to electron collisions with helium in the energy range 200 to 500 eV. In each case all intermediate states up to  $3^1P$  are included explicitly, and a closure approximation used for higher states, the energy parameter being chosen to fit the total cross section and dispersion relation values for Re f(0) and Im f(0). Calculations are carried out with and without  $V^4$  terms, and in a [1, 1]-Padé approximation, for the  $1^1S \rightarrow 1^1S$ ,  $2^1S$  and  $2^1P$  transitions. Results are compared with experiment and with those of other calculations. The present results cast doubt upon the practice of normalizing experiment to the first Born approximation at intermediate energies.

#### 1. Introduction

Recent improvements in the accuracy with which absolute differential cross sections, for elastic and inelastic scattering of fast electrons by helium and other simple atoms, may be measured (Chamberlain *et al* 1970, Bromberg 1970), and the availability of such data are encouraging theoretical workers to test their results against experiment, rather than against each others, and to go beyond the first Born approximation. We consider here various formulations of the second Born approximation, and apply it to elastic scattering of electrons by helium, and to excitation of the  $1^1S \rightarrow 2^1S$  and  $1^1S \rightarrow 2^1P$  transitions.

Previous detailed investigations of the second Born approximation for electron—atom collisions, largely by Moiseiwitsch and his collaborators (Holt and Moiseiwitsch 1968) were restricted to collisions involving atomic hydrogen. In the course of the preparation of this paper two related investigations of electron—helium collisions were published (Garibotti and Massaro 1971 and Holt *et al* 1971a, b) which will be discussed further below, as will an investigation of elastic scattering by Birman and Rosendorff (1969).

In § 2 of this paper we review the formulation of the second Born approximation and discuss the variants investigated here, in § 3 we consider elastic scattering, in § 4 the excitation of the 2<sup>1</sup>S and 2<sup>1</sup>P levels from the ground state, and we present our conclusions in § 5.

#### 2. The second Born approximation

## 2.1. The scattering amplitude

The cross section for a particular transition  $i \rightarrow f$  of a helium atom by electron impact

may be written as

$$Q_{if}(k_i^2) = 2\frac{k_f}{k_i} \int_0^{\pi} I(\theta) \sin \theta \, d\theta \qquad (\pi a_0^2)$$
 (1)

where  $\theta$  is the scattering angle and  $k_i$  and  $k_f$  are the initial and final wave vectors of the electron. The momentum transfer vector is then

$$K = k_i - k_f. (2)$$

The differential cross section can be written as

$$I(\theta) = |f(\theta)|^2 \tag{3}$$

where  $f(\theta)$  is the scattering amplitude for the transition of interest at impact energy  $\frac{1}{2}k_i^2$  and scattering angle  $\theta$ . The Born series for this amplitude may be written, neglecting exchange, as

$$f(\theta) = f_1(\theta) + f_2(\theta) + O(V^3) \tag{4}$$

to third order in the interaction potential V. Then the first Born approximation to  $f(\theta)$  is

$$f_1(\theta) = -\frac{1}{2\pi} \int \exp(i\mathbf{K} \cdot \mathbf{r}) V_{fi}(\mathbf{r}) d\mathbf{r}$$
 (5)

and the second Born correction is

$$f_2(\theta) = \frac{1}{\pi} \sum_{n} \int \int \exp\{i(\boldsymbol{k}_i \cdot \boldsymbol{r} - \boldsymbol{k}_f \cdot \boldsymbol{r}')\} V_{fn}(\boldsymbol{r}') V_{ni}(\boldsymbol{r}) \frac{\exp(i\boldsymbol{k}_n | \boldsymbol{r} - \boldsymbol{r}'|)}{4\pi | \boldsymbol{r} - \boldsymbol{r}'|} d\boldsymbol{r} d\boldsymbol{r}'$$
 (6)

where the summation over the intermediate states n includes an integration over the continuum. The matrix elements  $V_{nm}(r)$  are given by

$$V_{nm}(\mathbf{r}) = \int \int \psi_n^*(\mathbf{r}_1, \mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}) \psi_m(\mathbf{r}_1, \mathbf{r}_2) \, d\mathbf{r}_1 \, d\mathbf{r}_2$$
 (7)

where  $\psi_n(\mathbf{r}_1, \mathbf{r}_2)$  is the wavefunction of the *n*th state of the target helium atom having eigenenergy  $E_n$  with associated wavenumber  $k_n$  given by

$$k_n^2 = 2(E - E_n) \tag{8}$$

E being the total energy of relative motion, namely  $\frac{1}{2}k_i^2$ . The interaction potential V is

$$V(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}) = \frac{2}{r} - \frac{1}{|\mathbf{r} - \mathbf{r}_1|} - \frac{1}{|\mathbf{r} - \mathbf{r}_2|}.$$
 (9)

Replacing the Green function by its Fourier transform

$$\frac{\exp(\mathrm{i}\mathbf{k}_n|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|} = \lim_{\epsilon \to 0^+} \frac{1}{(2\pi)^3} \int \frac{\exp\{\mathrm{i}\mathbf{q} \cdot (\mathbf{r}-\mathbf{r}')\}}{q^2 - k_n^2 - \mathrm{i}\epsilon} \,\mathrm{d}\mathbf{q}$$

and interchanging the order of limiting operations (6) becomes

$$f_2(\theta) = \frac{1}{8\pi^4} \sum_{n=\epsilon \to 0^+} \lim_{r \to 0^+} \int d\mathbf{q} \int d\mathbf{r} \int d\mathbf{r}' \exp\{i(\mathbf{q} \cdot (\mathbf{r}' - \mathbf{r}) + \mathbf{k}_i \cdot \mathbf{r} - \mathbf{k}_f \cdot \mathbf{r}')\} \frac{V_{fn}(\mathbf{r}')V_{ni}(\mathbf{r})}{q^2 - k_n^2 - i\epsilon}$$

The r and r' integrals are readily evaluated (Bethe 1930) to give

$$f_2(\theta) = \frac{2}{\pi^2} \sum_{n} \lim_{\epsilon \to 0^+} \int \frac{\mathrm{d}\mathbf{q}}{q^2 - k_n^2 - \mathrm{i}\epsilon} \frac{I_{fn}(\mathbf{q} - \mathbf{k}_f) I_{ni}(\mathbf{k}_i - \mathbf{q})}{(\mathbf{q} - \mathbf{k}_i)^2 (\mathbf{q} - \mathbf{k}_f)^2}$$
(10)

where

$$I_{nm}(t) = \int \int \psi_n^*(r_1, r_2) \{ 2 \exp(it \cdot r_1) - 2 \} \psi_m(r_1, r_2) dr_1 dr_2.$$
 (11)

The exact second Born approximation to the scattering amplitude (10) involves summation over a complete set of intermediate states of the target atom and cannot, in general, be carried out in practice.

For given n and with appropriate analytic representations of the wavefunctions the evaluation of the real part of the q space integral in (10) may be effected by Feynman techniques, and has been discussed by earlier workers (cf Holt and Moiseiwitsch 1968). The extension to Im  $f_2(\theta)$ , and the necessary programs are discussed elsewhere (Woollings 1972).

Massey and Mohr (1934) replaced  $k_n$  in (10) by  $k_i$  and used closure to reduce the summation to a single term. This is unsatisfactory since among other things it implies that the imaginary part of the forward elastic scattering amplitude is infinite.

Kingston et al (1960) considered the  $1^1S \rightarrow 2^1S$  excitation of atomic hydrogen including contributions from the 1s, 2s,  $2p_{0,\pm 1}$  intermediate states only. Holt and Moiseiwitsch (1968) improved on this by evaluating exactly terms arising from coupling to the lowest N states and allowing for higher states by replacing  $k_n$  by  $k_{N+1}$  for n > N in (10), evaluating these terms by closure. We adopt a modification of this approach.

Bransden and McDowell (1970) have shown that a dispersion relation conjectured by Gerjuoy and Krall (1960) is well satisfied for electrons on helium at energies up to 500 eV. They fitted the available data on the total scattering cross section and showed via the dispersion relation and a phase shift analysis (Bransden and McDowell 1969) that the data was consistent with other low energy experiments. From this data they obtained the forward elastic scattering amplitude at various energies.

Now consider elastic scattering in the second Born approximation. We choose to retain the 1<sup>1</sup>S, 2<sup>1</sup>S, 3<sup>1</sup>S, 2<sup>1</sup>P, 3<sup>1</sup>P states explicitly and to take account of coupling to higher states by choosing  $k_n^2$  for all the higher states so that we reproduce Bransden and McDowell's forward elastic scattering amplitude. We find that different values of  $k_n^2$  are required, for any given  $k_1^2$ , to fit Re f(0) and Im f(0). They are presented in table 1 in terms of a parameter  $\Delta$  defined by

$$k_n^2 = k_i^2 - 2\Delta. (12)$$

We have investigated how  $\Delta$  varies with the number of intermediate states explicitly included in the second Born approximation and these results are also given in table 1. With N=1 we included only the 1<sup>1</sup>S intermediate state, N=2 the 1<sup>1</sup>S, 2<sup>1</sup>S, 2<sup>1</sup>P and N=3 all five states listed above.

Now the dispersion relation expresses the real part of the forward elastic scattering amplitude Re f(0) in terms of the total cross section at all energies. By choosing  $\Delta$  to reproduce these dispersion relation values we ensure that the calculated values of Re f(0) in the second Born approximation are consistent in this sense with the observed values of the total cross section. The optical theorem expresses Im f(0) in terms of the total cross section at that energy and so choosing  $\Delta$  to reproduce the optical theorem value

of Im f(0) we again ensure consistency in this sense with the observed total cross sections. It is then again consistent with this derivation of  $\Delta$  to make it independent of transition considered.

Garibotti and Massaro (1971) have argued that for elastic scattering  $\Delta$  should be a function of angle as well as of impact energy and our calculations reported below tend to confirm this. We see no simple way to make a choice of  $\Delta$  if it is to be angle dependent. (cf Bonham 1971.)

		Re f			$\operatorname{Im} f$	
$E\left( \mathrm{eV}\right)$	N = 1	N = 2	N = 3	N = 1	N=2	N = 3
200	5.65	6.7	7.1	3.15	3.6	3.8
300	7.4	8.9	9.55	3.2	3.7	3.9
400	8.9	10.9	11.65	3.5	4.1	4.35
500	10.2	12.5	13.45	3.7	4.45	4.7

**Table 1.** Calculated values of  $\Delta$  (in atomic units)

Holt et al (1971a) have compared the values of Re f(0) they obtained using their value of  $k_n^2$  with the values given by Bransden and McDowell (1970). The agreement is poor.

Birman and Rosendorff (1969) choose N=1 and replace  $k_n^2$  by  $k_i^2 - \Delta'$  where  $\Delta'$  is a free parameter. They found that to obtain agreement with experimental elastic scattering differential cross sections at angles greater than  $5^{\circ}$   $\Delta'$  must be chosen appreciably larger than the value implied in the work of Holt *et al* (1971a). They considered only Re f and found that  $\Delta'$  varies rapidly with incident electron energy, in agreement with our results.

Garibotti and Massaro (1971) also took N=1 and choose  $\Delta$  such that the [1, 1] Padé approximant (see § 2.3) to the elastic scattering amplitude in the forward direction is stationary at the energy considered. They find, in agreement with the work reported here, and with that of Birman and Rosendorff, that  $\Delta$  is required to be energy dependent. However their resultant values of Re f(0) are markedly lower than those obtained by Bransden and McDowell.

#### 2.2. Simplified second Born approximation

From (3) and (4), we have that in the second Born approximation  $I(\theta)$  includes some of the terms of order  $V^4$ . Kingston *et al* (1960) argued that other terms of this order arise from the third Born approximation to  $f(\theta)$ , and that it is preferable to omit all terms of order  $V^4$  in calculating  $I(\theta)$ . To second order in the Born approximation with the same notation as in (4), but omitting the explicit angle dependence,

$$f = f_1 + f_2. (13)$$

$$I(\theta) = |f_1 + f_2|^2 = |f_1|^2 \{ (1+\alpha)^2 + \beta^2 \} = |f_1|^2 \{ 1 + 2\alpha + \alpha^2 + \beta^2 \}$$

where

$$\alpha = \operatorname{Re}\left(\frac{f_2}{f_1}\right) \qquad \beta = \operatorname{Im}\left(\frac{f_2}{f_1}\right)$$
 (14)

and we call this the full second Born approximation (FB2). Retaining no terms of fourth order in V we have the modified second Born approximation (RB2)

$$I_3(\theta) = |f_1|^2 \{1 + 2\alpha\} \tag{15}$$

referred to by Holt et al as the third order approximation.

Holt et al (1971b) adopt the RB2 approximation and include  $1^1S$ ,  $2^1S$ ,  $2^1P$  intermediate states explicitly, putting  $\Delta = E(3^1S)$ . When an average  $\Delta$  is employed the approximations (14) and (15) are said to be simplified and we shall denote them by SFB2 and SRB2 respectively. We examine both elastic scattering and excitation of the  $2^1S$  and  $2^1P$  levels using both SRB2 and SFB2 approximations with the five intermediate states discussed above, and the values of  $\Delta$  given in table 1.

#### 2.3. Padé approximants

The [N, M] Padé approximant to a series

$$g(V) = g_0 + g_1 V + g_2 V^2 + \dots$$

is defined (Wall 1948) as the ratio

$$[N, M] = \frac{P_N(V)}{Q_M(V)}$$

where  $P_N(V)$  and  $Q_M(V)$  are polynomials in V of order N and M respectively. They are uniquely defined by the equations

$$Q_M(V)g(V) = P_N(V) + O(V^{N+M+1})$$
  
 $Q_M(0) = 1.$ 

Hence the [1,1] Padé approximant to the scattering amplitude as given in (4) is

$$f_p(\theta) = \frac{f_1^2}{f_1 - f_2} \tag{16}$$

and if we approximate  $f_2$  by choosing an average  $\Delta$  this is called the simplified [1, 1] Padé approximant.

Note that if the Schwinger variational principle is used with plane waves for the incident and scattered electron then the [1, 1] Padé approximant for the scattering amplitude is recovered. If  $\alpha$  and  $\beta$  (cf equation 14) are both small then

$$I_{p}(\theta) = |f_{p}(\theta)|^{2} = |f_{1}|^{2} \{ 1 + 2\alpha + 3\alpha^{2} - \beta^{2} + O(V^{3}) \}$$
(17)

which agrees with (14) and (15) to order  $V^3$  but differs in terms of order  $V^4$ . Again other terms of order  $V^4$  arise from higher approximants.

#### 2.4. Wavefunctions

Analytic Hartree–Fock wavefunctions are available in the literature for all states of the helium atom required in our work. For the ground 1 state we use Green wavefunction (Green et al 1954),

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = N\{\exp(-zr_1) + c \exp(-2zr_1)\}\{\exp(-zr_2) + c \exp(-2zr_2)\}$$
 (18)

with c = 0.6, z = 1.4558. McEachran has given analytic Hartree-Fock functions for

the  $(1snl)n^1L(l=0,1; n \le 3)$  states of interest (Cohen and McEachran (1969), Crothers and McEachran (1970)), in the form

$$\psi(r_1, r_2; n'l) = u(r_1)v(r_2) + u(r_2)v(r_1)$$
(19)

where

$$u(r) = 2 \exp(-r) Y_{00}(\hat{r})$$

$$v(r) = \sum_{j=2l+1}^{N} a_j \exp(-\alpha r) r^l L_j^{2l+1}(2\alpha r) Y_{lm}(\hat{r})$$
(20)

and  $\alpha = (1/n)$ . The  $L_j^{2l+1}(x)$  are associated Laguerre functions, and the  $Y_{lm}(f)$  the spherical harmonics. Scaled atomic units are used (the unit of length is  $za_0$ , that of energy is  $z^2$ au). We found that the recursive methods required to evaluate the second order matrix elements were impractical if more than four terms were used in (20) above.

The overlap integral  $\langle 1s|2s \rangle$ , using (18) and (19) for the wavefunctions was -0.015, an unacceptably large value, as the 2<sup>1</sup>S excitation cross section is of order  $10^{-3}$  times the elastic scattering cross section. An improved 2s orbital was obtained by minimizing

$$F = 100|\langle 1s|2s\rangle|^2 + \{Q_{\rm B1}(1s \to 2s) - Q_{\rm B1}^{(c)}(1s \to 2s)\}^2$$
 (21)

where  $Q_{\rm B1}^{\rm (c)}$  is the first Born 1<sup>1</sup>S  $\rightarrow$  2<sup>1</sup>S excitation cross section calculated using our trial (1s2s)2<sup>1</sup>S function and  $Q_{\rm B1}$  is the accurate first Born value of Bell *et al* (1969). The minimization was carried out at 200 eV, and the resulting 'improved' wavefunction gave good first Born cross sections at all energies considered. The coefficients of the Cohen–McEachran function and our modified function are given in table 2.

Table 2. Coefficients for the (1s2s)2<sup>1</sup>S wavefunction

	$a_1$	$a_2$	$a_3$	$a_4$	⟨1s 2s⟩
Cohen-McEachran	1.0	2.0986	-3.8653-1	4.6059-2†	-1.504-2
Modified	1.0	2.2786	$-3.6640^{-1}$	5.1369-2	$-1.035^{-6}$

<sup>†</sup> The superscript denotes the power of ten by which the entry should be multiplied.

The corresponding first Born excitation cross sections together with the accurate values of Bell  $et\ al\ (1969)$  are given in table 3. Note that in evaluating the matrix elements, the intermediate state energies  $E_n$  adopted (equation (8) above) are the Cohen-McEachran Hartree-Fock values.

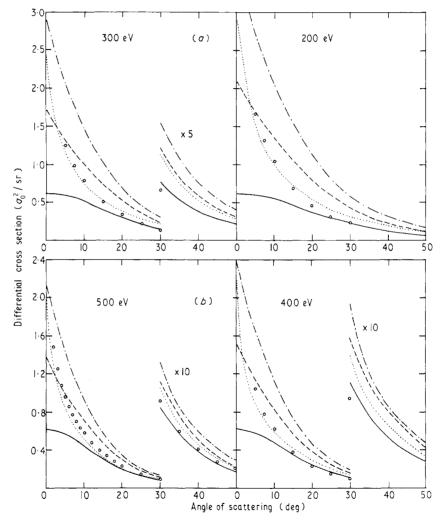
**Table 3.** First Born cross sections for the  $1^1S \rightarrow 2^1S$  process in units of  $10^{-3} \pi a_0^2$ 

E(eV)	200	300	400	√ <b>50</b> 0
Bell et al	11.7	8.0	6.0	4.8
Cohen-McEachran	9.7	6.6	5.0	4.1
Modified	11-6	7.9	6.0	4.8

### 3. Elastic scattering

#### 3.1. Differential cross sections

Calculated elastic differential cross sections are shown in figure 1, where they are compared with the srb2 calculation of Holt et al (1971b). The experimental data are those of Bromberg (1970) at 500 eV, and at the other energies those of Vriens et al (1968b) renormalized at 5° to Chamberlain et al (1970). With our choice of  $\Delta$  the srb2 results lie well above all other values at all angles considered. Our srb2 results are in less good agreement with experiment than those of Holt et al (1971b) who chose  $\Delta = E(3^1\text{S})$ . By forcing our differential cross section to the forward dispersion relation



values we overestimate the scattering at small non-zero angles. That is we are forcing the Born series to be represented by its first two terms, which is clearly unsatisfactory. Our results using the simplified Padé approximant lie just above the first Born curve at most angles and energies, and do not give the intense forward peak.

Garibotti and Massaro (1971) used a very simple ground state wavefunction and did not take explicit account of any other intermediate states. However at the three energies where we can compare results, these appear to be closest to our SFB2 results at small angles but approach the experimental values faster than our SFB2 results do at larger angles.

A comparison with the srb2 calculation by Birman and Rosendorff (1969), who included only the 1<sup>1</sup>S intermediate state explicitly, is possible at 200 eV. Their results, using  $\Delta = 5.0$ , are in agreement with our srb2 results using  $\Delta = 7.1$  but including more intermediate states explicitly, as would be expected (cf table 1).

These comparisons suggest that no matter what wavefunctions are used, or how many intermediate states considered explicitly, or what form for the differential cross section is adopted a suitable choice of  $\Delta$  will fit the forward elastic scattering cross section of Bransden and McDowell (1970). However this choice does not give accurate differential cross sections for larger angles, that is,  $5^{\circ} \rightarrow 30^{\circ}$  in these second order calculations. The values given by Bransden and McDowell (1970), while the best available, are not definitive.

Garibotti and Massaro (1971) do not quote the value of  $\Delta$  they used for electronhelium scattering but from independent calculations (Woollings 1972) it was found that a very large value of  $\Delta$  is required for  $|f_p(0)|^2$  to be stationary. In the case of elastic scattering of electrons by atomic hydrogen in its ground state, Prasad (1964) has evaluated Re  $f_2(0)$  (equation (4)) exactly in the second Born approximation. The large values of  $\Delta$  obtained by Garibotti and Massaro for this case lead to significantly lower values of Re  $f_2(0)$ . For example at  $k_1=4$  au, Prasad finds Re  $f_2(0)=0.8266$  including N=3 states explicitly, we find that with N=16 states included explicitly Re  $f_2(0)=0.8744$  and Holt (1972) includes N=100 states explicitly, finding Re  $f_2(0)=0.878$ . With the N=2 states included explicitly and  $\Delta=6.5$ , Garibotti and Massaro give Re  $f_2(0)=0.6868$ , whilst the maximum value of Re  $f_2(0)$  that can be obtained in this model is 0.8472 with  $\Delta=1.4$ . Hence it would appear that Garibotti and Massaro's choice of  $\Delta$  does not give the best approximation to the infinite summation occurring in (10), in the forward direction.

Finally it is clear from figure 1 that the approximations adopted by Holt et al give a more satisfactory account of the elastic scattering of electrons by helium than do our variants of the second Born approximation or than the simplified [1, 1] Padé approximant.

#### 3.2. Total elastic cross section

Our results for the total elastic scattering cross section obtained using (14), (15) and (16) are presented in table 4, and compared with experiment, and with the complete SRB2 calculation of Holt et al (1971b). They were obtained by numerical integration of our differential cross sections, and agree in first Born with the very accurate values of Bell et al (1969) to better than 0.5%. However our SRB2 results are much larger than the corresponding calculations of Holt et al, and our SFB2 results are larger still. The [1, 1] simplified Padé results, using our values of  $\Delta$ , are however in substantially better agreement with the experimental values than any of the second Born calculations.

However owing to the shape of the Padé differential cross section this good agreement is probably fortuitous. The situation remains unsatisfactory.

Energy (eV)	200	300	400	500
First Born	0.221	0.151	0.115	0.0922
SFB2	0.633	0.353	0.234	0.172
SRB2	0.430	0.252	0.175	0.133
Simplified Padé	0.240	0.158	0.121	0.0977
Holt et al	0.352	0.211	0.149	0.115
Vriens et al†	0.251	0.171	0.128	

**Table 4.** Total cross sections for the elastic scattering of electrons by helium (in  $\pi a_0^2$ )

## 4. Inelastic scattering

We have calculated differential and total cross sections for the  $1^1S \rightarrow 2^1S$ ,  $1^1S \rightarrow 2^1P$  transitions at energies of 200(100)500 eV in the sfb2, srb2 and simplified [1, 1] Padé approximations using the values of  $\Delta$  given in table 1.

For both inelastic transitions examined we have compared our differential cross sections only with the absolute experimental measurements of Chamberlain *et al* (1970). The relative measurements by Lassetre *et al* (1964) are normalized at four small angles to first Born calculations of the  $1^{1}S-2^{1}P$  differential cross section at 511 eV, and for both transitions agree closely with the first Born approximation over our range of angles and energies, and consequently with the calculations of Holt *et al* (1971).

4.1. 
$$1^1S \rightarrow 2^1P$$

In this case we found that we were unable to calculate the imaginary part of (10) for the  $2^1P$  intermediate state (Woollings 1972). That is with our representation of the wavefunctions the expression for  $\text{Im}(f_2/f_1)$  arising from the  $1s \to 2p \to 2p$  sequence led to intractable integrals. We feel that this may be an important contribution to the imaginary part so we only present our SRB2 results. The differential cross sections are compared with Holt  $et\ al\ (1971b)$  and experiment in table 5. The experimental forward differential cross sections were obtained, from the analytic fits to the experimental values given by Vriens  $et\ al\$ and used to calculate their total cross sections. The SRB2 results

**Table 5.** Differential cross sections for the excitation of the  $2^1P$  state of helium by electrons  $(\text{in } a_0^2/\text{sr})$ 

Energy (eV)		200			400	
Angle	0°	5°	10°	0°	5°	10°
First Born	15.13	3.47	0.69	32.96	1.90	0.21
SRB2	13.43	3.00	0.56	30.86	1.73	0.17
Holt et al	14.74	3.47	0.67	31.83	1.93	0.21
Vriens et al†	11.90	2.91	0.56	28.94	1.784	0.18

<sup>+</sup> Vriens et al (1968a) renormalized to Chamberlain et al (1970) at 5°.

<sup>†</sup> Vriens et al (1968a) renormalized to Chamberlain et al (1970) at 5°.

are a considerable improvement on the first Born results and are also superior to those of Holt *et al*, but still over estimate the forward peak.

In table 6 we compare total cross sections. Again our SRB2 results are in good agreement with the experiments of Vriens  $et\ al$  but not with the more recent preliminary results of de Jongh and van Eck (1971). Further, with our choice of  $\Delta$  the total cross section is decreased relative to the first Born while Holt  $et\ al$  (1971b) find that their SRB2 total cross section is larger than their first Born. Note that for this transition our agreement with the experiment of Vriens  $et\ al$  is maintained down to 200 eV, whereas the first Born approximation is outside the quoted errors on this experiment up to  $400\,\mathrm{eV}$ .

Table 6.	Total	cross	sections	for	the	excitation	of	the	21P	state	of	helium	by	electrons
$(in 10^{-2})$	$\pi a_0^2$													

Energy (eV)	200	300	400	500
First Born	10.6	8.3	7.0	6.1
SRB2	8.8	7.4	6.4	5.6
Holt et al†	10.91	8.55	7.11	
Vriens et al‡	8.6	7.4	6.2	
de Jongh and van Eck	9.98	8.25	6.83	5.87

<sup>†</sup> The values quoted are those given by Hunt (1971). Columns (3) and (4) of table 3 of the paper by Holt et al (1971b) appear to have been interchanged.

## 4.2. $1^{1}S \rightarrow 2^{1}S$

In table 7 we compare the differential cross sections for the  $1^1S \rightarrow 2^1S$  transition of helium atoms by electron impact, calculated in the first Born, srb2, sfb2 and simplified Padé approximations, with Holt *et al* (1971b) srb2 calculation and the Vriens *et al* (1968a) experimental results (renormalized to the Chamberlain *et al* (1970) experimental results at  $5^\circ$ ). The imaginary part of the forward scattering amplitude is of the same order of magnitude as the first Born scattering amplitude in the forward direction, and this accounts for the very large sfb2 differential cross sections. The simplified [1, 1] Padé approximant gives a forward differential cross section which decreases with decreasing angle ( $\theta \le 5^\circ$ ) whereas all the other cases show an increase of differential

**Table 7.** Differential cross sections for the excitation of the 2<sup>1</sup>S state of helium by electrons (in  $a_0^2/\text{sr}$ )

Energy (eV)		200			400	
Angle	0°	5°	10°	0°	5°	10°
First Born	0.188	0.162	0.106	0.199	0.147	0.0644
SRB2	0.206	0.153	0.0968	0.217	0.141	0.0613
SFB2	0.818	0.323	0.133	0.707	0.187	0.0691
Simplified Padé	0.0454	0.0769	0.0743	0.059	0.108	0.0551
Holt et al	0.191	0.162	0.106	0.203	0.147	0.0661
Vriens et al†	0.155	0.128	0.0698	0.185	0.128	0.05
			41.4			

<sup>†</sup> Vriens et al (1968a), renormalized.

<sup>‡</sup> Vriens et al (1968a), renormalized.

cross section to small angles. The SRB2 approximation gives a differential cross section that is larger than the first Born one near the forward direction (in disagreement with experiment which is smaller) but at slightly larger angles ( $\geq 5^{\circ}$ ) becomes smaller than the first Born in agreement with experiment. However the improvement is not as dramatic as in the  $1^{1}S \rightarrow 2^{1}P$  transition. Holt *et al* (1971b) find that the SRB2 approximation, with their choice of parameters, is almost identical to the first Born for this transition at the angles and energies considered above, whereas we find a change of close to 10% from the first Born.

In table 8 we compare the total  $1^1S \rightarrow 2^1S$  cross sections. As expected from consideration of the differential cross sections the SFB2 result is much too large. Although the simplified [1, 1] Padé result appears to be in best agreement with experiment it does not correctly reproduce the shape of the small angle differential cross section. The SRB2 approximation decreases the first Born total cross section but is still only in moderate agreement with experiment. As with the  $1^1S \rightarrow 2^1P$  total cross sections we find that our choice of  $\Delta$  decreases the total cross section relative to first Born whereas Holt  $et\ al$  found it increased over their first Born values. We find that the total  $1^1S \rightarrow 2^1S$  cross section evaluated in the SRB2 approximation lies at least 5% lower than our first Born values at all energies up to 500 eV, whereas Holt  $et\ al$  find negligible differences (<1%) in our energy range. However, none of the Born calculations lie within the error brackets ( $\pm 10\%$ ) of the experimental data even at 400 eV. Further work is required.

Energy (eV)	200	300	400	500
Elicity (CV)	200			
First Born	11.6	7.87	5.97	4.81
SRB2	10.4	7.28	5.64	4.57
SFB2	20.6	12.0	8.34	6.35
Simplified Padé	7.02	5.40	4.42	3.73
Holt et al	11.63	7.84	5.92	4.75
Vriens et al†	6.7	5.3	4.7	

**Table 8.** Total cross section for the excitation of the  $2^{1}S$  state of helium by electrons (in  $10^{-3} \pi a_{0}^{2}$ )

#### 5. Conclusions

We have investigated various forms of the second Born approximation for elastic and inelastic collisions of electrons with helium atoms. Our results differ significantly in some respects from those of earlier workers (Holt et al 1971a, b). In particular by choosing the intermediate state energy parameter  $\Delta$  to fit the forward dispersion relation values for Re f(0) our srb2 results give poor agreement with experimental elastic scattering data at small angles, but improved agreement with experiment for the  $1^1S \rightarrow 2^1S$  and  $1^1S \rightarrow 2^1P$  inelastic differential cross sections.

The full second Born approximation (sFB2) includes contributions from Im  $f(\theta)$ , and by choosing the parameters so that Im  $f_{\rm el}(0)$  takes the optical theorem values, the differential and total cross sections for some individual cross sections appear excessively large. However approximations to the second Born approximation do not

<sup>†</sup> Vriens et al (1968a), renormalized.

in general satisfy the optical theorem. The SRB2 approximation, which sets Im f(0) = 0, of course cannot satisfy the optical theorem.

Our results for inelastic processes indicate that a third order calculation of this kind can produce changes of between 5 and 10% in the total cross sections for individual transitions at impact energies up to twenty times the threshold, implying that the Born series for such processes may not converge to this accuracy until at least this high an energy. Experimental relative cross sections normalized to the first Born approximation at energies below say fifty times threshold may be less reliable than is usually supposed. However a different conclusion would follow from Holt *et al*'s version of the SRB2 approximation.

Further work on doubly excited transitions and on  $1^1S \rightarrow n^1D$  transitions is in progress.

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