

PERTURBATIVE METHODS IN ELECTRON- AND POSITRON-ATOM SCATTERING

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NORTH-HOLLAND – AMSTERDAM

Abstract:

This article reviews a particular area of perturbation theory in which there has been much activity during the past ten years. This area embraces distorted-wave Born series, the Glauber approximation, the eikonal-Born series, the modified Glauber approximation, the Wallace approximation, the unitarized eikonal-Born series and ab-initio optical potential methods. Central to the developments which have taken place is the rôle of the second-order, or second Born, term. The physical content of this term and methods for its calculation are therefore discussed in detail.

1. Introduction

Despite the generality of the title this article is restricted to a particular area of perturbation theory in which there has been much activity in the past ten years. This area encompasses distorted-wave Born approximations, methods based upon the Glauber and Wallace approximations and ab-initio optical potential theory. These three sub-areas share a common set of ideas and techniques. Foremost amongst these ideas is the rôle of the second-order, or second Born, term. Indeed, this article is very much a study of the second-order term.

Our attention will be directed primarily towards electron-atom collisions since the amount of information and work in this field overshadows that on positron collisions. Also, since perturbation theory is of most use at the higher energies where exchange scattering is small, we shall initially be concerned mainly with direct electron-atom scattering. Not until section 8 shall we start to look at exchange scattering in a detailed way.

After defining notation in section 2, I start in section 3 with the simplest form of perturbation theory, the plane wave Born series expansion. This section sets the tone for the more sophisticated developments of sections 5, 6 and 7, but also contains some very interesting results in its own right.

For other review articles in the same kind of area the reader is directed to [1–9].

2. Notation

Atomic units (a.u.) will be used. In this system $\hbar = m_e = e = 1$, where \hbar is Planck's constant divided by 2π , m_e is the mass of the electron/positron and e is the magnitude of the electronic charge. The Bohr radius, \hbar^2/me^2 , will be denoted by the symbol a_0 .

I shall consider the collision of an e^\pm with an N -electron atom. The Hamiltonian for this system is

$$H = K_0 + H_a + V, \quad (2.1)$$

where

$$K_0 \equiv -\frac{1}{2}\nabla_0^2, \quad (2.2a)$$

$$H_a \equiv \sum_{i=1}^N \left(-\frac{1}{2}\nabla_i^2 - N/r_i \right) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N 1/r_{ij}, \quad (2.2b)$$

$$V \equiv V(\mathbf{r}_0, \mathbf{X}) \equiv \bar{Q} \left(N/r_0 - \sum_{i=1}^N 1/r_{0i} \right). \quad (2.2c)$$

In (2.2) \mathbf{r}_0 is the position vector of the incident e^\pm relative to the atomic nucleus, and \bar{Q} is its charge ($= \pm 1$); \mathbf{r}_i labels the position vector of the i th atomic electron and \mathbf{r}_{ij} stands for $\mathbf{r}_i - \mathbf{r}_j$; since the atom is assumed to be electrically neutral the nuclear charge is N . The symbols K_0 , H_a and V represent respectively the kinetic energy of the incident e^\pm , the atomic Hamiltonian and the interaction potential between the incident e^\pm and the atom. \mathbf{X} stands for the aggregate of space and spin coordinates of the N atomic electrons.

The atomic eigenstates will be written as $\psi_n(\mathbf{X})$. Thus

$$H_a \psi_n = \varepsilon_n \psi_n, \quad (2.3)$$

where ε_n is the energy of the state ψ_n . When ψ_n is a bound state it will be normalized to unity. In sums involving continuum states, e.g., the completeness relation

$$\sum_n |\psi_n\rangle\langle\psi_n| = 1 \quad (2.4)$$

a discrete notation will often be used, it being understood that the continuum states are integrated over and have the appropriate normalization.

Let the e^\pm be incident with momentum \mathbf{k}_0 upon the atom in the state ψ_0 . The wavefunction Ψ^+ for the entire $(N + 1)$ -particle system must therefore satisfy the Schrödinger equation

$$H\Psi^+ = (\frac{1}{2}k_0^2 + \varepsilon_0)\Psi^+. \quad (2.5)$$

Treating the incident particle as distinguishable* from the atomic electrons, Ψ^+ must satisfy the boundary condition

$$\Psi^+ \xrightarrow{r_0 \rightarrow \infty} \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0) \psi_0(\mathbf{X}) + \text{outgoing scattered waves}. \quad (2.6)$$

(The solution of (2.5) with ingoing scattered waves in (2.6) will be denoted Ψ^-). If the e^\pm is subsequently scattered with momentum \mathbf{k}_f and the atom is left in the state ψ_f , it is well known from elementary scattering theory that the corresponding scattering amplitude is given by

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -\frac{1}{2\pi} \langle \mathbf{k}_f \psi_f | V | \Psi^+ \rangle \quad (2.7)$$

where

$$\langle \mathbf{k}_f \psi_f | V | \Psi^+ \rangle \equiv \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_f^*(\mathbf{X}) V(\mathbf{r}_0, \mathbf{X}) \Psi^+(\mathbf{r}_0, \mathbf{X}) d\mathbf{r}_0 d\mathbf{X}, \quad (2.8)$$

and * stands for complex conjugation.

* This means that the spin coordinate of the incident e^\pm can be ignored – under the Hamiltonian (2.1) its spin will be conserved. For positron scattering this is no restriction, but for electron scattering it means that (2.7) is just the direct scattering amplitude.

The differential cross section for the transition $\psi_0 \rightarrow \psi_f$ is given by

$$\frac{d\sigma_{f0}}{d\Omega} = \frac{k_f}{k_0} |f_{f0}(k_f, k_0)|^2, \quad (2.9)$$

where

$$k_f^2 = k_0^2 + 2(\epsilon_0 - \epsilon_f), \quad (2.10)$$

and the corresponding integrated cross section by

$$\sigma_{f0} = \int \frac{d\sigma_{f0}}{d\Omega} d\Omega. \quad (2.11)$$

Also of interest is the so-called total cross section. For an e^\pm incident upon the state ψ_0 this is

$$\sigma_{\text{total}} = \sum_f \sigma_{f0}, \quad (2.12)$$

where the sum is over all states ψ_f (including $f = 0$) which can be excited at the given impact energy. By the optical theorem

$$\sigma_{\text{total}} = (4\pi/k_0) \operatorname{Im} f_{00}(\theta = 0), \quad (2.13)$$

where θ is the scattering angle.

The momentum transfer \mathbf{q} in the collision is

$$\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_f. \quad (2.14)$$

The magnitude of \mathbf{q} is related to θ by

$$q^2 = k_0^2 + k_f^2 - 2k_0k_f \cos \theta. \quad (2.15)$$

Finally, unit vectors are labelled by a caret, i.e.,

$$\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|. \quad (2.16)$$

3. The Born series

The Schrödinger equation (2.5) together with the boundary condition (2.6) is easily recast in the form of an integral equation, the so-called Lippmann–Schwinger equation [10]

$$\Psi^+ = \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0) \psi_0 + G_0^+ V \Psi^+, \quad (3.1a)$$

where

$$G_0^\pm \equiv \lim_{\eta \rightarrow 0^+} (E - H_0 \pm i\eta)^{-1}, \quad (3.1b)$$

$$H_0 \equiv K_0 + H_a, \quad (3.1c)$$

$$E \equiv \frac{1}{2}k_0^2 + \varepsilon_0. \quad (3.1d)$$

A formal series solution of (3.1a) in powers of V is obtained by iteration starting with $\Psi^+ = \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)\psi_0$:

$$\Psi^+ = (1 + G_0^+ V + (G_0^+ V)^2 + \dots + (G_0^+ V)^p + \dots) \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)\psi_0. \quad (3.2)$$

This is the Born series for the wavefunction. Using (3.2) in (2.7) gives the Born expansion of the scattering amplitude:

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle \mathbf{k}_f \psi_f | (V + VG_0^+ V + V(G_0^+ V)^2 + \dots + V(G_0^+ V)^p + \dots) |\mathbf{k}_0 \psi_0 \rangle. \quad (3.3)$$

When the infinite series (3.3) is truncated after the n th term we obtain the n th Born *amplitude*:

$$f_{f0}^{\text{Born } n} = \sum_{p=1}^n f_{f0}^{Bp}, \quad (3.4a)$$

where I shall call

$$f_{f0}^{Bp} \equiv -(1/2\pi)\langle \mathbf{k}_f \psi_f | V(G_0^+ V)^{p-1} |\mathbf{k}_0 \psi_0 \rangle \quad (3.4b)$$

the p th Born *term*.

3.1. The first Born approximation (FBA)

From (3.4) the first Born amplitude is given by

$$f_{f0}^{\text{Born } 1} = f_{f0}^{B1} = -(1/2\pi)\langle \mathbf{k}_f \psi_f | V |\mathbf{k}_0 \psi_0 \rangle \quad (3.5a)$$

$$= -\frac{1}{2\pi} \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_f^*(\mathbf{X}) \bar{Q}\left(\frac{N}{r_0} - \sum_{i=1}^N \frac{1}{r_{0i}}\right) \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0) \psi_0(\mathbf{X}) d\mathbf{r}_0 d\mathbf{X}. \quad (3.5b)$$

The FBA has received considerable attention (for example, [11]). Here I would just like to highlight a few points which will be useful in later sections and/or which deserve further publicity.

(i) Large momentum transfer scattering (or equivalently, high energy large angle scattering) can only take place (with reasonable probability) if the incident e^\pm collides with the much heavier atomic nucleus. This is a fact which will play an important rôle in this article. For inelastic scattering the orthogonality $\langle \psi_f | \psi_0 \rangle = 0$ removes the e^\pm –nucleus interaction, $\bar{Q}N/r_0$, from the FBA amplitude (3.5). As a result the

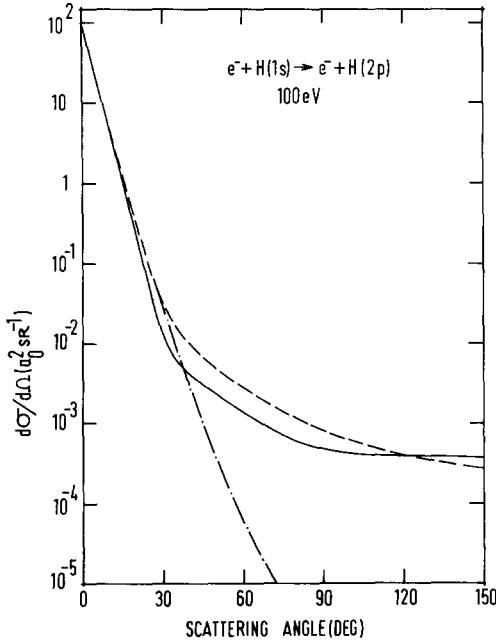


Fig. 1. Differential cross section for $e^- + H(1s) \rightarrow e^- + H(2p)$ at 100 eV. Curves: (—) realistic estimate (i.e. DWSBA calculation of [32]); (---) first Born approximation; (----) second Born approximation (3.10) (calculated in the closure approximation of [32]).

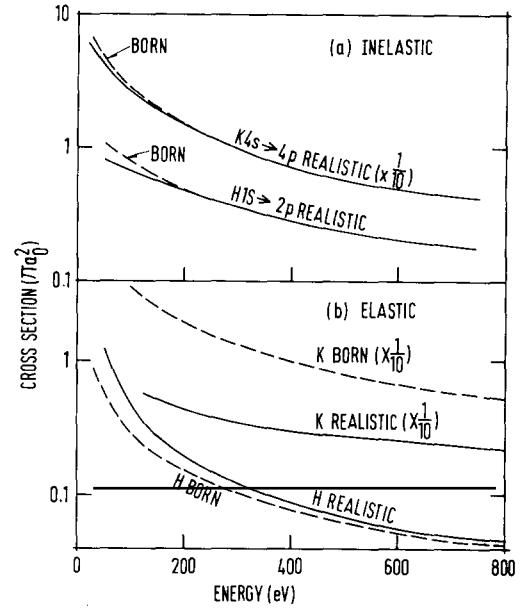


Fig. 2. Integrated cross sections for electron scattering by H and K: (a) $H(1s) \rightarrow H(2p)$ and $K(4s) \rightarrow K(4p)$; (b) elastic scattering. Curves: (—) realistic estimates based upon experimental data and calculations recorded in [13, 32]; (---) first Born approximation (from [13] in the case of K).

FBA cross section for high energy large angle inelastic scattering is orders of magnitude too small. This is illustrated in fig. 1 for the $1s \rightarrow 2p$ excitation of H.

(ii) If ψ_0 and ψ_f differ in orbital angular momentum by one unit, have opposite parities, but the same spin, the transition $\psi_0 \rightarrow \psi_f$ is optically allowed (i.e., can be excited by photon impact). For such transitions the FBA amplitude (3.5) has a pole at $q = 0$. For example, for the $1s \rightarrow 2p_m$ excitation of atomic hydrogen (3.5) is

$$-8\sqrt{6\pi}i\bar{Q}Y_{1m}^*(\hat{q})/q(q^2 + q^2)^3, \quad (3.6)$$

where Y_{1m} is a spherical harmonic [12]. The exact scattering amplitude also has a pole at $q = 0$ and this pole is identical with that in the first Born term. For scattering at small enough q the pole term will dominate the amplitude making the FBA quite accurate. Figure 1 also illustrates this point.

(iii) For elastic scattering (3.5) has the structure

$$f_{00}^{Born\ 1} = -(1/2\pi) \int \exp(-ik_f \cdot r_0) V_{00}(r_0) \exp(ik_0 \cdot r_0) dr_0, \quad (3.7a)$$

where

$$V_{00}(r_0) = \int \psi_0^*(X) \bar{Q} \left(\frac{N}{r_0} - \sum_{i=1}^N \frac{1}{r_{0i}} \right) \psi_0(X) dX \quad (3.7b)$$

is the *static potential* of the state ψ_0 . As N is increased, i.e., as we go to heavier and heavier atoms, the potential V_{00} gets stronger and stronger and the amplitude (3.7a) grows in magnitude [13]. This growth on going from atomic hydrogen ($N = 1$) to potassium ($N = 19$) is illustrated in fig. 2b; note that while the FBA for atomic hydrogen is reasonable it is much too large for potassium. It is therefore clear that a perturbation expansion of the scattering amplitude in powers of V , i.e., the ordinary Born series (3.3), is going to be of practical value, if at all, only for the very light atoms. The gross failure of the FBA for elastic electron scattering by the heavier atoms has some important implications in heavy particle collisions [14].

(iv) If ψ_0 and ψ_f can be represented by single Slater determinants composed out of orthonormal spin-orbitals, and if ψ_0 and ψ_f differ only in that the electron in spin-orbital ϕ_0 if promoted to the spin-orbital ϕ_f , then the FBA amplitude (3.5) is

$$f_{f0}^{\text{Born}\,1} = \frac{\bar{Q}}{2\pi} \int \exp(-ik_f \cdot r_0) \phi_f^*(x) \frac{1}{|r_0 - r|} \phi_0(x) \exp(ik_0 \cdot r_0) dr_0 dx, \quad (3.8)$$

where $x \equiv (r, s)$ stands for the space, r , and spin, s , coordinates of the atomic electron. Formula (3.8) makes no reference to the other ($N - 1$) electrons (or the nucleus) in the atom. As N is increased (3.8) will therefore not grow in size as the elastic amplitude (3.7) does. As a result the FBA can give reasonable inelastic cross sections for the heavier atoms at finite energies (even when ψ_0 and ψ_f cannot be simply represented as described above). This is illustrated in fig. 2a for the $4s \rightarrow 4p$ transition in potassium; it is seen that the FBA for the $1s \rightarrow 2p$ transition in atomic hydrogen and the $4s \rightarrow 4p$ transition in potassium converge to realistic values at much the same energy. Figures 2a and 2b should be contrasted! Serious problems for the Born series approximation to inelastic scattering by the heavier atoms start to arise at second and higher orders where elastic matrix elements of the form (3.7) begin to appear (see (4.3b)).

3.2. The second Born approximation (SBA)

The second Born amplitude is

$$f_{f0}^{\text{Born}\,2} = f_{f0}^{\text{B1}} + f_{f0}^{\text{B2}}, \quad (3.9)$$

and the corresponding differential cross section is

$$d\sigma_{f0}/d\Omega = (k_f/k_0)|f_{f0}^{\text{B1}} + f_{f0}^{\text{B2}}|^2. \quad (3.10)$$

Figure 3 compares the cross section (3.10) with the accurate experimental data of Bromberg [15] for the elastic scattering of electrons by He at 500 eV. It is clear that overall the SBA is poor. However, a more careful inspection reveals that at small angles there is quite good agreement between theory and experiment; it is at large angles where the big discrepancies arise. This observation gives the clue to what exactly is wrong with the SBA.

As previously mentioned, high energy large angle scattering requires a collision between the incident e^\pm and the nucleus. This is demonstrated in fig. 3 where the Rutherford cross section for pure Coulomb scattering by the nuclear potential $\bar{Q}N/r_0$ is also plotted; it is seen that the experimental data approach this cross section at large angles. The failure of the SBA at large angles therefore indicates that the SBA is having difficulty in dealing with the nuclear term.

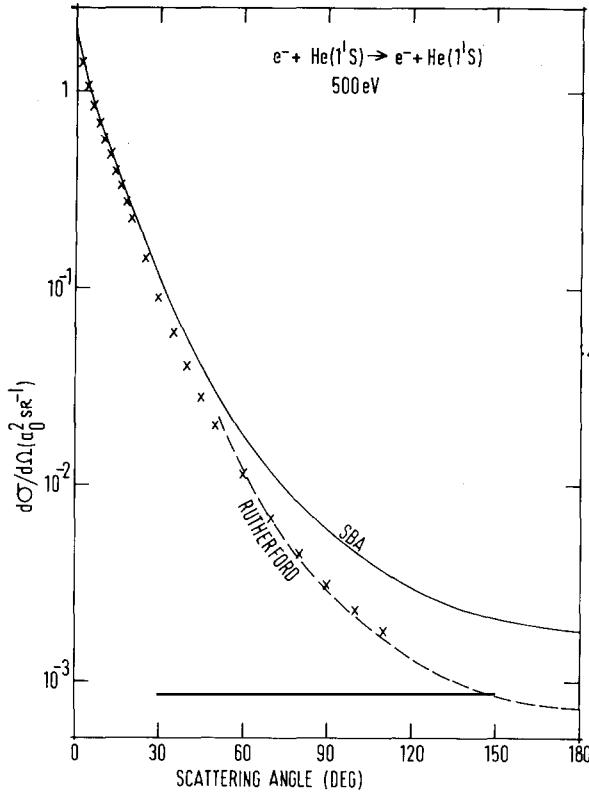


Fig. 3. Differential cross section for elastic scattering of electrons by He(¹S) at 500 eV. Curves: (—) second Born approximation (3.10) (the FSSB1 numbers of [42]); (— —) Rutherford cross section for scattering by bare He nucleus. Experimental data: (x) Bromberg [15].

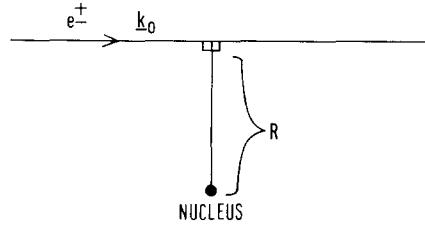


Fig. 4. Connection between distance of closest approach, R , and angular momentum, l , of an e^\pm moving with momentum k_0 along a straight line past a nucleus.

The reason why the nuclear potential $\bar{Q}N/r_0$ presents problems for perturbation theory is that it is singular as $r_0 \rightarrow 0$, i.e., as r_0 tends to zero it grows indefinitely in strength. A crude classical argument may be used to throw light upon this point. Consider an e^\pm with angular momentum l moving along a straight line past the potential $\bar{Q}N/r_0$ (fig. 4). The distance of closest approach to the nucleus, R , is given by

$$R \sim l/k_0. \quad (3.11)$$

For fixed l , as k_0 increases, R gets smaller. Thus, while the e^\pm is moving faster, which is good for perturbation theory, it is moving in a region of stronger potential, which is bad for perturbation theory. Consequently the $1/r_0$ singularity slows the convergence of perturbation theory.

This leads to an important guiding principle in perturbation work, namely, that the singularity at $r_0 = 0$ in the e^\pm -nucleus interaction, QN/r_0 , is a primary cause of the slow convergence of perturbation theory.

The good accord between theory and experiment at small angles seen in fig. 3 suggests that the SBA is handling the interaction between the incident electron and the target electrons very well—for small angle elastic scattering effects arising from polarization of the target electrons by the incident e^\pm are very important. It would therefore appear that if scattering by the nuclear potential could be treated

more exactly, i.e., non-perturbatively or in a higher order of perturbation theory, while still dealing in second order with the many-body interaction between the incident and target electrons, a very good approximation might result. The correctness of this idea will be confirmed in section 5.3.1.

In early work on the SBA [1, 16, 17] it was suggested that (3.10) was inconsistent. Thus it contains a term, $|f_{f0}^{B2}|^2$, of fourth order in V but neglects another term, arising from the product of f_{f0}^{B1} and f_{f0}^{B3} , which is also of fourth order. If the scattering amplitude is known only up to second order, then, it was argued, the cross section could only be calculated consistently to third order, i.e.,

$$d\sigma_{f0}/d\Omega = (k_f/k_0)[|f_{f0}^{B1}|^2 + 2 \operatorname{Re}(f_{f0}^{B1*} f_{f0}^{B2})]. \quad (3.12)$$

The third-order cross section (3.12) is shown in fig. 5. It behaves in exactly the opposite way to the full second Born cross section (3.10), i.e., at small angles it is poor, at large angles it is quite good.

The discrepancy at small angles is easily understood. The large forward peak in the experimental cross section is primarily the result of target polarization, which appears in f_{00}^{B2} (section 4.1.1); by dropping $|f_{00}^{B2}|^2$ from (3.10) the approximation (3.12) throws away the major part of the polarization effect and hence gives too small a cross section [3].

As stated earlier, the large angle cross section is mainly Coulomb scattering by the nucleus. The Coulomb amplitude, f_c , for the potential $\bar{Q}N/r_0$ is [10]

$$f_c = -\frac{2\bar{Q}N}{q^2} \frac{\Gamma(1+i\bar{Q}N/k_0)}{\Gamma(1-i\bar{Q}N/k_0)} \exp\left[-\frac{2i\bar{Q}N}{k_0} \ln\left(\frac{q}{k_0}\right)\right]. \quad (3.13)$$

This amplitude has the structure

$$f_c = -(2\bar{Q}N/q^2) e^{i\bar{Q}N\beta}, \quad (3.14)$$

where β is a real phase which can be expanded in powers of $\bar{Q}N$, the potential strength. Expanding

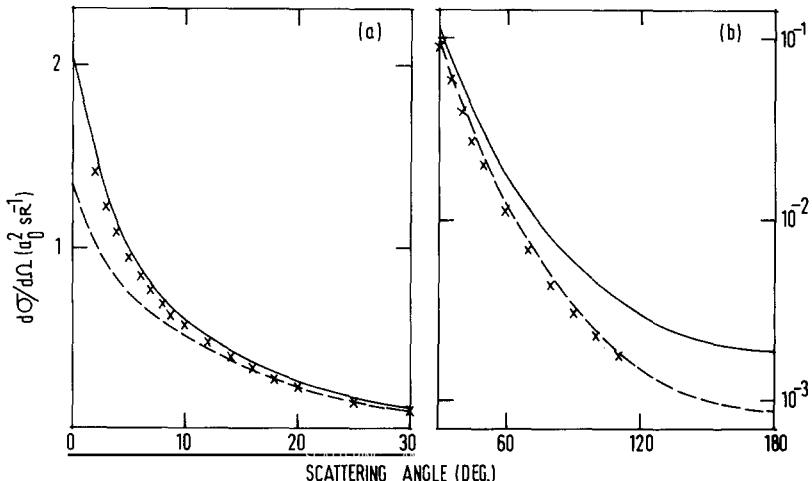


Fig. 5. Differential cross section for elastic scattering of electrons by He(1^1S) at 500 eV: (a) 0° to 30° ; (b) 30° to 180° . Curves: (—) second Born approximation (3.10) (the FSSB1 numbers of [42]); (---) third-order cross section (3.12) (the TSSB1 numbers of [42]). Experimental data: (x) Bromberg [15].

(3.14) to second order in $\bar{Q}N$, the second Born approximation, gives

$$f_c^{\text{Born}\,2} = -(2\bar{Q}N/q^2)(1 + i\bar{Q}N\beta_0), \quad (3.15)$$

where β_0 is the value of β at $\bar{Q}N = 0$. Using (3.15) in (3.10) leads to a cross section

$$(4N^2/q^4)(1 + N^2\beta_0^2), \quad (3.16)$$

which is *larger* than the exact Rutherford value $4N^2/q^4$; putting (3.15) in (3.12) produces the exact answer. These results explain the success of the third-order cross section and the failure of the full cross section at large angles in figs. 3 and 5. Of course, large angle scattering is not exactly pure Coulomb scattering, but as long as the amplitude has a structure similar to (3.14) the explanation will hold.

Generally speaking the SBA (3.10) for inelastic scattering is also poor [18]. Again, the flaw in the approximation is to be mainly identified with the nuclear term $\bar{Q}N/r_0$. Yet, this term confers upon the SBA one very important advantage over the FBA, high energy large angle SBA cross sections are the right order of magnitude, see fig. 1; this is because the second Born term, f_{f0}^{B2} , for inelastic scattering contains the e^\pm -nucleus interaction (section 4.1.2) [2, 3, 5, 18–21].

Totally unlike the elastic case, the third-order cross section (3.12) for high energy large angle inelastic scattering, like the FBA, is much too small [18]. Dropping the term $|f_{f0}^{\text{B2}}|^2$ from (3.10) leaves out most of the e^\pm -nucleus interaction.

A quantity of interest in e^\pm -photon coincidence experiments is the sign of the orientation vector [22]. When ψ_0 is an S-state and ψ_f a P-state this sign is given by[†]

$$\text{Im}(f_0 f_1^*), \quad (3.17)$$

where f_m is the amplitude for exciting the m th magnetic substate. If the impact energy is high enough for f_m to be approximated by the first two terms of the Born series (3.17) is[‡]

$$\text{Im}(f_0^{\text{B1}} f_1^{\text{B2}*} + f_0^{\text{B2}} f_1^{\text{B1}*} + f_0^{\text{B2}} f_1^{\text{B2}*}). \quad (3.18)$$

Now, at high enough energy, f^{B1} will dominate f^{B2} at small angles (section 3.1(ii)) so that (3.18) is, in effect,

$$\text{Im}(f_0^{\text{B1}} f_1^{\text{B2}*} + f_0^{\text{B2}} f_1^{\text{B1}*}). \quad (3.19)$$

Changing the projectile from e^- to e^+ reverses the sign of f^{B1} but not of f^{B2} . We therefore have the prediction that for high energy small angle scattering the sign of the orientation vector changes on replacing e^- by e^+ . For high energy large angle scattering, on the other hand, f^{B1} is negligible in comparison with f^{B2} (section 3.1(i)) so (3.18) is

$$\text{Im}(f_0^{\text{B2}} f_1^{\text{B2}*}). \quad (3.20)$$

[†] A factor of $e^{-i\phi}$ has been assumed removed from f_1 , where ϕ is the azimuthal angle of k_f about k_0 as z-axis.

[‡] $f_0^{\text{B1}} f_1^{\text{B1}*}$ is real.

Changing the projectile does not therefore alter the sign of the orientation vector in this case. These predictions are due to Madison and Winters [23].

Recently some interesting applications of the SBA (3.10) have been made to the triple differential cross section for high energy electron impact ionization of H and He [24, 25, 26]. This cross section, $d^3\sigma/d\Omega_A d\Omega_B dE_B$, is a measure of the probability that an electron incident upon the atom with momentum \mathbf{k}_0 will produce two electrons in the final state (i.e., scattered incident electron and ionized electron) with momenta \mathbf{k}_A and \mathbf{k}_B . The energies of these electrons are denoted by E_A and E_B and the solid angles into which they are scattered by $d\Omega_A$ and $d\Omega_B$. In the SBA (3.10) the cross section is

$$d^3\sigma/d\Omega_A d\Omega_B dE_B = (k_A k_B/k_0) |f^{B1} + f^{B2}|^2. \quad (3.21)$$

There are two “geometries” in which the SBA (3.21) has achieved notable success at high impact energies:

(i) when the ionized electron emerges with a low velocity and the incident electron is scattered only through a small angle (fig. 6);

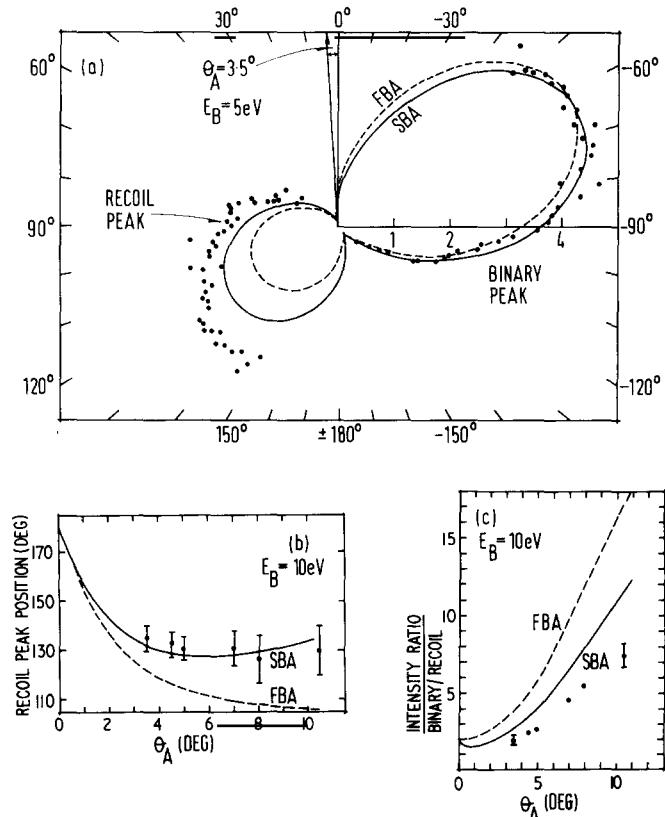


Fig. 6. Triple differential cross section $d^3\sigma/d\Omega_A d\Omega_B dE_B$ (a.u.) for the ionization process $e^- + \text{He}(1^1S) \rightarrow \text{He}^+(1s) + e^- + e^-$ at 500 eV in coplanar geometry (i.e., $\mathbf{k}_0, \mathbf{k}_A, \mathbf{k}_B$ coplanar): (---) first Born approximation; (—) second Born approximation (3.21); (●) experimental data. (Taken from Ehrhardt et al. [24], figs. 1, 2 and 3.) (a) Polar diagram of $d^3\sigma/d\Omega_A d\Omega_B dE_B$ as a function of θ_B for fixed $E_B = 5 \text{ eV}$ and $\theta_A = 3.5^\circ$ (θ_B is the angle between \mathbf{k}_0 and \mathbf{k}_B etc.). The experimental data and the first Born approximation have been normalized to the second Born curve at $\theta_B = -60^\circ$. (b) Angular position of the recoil peak at its maximum as a function of θ_A for $E_B = 10 \text{ eV}$. (c) Ratio of the intensity of the binary peak to that of the recoil peak, at the maximum, as a function of θ_A , for $E_B = 10 \text{ eV}$.

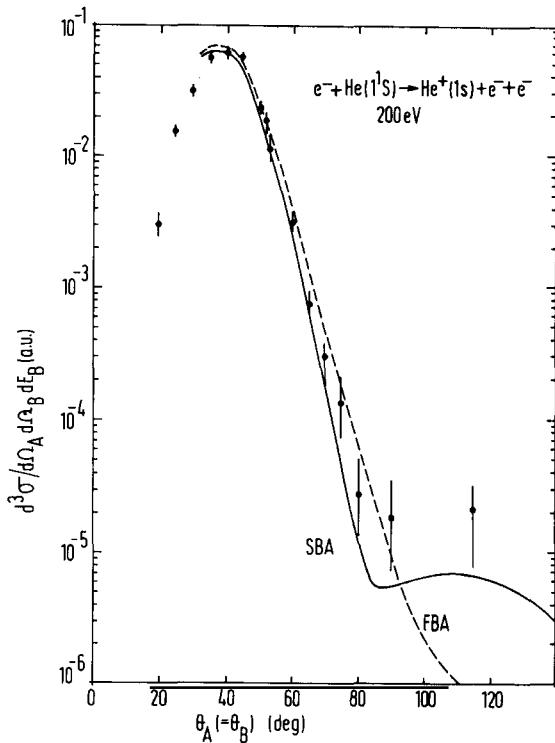


Fig. 7. Triple differential cross section $d^3\sigma/d\Omega_A d\Omega_B dE_B$ (a.u.) for the ionization process $e^- + \text{He}(1^1S) \rightarrow \text{He}^+(1s) + e^- + e^-$ at 200 eV in coplanar symmetric energy-sharing geometry (i.e. $\mathbf{k}_0, \mathbf{k}_A, \mathbf{k}_B$ coplanar, $k_A = k_B$, $\theta_A = \theta_B$), shown as a function of the angle $\theta_A (= \theta_B)$: (---) first Born approximation; (—) second Born approximation (more correctly leading contribution to second Born approximation, see [26]); (●) experimental data normalized to the second Born curve at 40°. (Taken from Pochat et al. [26], fig. 2.)

(ii) when \mathbf{k}_A and \mathbf{k}_B are coplanar with \mathbf{k}_0 , $k_A = k_B$, $\theta_A = \theta_B$ (where θ_A is the angle between \mathbf{k}_A and \mathbf{k}_0 etc.) and θ_A is large ($> 70^\circ$).

In the first case [24] the collision is not dissimilar to discrete excitation where the target electron is left within the field of the nucleus long after the incident electron has passed by. While, as stated earlier, it is true that the SBA is generally poor for discrete excitations, a more refined assessment reveals that (3.10) can give a fairly good cross section provided the incident energy is high and the momentum transfer is sufficiently small. These are precisely the circumstances of (i).

In the second case [25, 26] the cross section at high energies is dominated by a mechanism in which the incident electron first collides with the nucleus, suffering a large angle deflection, it then strikes a target electron, the two electrons finally emerging in the symmetric geometry (ii). This mechanism is absent from the FBA which does not contain the electron-nucleus interaction (section 3.1 (i)) but is present in the second Born term. The overall result at high energies is that the large θ_A cross section exhibits a pronounced peak coming from the second Born term. This peak has been observed in experiment [26] (fig. 7).

3.3. Higher Born terms

The accurate evaluation of the second Born term, f_{10}^{B2} , is at the limit of present expertise (section 4.3); what is known about higher-order Born terms is much more approximate. Nevertheless, some very useful information has been gleaned.

Byron and Joachain [5] have analyzed the leading behaviour of the Born terms for $S \rightarrow S$ transitions in the high k_0 limit. Their results are given in table 4 and will be discussed more fully in section 6.2.2. Byron, Joachain and collaborators [5] have also shown that the Glauber approximation may generate some of the higher Born terms with fairly good accuracy at high energies; again this is a subject better left to section 6.2.1.

Dewangan [27] has proved a very useful result concerning forward elastic scattering. He has shown that in a closure approximation (section 4.2.1) in which all atomic states ψ_n are given the same (average) energy[†]

$$f_{00}^{B(2n+1)}(\theta = 0) = 0, \quad n \geq 1, \quad (3.22)$$

i.e., all odd Born terms from f_{00}^{B3} upwards are zero. This result has a very important implication [28]. From the optical theorem (2.13) the total scattering cross section is given by

$$\begin{aligned} \sigma_{\text{total}} &= (4\pi/k_0) \operatorname{Im} f_{00}(\theta = 0) \\ &= (4\pi/k_0) \sum_{\text{even } n} \operatorname{Im} f_{00}^{Bn}(\theta = 0), \end{aligned} \quad (3.23)$$

using (3.22) and the fact that f_{00}^{B1} is real. Since f_{00}^{Bn} contains V to the power n , (3.23) implies that σ_{total} is unchanged when V changes sign – in other words electrons and positrons will have the same total cross section!

$$\sigma_{\text{total}}(\text{electron}) = \sigma_{\text{total}}(\text{positron}). \quad (3.24)$$

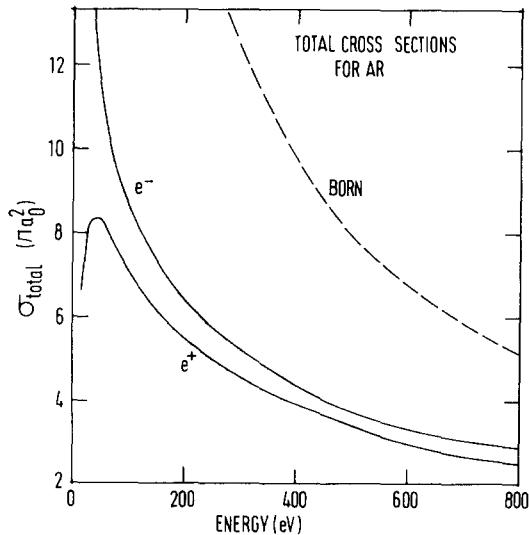


Fig. 8. Total cross sections for e^\pm scattering by Ar. Curves: (—) experimental data of reference [29]; (---) first Born approximation.

[†] His result is a little more general than this statement would imply since it is still true if different average energies for the atomic states are used in different Green's functions. Furthermore the result can be generalized to inelastic scattering at (unphysical) zero-momentum transfer.

The two assumptions behind (3.24) are: (i) electron exchange can be ignored in electron scattering so that only the direct amplitude need be considered; (ii) the closure approximation is valid so that (3.22) holds.

In fig. 8 the experimental total cross sections of Kauppila et al. [29] for e^+ and e^- scattering by Ar are compared. At low energies the two cross sections are radically different, but beyond about 200 eV they seem to reflect the approximate result (3.24). At low energies (3.24) will be invalid if only on account of assumption (i).

Asymptotically in energy the e^+ and e^- total cross sections should converge to the same first Born limit. In fig. 8 the FBA total cross section is also shown*. At the energies of fig. 8 the experimental e^+ and e^- cross section are far from the FBA limit, thus their agreement is not a trivial consequence of them being near this limit, i.e., (3.24) is a powerful approximate result valid at non-asymptotic energies.

3.4. High energy limit of the scattering amplitude

What is the high energy limit of the scattering amplitude? The answer to this question depends upon what variables are used to describe it. Let us first assume that ψ_0 and ψ_f are S-states. In this case the scattering amplitude might be considered to be a function of k_0 and momentum transfer q or a function of k_0 and scattering angle θ . The relationship between q and θ is

$$q^2 = k_0^2 + k_f^2 - 2k_0k_f \cos \theta. \quad (3.25)$$

Naively, one might expect the high energy limit of the scattering amplitude to be the first Born term f^{B1} . This is indeed true for the limits $k_0 \rightarrow \infty$ at fixed q and $k_0 \rightarrow \infty$ at $\theta = 0$:**

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } q}} f_{f0} = f_{f0}^{B1}, \quad (3.26)$$

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at } \theta = 0}} f_{f0} = f_{f0}^{B1}. \quad (3.27)$$

From (3.25) and (2.10) the limit $k_0 \rightarrow \infty$ at fixed non-zero θ is a limit in which both k_0 and q simultaneously go to infinity. This limit therefore corresponds to large momentum transfer scattering of the incident e^\pm . However, in sections 3.1(i) and 3.2 it was pointed out that for inelastic scattering the first Born term does not handle large momentum transfer collisions correctly, because it lacks the e^\pm -nucleus interaction, but the second Born term does. It follows that

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } \theta \neq 0}} f_{f0} = f_{f0}^{B2}, \quad f \neq 0. \quad (3.28)$$

For elastic scattering the first Born term retains the e^\pm -nucleus interaction so that (3.27) holds even for non-zero θ , i.e.,

* The very large FBA cross section is another illustration of section 3.1 (iii). Note that $\sigma_{\text{total}} = \sigma_{\text{elastic}} + \sigma_{\text{inelastic}}$. It is σ_{elastic} which is grossly overestimated by the FBA of fig. 8.

** By $\lim_{k_0 \rightarrow \infty} a = b$ I mean $\lim_{k_0 \rightarrow \infty} a/b = 1$. Note that this does *not* imply that both $\lim_{k_0 \rightarrow \infty} \text{Re } a = \text{Re } b$ and $\lim_{k_0 \rightarrow \infty} \text{Im } a = \text{Im } b$.

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } \theta}} f_{00} = f_{00}^{B1}. \quad (3.29)$$

The results (3.26) to (3.29) are supported by the detailed analysis of Byron and Joachain which is given in table 4.

When ψ_0 and ψ_f are not both S-states the situation is somewhat more tricky. While it is probably true that (3.26) to (3.29) hold in most cases they cannot hold in all cases. For example, for S→P transitions the FBA is identically zero for excitation to the $m = 0$ magnetic substate when the quantization axis is taken to be perpendicular to \mathbf{q} , thus (3.26) cannot be correct in this case (except in the trivial sense that the amplitude will go to zero at infinite k_0). What is most likely true, however, although no proof exists, is that the differential cross section analogues of (3.26) to (3.29) hold, provided that the differential cross section is averaged over the magnetic substates of the initial state and summed over the magnetic substates of the final state, i.e.,

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } q \\ \text{or fixed } \theta}} d\sigma_{\text{elastic}}/d\Omega = d\sigma_{\text{elastic}}^{B1}/d\Omega, \quad (3.30a)$$

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } q \\ \text{or at } \theta=0}} d\sigma_{\text{inelastic}}/d\Omega = d\sigma_{\text{inelastic}}^{B1}/d\Omega, \quad (3.30b)$$

$$\lim_{\substack{k_0 \rightarrow \infty \\ \text{at fixed } \theta \neq 0}} d\sigma_{\text{inelastic}}/d\Omega = d\sigma_{\text{inelastic}}^{B2}/d\Omega. \quad (3.30c)$$

4. The second Born term

The second Born term, f_{f0}^{B2} , plays a profound rôle in e^\pm -atom scattering. It is therefore fitting that some space should be devoted to its study. In analyzing and approximating f_{f0}^{B2} it is useful to make a spectral resolution of the Green's function (3.1b) according to

$$G_0^\pm = \sum_n \lim_{\eta \rightarrow 0^+} \frac{1}{4\pi^3} \int \frac{dk |k\psi_n\rangle \langle k\psi_n|}{k_n^2 - k^2 \pm i\eta}. \quad (4.1)$$

Here the sum on n is a sum over all bound and continuum states ψ_n of the atom; k_n is defined by

$$k_n^2 = k_0^2 + 2(\epsilon_0 - \epsilon_n). \quad (4.2)$$

Substitution of (4.1) in (3.4b) then gives

$$f_{f0}^{B2} = \sum_n f_{f0}^{B2; n} \quad (4.3a)$$

where

$$f_{f0}^{B2; n} \equiv -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0^+} \int \frac{dk \langle k_f \psi_f | V | k \psi_n \rangle \langle k \psi_n | V | k_0 \psi_0 \rangle}{k_n^2 - k^2 \pm i\eta}. \quad (4.3b)$$

4.1. Physical content

4.1.1. Elastic scattering*

In the case of elastic scattering, $\psi_0 = \psi_f$, (4.3a) falls naturally into two pieces: (i) the contribution from the $n = 0$ intermediate state, i.e., $f_{00}^{B2;0}$; (ii) the contribution from the remaining states. The former may be recognized as the second Born term for scattering by the static potential $V_{00}(\mathbf{r}_0)$ (see (3.7b)). The latter couples the state ψ_0 to the other states ψ_n ($n \neq 0$) of the system and therefore contains the response of the atomic electrons to the field of the incident e^\pm .

The amplitudes (4.3b) are complex numbers which may be split into their real and imaginary parts by writing the integral over k as a principal value part and a contribution from the pole at $k = k_n$. Thus, for elastic scattering,

$$\begin{aligned} f_{00}^{B2; n} = & -\frac{1}{8\pi^4} P \int \frac{d\mathbf{k}}{k_n^2 - k^2} \langle \mathbf{k}_f \psi_0 | V | \mathbf{k} \psi_n \rangle \langle \mathbf{k} \psi_n | V | \mathbf{k}_0 \psi_0 \rangle \\ & + \frac{i k_n}{16\pi^3} \int d\hat{\mathbf{k}} \langle \mathbf{k}_f \psi_0 | V | k_n \hat{\mathbf{k}} \psi_n \rangle \langle k_n \hat{\mathbf{k}} \psi_n | V | \mathbf{k}_0 \psi_0 \rangle, \end{aligned} \quad (4.4)$$

where P stands for principal value and $d\hat{\mathbf{k}}$ indicates an integration over angular coordinates only. In writing (4.4) it has been assumed that $k_n^2 > 0$. If k_n^2 is negative, which arises when the impact energy is insufficient to excite the state ψ_n (see (4.2)), there is no second term in (4.4) and the principal value integral is merely an ordinary integral. The first term on the right-hand side of (4.4) is purely real, the second is pure imaginary**.

If we specialize to forward elastic scattering, the imaginary part of (4.4) may be identified with the first Born cross section for exciting the state ψ_n . Thus, using (2.9), (2.11) and (3.5a),

$$\begin{aligned} \text{Im } f_{00}^{B2; n}(\theta = 0) &= \frac{k_0}{4\pi} \int \frac{k_n}{k_0} |f_{n0}^{B1}(k_n \hat{\mathbf{k}}, \mathbf{k}_0)|^2 d\hat{\mathbf{k}} \\ &= \frac{k_0}{4\pi} \sigma_{n0}^{B1}. \end{aligned} \quad (4.5)$$

Combining (4.3a) and (4.5)

$$\text{Im } f_{00}^{B2}(\theta = 0) = \sum_{\substack{\text{all energetically} \\ \text{accessible states } n}} \frac{k_0}{4\pi} \sigma_{n0}^{B1} = \frac{k_0}{4\pi} \sigma_{\text{total}}^{B1}, \quad (4.6)$$

where $\sigma_{\text{total}}^{B1}$ is the total cross section calculated in the first Born approximation. Thus the *second Born term satisfies the optical theorem* (2.13) *in the sense of* (4.6). In particular this implies that the second Born term takes account of the important physical effect of flux loss from the incident channel. Note that flux loss is associated with the imaginary part of f_{00}^{B2} .

A very important physical effect in elastic scattering is the polarization of the atom by the incident e^\pm . Normally one is first introduced to this idea in an adiabatic approximation to the interaction

* In this section it is tacitly assumed that ψ_0 is an S-state.

** For the purpose of this statement it is assumed that the magnetic substates of ψ_n are summed over in (4.4).

between the e^\pm and the atom. Thus it is shown in elementary perturbation theory that the second-order energy of an atom in the field of an e^\pm fixed at the point \mathbf{r}_0 is

$$V_{00}^{\text{AD2}}(\mathbf{r}_0) = \sum_{n \neq 0} \frac{\langle \psi_0 | V | \psi_n \rangle \langle \psi_n | V | \psi_0 \rangle}{\varepsilon_0 - \varepsilon_n}. \quad (4.7)$$

For large r_0 the potential V_{00}^{AD2} has the characteristic polarization form

$$V_{00}^{\text{AD2}}(\mathbf{r}_0) \xrightarrow{r_0 \rightarrow \infty} -\alpha_{00}/2r_0^4, \quad (4.8)$$

where α_{00} is known as the (dipole) polarizability of the state ψ_0 .

Physical intuition suggests that the second Born term f_{00}^{B2} must contain this effect; (4.7) and f_{00}^{B2} are, after all, both of second order in V . For distant collisions of the e^\pm with the atom the field of the e^\pm at the atom will vary slowly with time. Therefore, as far as the atom is concerned it will be as if the e^\pm is almost stationary and is polarizing it according to (4.8).

To reveal the presence of the atomic polarizability α_{00} in the second Born term it is necessary to look at this amplitude under distant collision conditions. In (3.11) collision distance was related to angular momentum, it being shown that the collision distance increases with the angular momentum. To see α_{00} the second Born term must therefore be examined at large angular momenta.

Decomposing f_{00}^{B2} into partial waves according to

$$f_{00}^{\text{B2}}(\theta) = \frac{1}{2} \sum_{l=0}^{\infty} (2l+1) f_{00,l}^{\text{B2}} P_l(\cos \theta), \quad (4.9)$$

where P_l is a Legendre polynomial, it is easily verified that*

$$f_{00,l}^{\text{B2}} = -4 \langle j_l Y_{l0}, \psi_0 | V G_0^+ V | j_l Y_{l0}, \psi_0 \rangle, \quad (4.10)$$

where $j_l \equiv j_l(k_0 r_0)$ is a spherical Bessel function and $Y_{lm} \equiv Y_{lm}(\hat{\mathbf{r}}_0)$ is a spherical harmonic [12]. If f_{00}^{B2} contains the polarization interaction (4.8) it is therefore to be expected that (4.10) will approach its adiabatic analogue

$$f_l^{\text{AD2}} \equiv -4 \langle j_l Y_{l0} | V_{00}^{\text{AD2}} | j_l Y_{l0} \rangle \quad (4.11)$$

for large l . That it does is illustrated in table 1 where (4.10) is compared with (4.11) for electron scattering by a model Li atom [30]. Note that (4.10) is complex while (4.11) is real; at large l the imaginary part of (4.10) dies away and the real part converges to (4.11).

The use of partial wave matrix elements, such as (4.10) and (4.11), at large angular momenta to study the long-range behaviour of collision quantities, such as potentials, is an important idea which will find much application in this article.

Since distant collisions contribute to near forward scattering, it should also be possible to see the atomic polarizability in the second Born term at small momentum transfers q . Thus it has been shown

* Still assuming ψ_0 is an S-state. Note that in this case the value of the right-hand side of (4.10) is unchanged if Y_{l0} is replaced by Y_{lm} with $m \neq 0$.

Table 1
 Partial wave scattering amplitudes $f_{00,l}^{B2}$ and f_l^{AD2} for electron scattering by a model ground state Li atom at an impact energy of 2 eV. The numbers are taken from reference [30] table 1

l	$\text{Im } f_{00,l}^{B2}$	$\text{Re } f_{00,l}^{B2}$	f_l^{AD2}
0	0.78×10^{-1}	0.135×10^2	0.355×10^2
1	0.67×10	0.137×10^2	0.111×10^2
2	0.38	0.38×10	0.33×10
3	0.21×10^{-1}	0.13×10	0.12×10
4	0.1×10^{-2}	0.57	0.56
5	about 10^{-4}	0.30	0.30

that at high energies and small q the leading contribution to $\text{Re } f_{00}^{B2}$ takes the form [20, 31]*

$$\text{Re } f_{00}^{B2} \xrightarrow[q \text{ small}]{k_0 \text{ large}} \pi \sum_n \frac{1}{k_n} |\langle \psi_0 | Z | \psi_n \rangle|^2 \left(1 - \frac{k_n q}{(k_n^2 q^2 + 4(\varepsilon_0 - \varepsilon_n)^2)^{1/2}} \right), \quad (4.12a)$$

$$Z \equiv z_1 + z_2 + \dots + z_N. \quad (4.12b)$$

Noting that the polarizability α_{00} of (4.8) may be written

$$\alpha_{00} = 2 \sum_{n \neq 0} |\langle \psi_0 | Z | \psi_n \rangle|^2 / (\varepsilon_n - \varepsilon_0) \quad (4.13)$$

we see its obvious manifestation in (4.12).

To summarize: (i) the imaginary part of f_{00}^{B2} satisfies the optical theorem in the sense of (4.6), f_{00}^{B2} therefore incorporates flux loss effects; (ii) the real part of f_{00}^{B2} contains the dipole polarizability of the atomic state ψ_0 , expressed in the correct dynamic way.

4.1.2. Inelastic scattering

The importance of the e^\pm -nucleus interaction in high energy large angle scattering has been emphasized previously. For inelastic scattering it is absent from the first Born term and first occurs in the second Born term. In f_{f0}^{B2} it appears in, and only in, the $f_{f0}^{B2;0}$ and $f_{f0}^{B2;f}$ contributions to (4.3a). These contributions have the structure

$$f_{f0}^{B2;0} = -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int \frac{d\mathbf{k} \langle \mathbf{k}_f \psi_f | V | \mathbf{k} \psi_0 \rangle \langle \mathbf{k} | V_{00} | \mathbf{k}_0 \rangle}{k_0^2 - k^2 + i\eta} \quad (4.14a)$$

$$f_{f0}^{B2;f} = -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int \frac{d\mathbf{k} \langle \mathbf{k}_f | V_{ff} | \mathbf{k} \rangle \langle \mathbf{k} \psi_f | V | \mathbf{k}_0 \psi_0 \rangle}{k_f^2 - k^2 + i\eta}, \quad (4.14b)$$

where V_{00} and V_{ff} are the static potentials (see (3.7)) of the states ψ_0 and ψ_f .

* Note that only P-states ψ_n contribute to (4.12) and (4.13). Also (4.12) was given under the assumption $\varepsilon_n \geq \varepsilon_0$ for all P-states ψ_n .

Formulae (4.14) have a simple physical interpretation for large angle scattering. Since the e^\pm -nucleus interaction occurs only in the matrix elements of the static potentials and not in the inelastic transition matrix element $\langle k'\psi_f|V|k''\psi_0\rangle$, due to orthogonality of ψ_0 and ψ_f , a large angle deflection can only be brought about by V_{00} and V_{ff} . Thus, in (4.14a), the incident e^\pm is first elastically scattered through a large angle by V_{00} , it then collides with an atomic electron, exciting the atom to the state ψ_f , but in this collision is only deflected through a small angle; overall the effect is large angle inelastic scattering. In (4.14b) small angle excitation of the atom takes place first followed by large angle elastic scattering by the static potential of the final state.

The expected convergence of f_{f0}^{B2} to the sum $(f_{f0}^{B2;0} + f_{f0}^{B2;f})$ at large angles is illustrated in fig. 9 for the $1s \rightarrow 2s$ excitation of H at 200 eV.

A point worth noting from (4.14), for future developments (section 5), is that the e^\pm -nucleus interaction appears most naturally as part of a static potential, V_{nn} , in which it is fully screened by the atomic electrons so as to present to a distant e^\pm an overall neutral target.

Analogous to (4.12), it can be shown that for S \rightarrow S inelastic transitions the leading contribution (in k_0) at small q to $\text{Re } f_{f0}^{B2}$ is [20]*

$$\text{Re } f_{f0}^{B2} \xrightarrow[k_0 \text{ large}]{q \text{ small}} \pi \sum_n \frac{1}{k_n} \langle \psi_f | Z | \psi_n \rangle \langle \psi_n | Z | \psi_0 \rangle \left(1 - \frac{k_n q}{[k_n^2 q^2 + 4(\varepsilon_0 - \varepsilon_n)(\varepsilon_f - \varepsilon_n)]^{1/2}} \right). \quad (4.15)$$

In (4.15) we perceive a generalization of the idea of polarizability to inelastic transitions (i.e.,

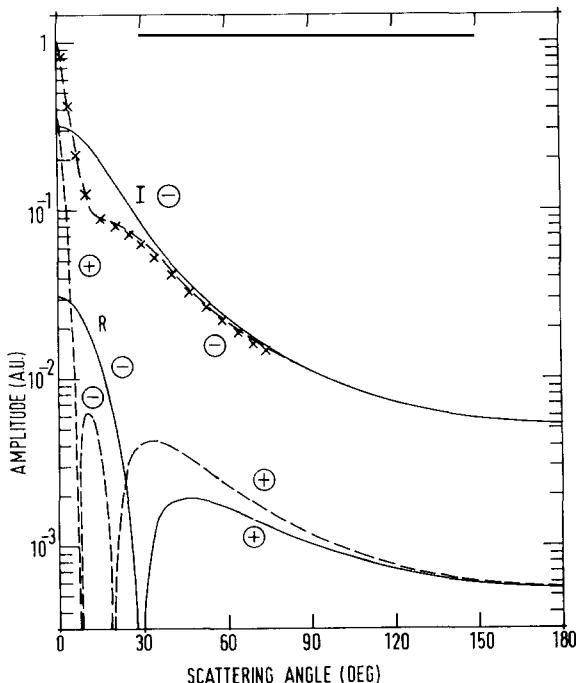


Fig. 9. Second Born terms for $e^\pm + H(1s) \rightarrow e^\pm + H(2s)$ at 200 eV. Notation: R = real part; I = imaginary part; \oplus = positive; \ominus = negative. Curves: (—) full second Born term $f_{2s,1s}^{B2}$; (—) $(f_{2s,1s}^{B2,1s} + f_{2s,1s}^{B2,2s})$; (\times) second-order Glauber term $f_{2s,1s}^{G2}$.

* Note that only P-states contribute to (4.15). Also (4.15) was given under the assumption $\varepsilon_n \geq \varepsilon_0$ and $\varepsilon_n \geq \varepsilon_f$ for all P-states ψ_n .

non-diagonal polarizabilities), namely,

$$\alpha_{f0} = 2 \sum_{n \neq 0, f} \frac{\langle \psi_f | Z | \psi_n \rangle \langle \psi_n | Z | \psi_0 \rangle}{[(\epsilon_0 - \epsilon_n)(\epsilon_f - \epsilon_n)]^{1/2}} \quad (4.16)$$

(Compare (4.12), (4.13), (4.15) and (4.16)); the idea can also be extended to non-S-states [32, 33]. It should be noted that (4.16) is symmetrical between the initial and final states, as any reasonable definition should be. Some time ago non-diagonal polarizabilities were considered in work on low energy electron–atom collisions [33], however, the definitions of α_{f0} adopted were not symmetrical.

4.2. Approximate methods of calculation

The second Born term (4.3) is

$$f_{f0}^{B2} = -\frac{1}{8\pi^4} \sum_n \lim_{\eta \rightarrow 0^+} \int \frac{dk \langle k_f \psi_f | V | k \psi_n \rangle \langle k \psi_n | V | k_0 \psi_0 \rangle}{k_n^2 - k^2 + i\eta}. \quad (4.17)$$

The main difficulty in calculating (4.17) lies with the sum over intermediate states ψ_n ; this is a sum over all bound and all continuum states of the atom.

4.2.1. Closure methods

In the earliest work, Massey and Mohr (1934) [34], the intermediate states were assigned an average energy, $\bar{\epsilon}$, so that k_n^2 became (see (4.2))

$$\bar{k}^2 = k_0^2 + 2(\epsilon_0 - \bar{\epsilon}), \quad (4.18)$$

independent of n . With the n dependence in (4.17) now only with the states ψ_n themselves, the completeness of these states may be invoked, i.e.,

$$\sum_n |\psi_n\rangle \langle \psi_n| = 1, \quad (4.19)$$

to trivially perform the sum and yield the approximation

$$\bar{f}_{f0}^{B2} = -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0^+} \int \frac{dk \langle k_f \psi_f | V | k \rangle \langle k | V | k_0 \psi_0 \rangle}{k^2 - \bar{k}^2 + i\eta}, \quad (4.20)$$

where in (4.20) it is to be understood that

$$\begin{aligned} \langle k_f \psi_f | V | k \rangle \langle k | V | k_0 \psi_0 \rangle &= \int \psi_f^*(X) \left\{ \int \exp[i(\mathbf{k} - \mathbf{k}_f) \cdot \mathbf{r}_0] V(\mathbf{r}_0, X) d\mathbf{r}_0 \right. \\ &\quad \times \left. \int \exp[i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}'_0] V(\mathbf{r}'_0, X) d\mathbf{r}'_0 \right\} \psi_0(X) dX. \end{aligned} \quad (4.21)$$

Formula (4.20) provides a practical approximation to f_{f0}^{B2} . Massey and Mohr studied elastic scattering and chose $\bar{\varepsilon} = \varepsilon_0$. This choice has two unsatisfactory outcomes. Firstly, it makes $\text{Im } \bar{f}_{00}^{B2}(\theta = 0)$ infinite [34, 35]. The infinity comes from the contributions of intermediate states for which the transition $\psi_0 \rightarrow \psi_n$ is optically allowed. This can easily be seen from (4.5). For example, if ψ_0 were the 1s state of H and ψ_n the 2p state then (4.5), (3.6) and (2.15) give

$$\text{Im } f_{1s, 1s}^{B2; 2p}(\theta = 0) = \frac{144}{k_0} \int_{t_{\min}}^{t_{\max}} \frac{dt}{t^4(t^2 + t^{2/6})}, \quad (4.22a)$$

$$t_{\min} = k_0 \mp [k_0^2 + 2(\varepsilon_{1s} - \varepsilon_{2p})]^{1/2}, \quad (4.22b)$$

where in (4.22) the magnetic substates of the 2p level have been summed over and q in (3.6) has been renamed t . If now ε_{2p} is set equal to ε_{1s} (i.e., ε_0), t_{\min} becomes zero and the integral in (4.22a) diverges due to the pole at $t = 0$. As previously mentioned (section 3.1(ii)) the pole at $t = 0$ is a characteristic feature of optically allowed transitions. It can be further shown that the manner in which $\text{Im } \bar{f}_{00}^{B2}(\theta)$ diverges as $\theta \rightarrow 0$ is as $\ln q$ where q is the momentum transfer (2.15).

The second unsatisfactory feature concerns the leading behaviour (4.12) (assuming ψ_0 is an S-state). If ε_n is set equal to ε_0 in (4.12a) a zero result is obtained. This means that $\text{Re } f_{00}^{B2}$ falls off more rapidly with increasing energy, at small q , than it ought to; in fact as $1/k_0^2$, which should be compared with the $1/k_0$ decay of (4.12a) [17].

Overall the choice $\bar{\varepsilon} = \varepsilon_0$ is obviously a bad one. However, the two difficulties described above may be trivially overcome by taking $\bar{\varepsilon} \neq \varepsilon_0$.

Holt and Moiseiwitsch [17] have generalized the simple closure approximation (4.20) by evaluating a few of the contributions $f_{f0}^{B2; n}$ to the second Born term with their exact energies and using an average energy for the rest. Again the closure relation (4.19) can be employed to yield the tractable approximation

$$f_{f0}^{B2, HM} = \sum_{n=0}^M (f_{f0}^{B2; n} - \bar{f}_{f0}^{B2; n}) + \bar{f}_{f0}^{B2}, \quad (4.23)$$

where it is assumed that the contributions of the first ($M + 1$) states are handled exactly. In (4.23) $\bar{f}_{f0}^{B2; n}$ stands for (4.3b) with k_n^2 replaced by \bar{k}^2 of (4.18); \bar{f}_{f0}^{B2} is given in (4.20). Holt and Moiseiwitsch call (4.23) the “simplified second Born approximation.” I shall use the term “closure approximation” to describe both (4.23) and (4.20), thinking of (4.20) as being merely a special case of (4.23). Holt and Moiseiwitsch take $\bar{\varepsilon}$ to be ε_{M+1} , the energy of the first state not treated exactly; this choice is arbitrary.

When the intermediate state ψ_n is degenerate in energy with the initial or final states its contribution to f_{f0}^{B2} should really be treated exactly, especially when $\psi_n = \psi_0$ or ψ_f . Failure to do so can lead to quite spurious behaviour [20, 36]. Take, for example, the $1s \rightarrow 2s$ excitation of H and let ψ_n be the 2p state. Since $\varepsilon_{2p} = \varepsilon_{2s}$, (4.15) tells us that the 2p state makes no contribution to the leading term of $f_{2s, 1s}^{B2}$ at small q . However, if all P-states are assigned an average energy $\bar{\varepsilon} \neq \varepsilon_{2s}$ in a closure approximation, then the 2p-state will contribute to (4.15). What is worse, as it turns out, this contribution will be of opposite sign and larger than that of the other P-states – the result will be a totally spurious leading behaviour for the calculated $\text{Re } f_{2s, 1s}^{B2}$ at small q [20]. Unfortunately not all authors have adopted the practice advised above (for example, the work of Gien quoted in section 6.3).

The closure approximations (4.23) and (4.20) involve only a single average energy $\bar{\varepsilon}$. For H and He this is reasonable but for heavier atoms with a well developed shell structure different average energies should be associated with different shells [37]. That this is not entirely an unnecessary over-complication of the closure approximation is illustrated in reference [38], albeit in a slightly different context from that considered here. In what follows I shall ignore this complication.

Let us now consider how the average energy $\bar{\varepsilon}$ should be chosen*. It is desirable that the choice should be dictated by the physics contained in the second Born term (section 4.1); the choices of Massey and Mohr and of Holt and Moiseiwitsch are not.

For elastic scattering we saw (section 4.1.1) that $\text{Re } f_{00}^{\text{B2}}$ contains the polarizability of the state ψ_0 while $\text{Im } f_{00}^{\text{B2}}$ is connected to the first Born total cross section through (4.6). There are various ways of fixing $\bar{\varepsilon}$ by these properties.

(i) $\bar{\varepsilon}$ may be chosen so that the optical theorem relation (4.6) is satisfied. In principle this choice should be made at each impact energy thereby giving an energy dependent $\bar{\varepsilon}$ [43]. However, in practice, it has been more usual to use an energy independent $\bar{\varepsilon}$, the value being determined from (4.6) at a given high energy [42, 44].

(ii) $\bar{\varepsilon}$ may be chosen so as to build the correct dipole polarizability of the state ψ_0 into the approximate amplitude (4.23) [37, 45, 46]. This is achieved by calculating (4.13) in the same approximation as (4.23) and adjusting $\bar{\varepsilon}$ to reproduce the exact value of α_{00} .

(iii) Better still would be to combine (i) and (ii), choosing separate average energies, $\bar{\varepsilon}_R$ and $\bar{\varepsilon}_I$, for the real and imaginary parts of f_{00}^{B2} ; $\bar{\varepsilon}_R$ being fixed by (ii) and $\bar{\varepsilon}_I$ by (i) [43].

For inelastic scattering an obvious physical property to concentrate on is the non-diagonal polarizability (section 4.1.2). This has been used by Kingston and Walters to determine $\bar{\varepsilon}$ in inelastic electron-H scattering [32]. Unlike diagonal polarizabilities α_{00} , non-diagonal polarizabilities are not readily available, only in a few cases can they be used to fix $\bar{\varepsilon}$. To make a good physical choice of $\bar{\varepsilon}$ in inelastic scattering is a problem.

In cases of extreme desperation, i.e., when there is no simple physical quantity on which to pin $\bar{\varepsilon}$, a “reasonable” choice of $\bar{\varepsilon}$ is made [47], for example, choose $\bar{\varepsilon}$ to coincide with the ionization limit, i.e., $(\bar{\varepsilon} - \varepsilon_0) = I_0$ where I_0 is the ionization potential of the state ψ_0 .

On the basis of present experience it is fair to say that the closure approximation, although by no means perfect, works quite well. This statement, of course, assumes that the closure approximation has been calculated in a sensible way using a suitable value of $\bar{\varepsilon}$. In table 2 the closure approximation for elastic H (1s) scattering at 30 eV is compared with exact results [43]. The particular closure approximation shown has been calculated under the best circumstances (iii) (above) with the 1s, 2s and 2p intermediate states being treated exactly in (4.23) [32]. However, the comparison of table 2 is under adverse conditions since 30 eV is a relatively low energy and the closure approximation is expected to work best at high energies. From table 2 it is clear that, all in all, the closure approximation is doing fairly well**.

In table 3 the closure approximated second Born term of Kingston and Walters [32] for the $1s \rightarrow 2s$ excitation of H at 54.4 eV is compared with exact numbers [49]. The imaginary part of the closure approximated amplitude is seen to be quite good but the real part is much poorer. However, since the real part is generally a lot smaller than the imaginary part, the overall result is not bad**.

* In what follows I give only those methods which have found favour in recent years. Other older ideas not already mentioned will be found in [39–41]. The reader is warned that most of the early calculations on He are in error [42].

** This is contrary to an incorrect statement made on page 829 of reference [48].

θ (deg.)	Exact [43]	Closure approximation of [32]	θ (deg.)	Exact [43]	Closure approximation of [32]
0	2.465	2.522	0	1.460	1.459
5	2.010	2.062	5	1.416	1.422
10	1.583	1.633	10	1.298	1.323
20	0.937	0.977	20	0.970	1.044
30	0.560	0.589	30	0.683	0.786
40	0.358	0.382	40	0.494	0.594
60	0.198	0.220	60	0.324	0.378
90	0.132	0.154	90	0.259	0.259
140	0.096	0.115	140	0.227	0.206
180	0.089	0.107	180	0.219	0.197

Table 3
Second Born term for $e^- + H(1s) \rightarrow e^- + H(2s)$ at 54.4 eV

θ (deg.)	Exact [49]	Closure approximation of [32]	θ (deg.)	Exact [49]	Closure approximation of [32]
0	+0.777	+0.668	0	-0.151 × 10	-0.137 × 10
6	+0.511	+0.396	6	-0.981	-0.872
10	+0.305	+0.196	10	-0.612	-0.534
20	+0.648 × 10 ⁻¹	+0.398 × 10 ⁻²	20	-0.240	-0.215
30	+0.582 × 10 ⁻²	-0.154 × 10 ⁻¹	30	-0.194	-0.180
40	-0.974 × 10 ⁻³	-0.361 × 10 ⁻²	40	-0.192	-0.180
60	+0.675 × 10 ⁻²	+0.131 × 10 ⁻¹	60	-0.152	-0.146
90	+0.964 × 10 ⁻²	+0.147 × 10 ⁻¹	90	-0.901 × 10 ⁻¹	-0.891 × 10 ⁻¹
140	+0.785 × 10 ⁻²	+0.105 × 10 ⁻¹	140	-0.519 × 10 ⁻¹	-0.516 × 10 ⁻¹
180	+0.76 × 10 ⁻²	+0.944 × 10 ⁻²	180	-0.469 × 10 ⁻¹	-0.453 × 10 ⁻¹

Byron and Latour [20] have introduced a variation on the closure approximation (4.23) for $S \rightarrow S$ transitions in which the polarizability, diagonal or non-diagonal, is automatically built into the second Born term. This is achieved by adding on to (4.23) a correction term

$$\Delta f_{f0}^{B2} = \pi q \sum_{n=M+1}^{\infty} \langle \psi_f | Z | \psi_n \rangle \langle \psi_n | Z | \psi_0 \rangle$$

$$\times \left(\frac{1}{[k_0^2 q^2 + 4(\varepsilon_0 - \bar{\varepsilon})(\varepsilon_f - \bar{\varepsilon})]^{1/2}} - \frac{1}{[k_0^2 q^2 + 4(\varepsilon_0 - \varepsilon_n)(\varepsilon_f - \varepsilon_n)]^{1/2}} \right) \quad (4.24)$$

derived from (4.15) in the high k_0 limit, i.e., $k_n \rightarrow k_0$. Whatever the value of $\bar{\varepsilon}$, the corrected closure amplitude will at least have the exact polarizability.

Byron and Joachain [50] have extended the correction (4.24) to take into account the leading order term (in $k_0^{-1} \ln k_0$) at small q of $\text{Im } f^{B2}$, while in reference [51] they also mix a pseudostate in with the

closure approximation in an attempt to get further improvement; the reader is directed to [50] and [51] for details.

4.2.2. Pseudostate methods

Another convenient way of approximating (4.17) is to replace the infinite sum over eigenstates ψ_n by a sum over a finite number of orthonormal pseudostates $\bar{\psi}_n$ [52, 53]:

$$f_{f0}^{\text{B2, PS}} = -\frac{1}{8\pi^4} \sum_{n=0}^P \lim_{\eta \rightarrow 0+} \int \frac{dk \langle \mathbf{k}_f \psi_f | V | \mathbf{k} \bar{\psi}_n \rangle \langle \mathbf{k} \bar{\psi}_n | V | \mathbf{k}_0 \psi_0 \rangle}{k_n^2 - k^2 + i\eta}, \quad (4.25a)$$

$$\bar{k}_n^2 = k_0^2 + 2(\varepsilon_0 - \bar{\varepsilon}_n), \quad (4.25b)$$

where $(P+1)$ is the number of such states and $\bar{\varepsilon}_n$ the energy associated with $\bar{\psi}_n$. The set $\bar{\psi}_n$ will normally contain some eigenstates.

Usually the pseudostates are constructed by diagonalizing the atomic Hamiltonian H_a of (2.2b) in some basis:

$$\langle \bar{\psi}_n | H_a | \bar{\psi}_m \rangle = \bar{\varepsilon}_n \delta_{m,n}. \quad (4.26)$$

The tricky problem is what to choose for the basis, since this choice will determine how “effectively” complete is the set $\bar{\psi}_n$ ($n = 0$ to P). The choice of a basis is an art and a matter for experimentation. Obviously, as with the closure approximation, one should try to choose the basis so that basic physical effects, such as dipole polarizability and the optical theorem (4.6) are correctly incorporated into the amplitude. An instructive testing ground for pseudostate methods is provided by some exact calculations on atomic hydrogen [43, 49, 54] (section 4.3).

The closure and pseudostate methods are in a sense complementary. Thus the closure approximation concentrates upon maintaining the completeness property of the eigenstates (4.19) at the expense of abandoning all but a few energy differences, i.e., an average energy $\bar{\varepsilon}$ is used. In the pseudostate method the set $\bar{\psi}_n$ ($n = 0$ to P) is not complete but energy differences are respected (see (4.26)).

The combination of closure and pseudostate methods should be quite powerful. The particular combination I would recommend is the following [55]: calculate the second Born term in the Massey–Mohr closure approximation (4.20) using some reasonable average energy $\bar{\varepsilon}$; evaluate (4.25) with $\bar{\varepsilon}_n$ set equal to $\bar{\varepsilon}$; compare the two amplitudes; adjust the pseudostate basis until the two amplitudes agree within acceptable limits; now evaluate (4.25) giving the pseudostates their correct energies (4.26) – adopt this as the approximation to the second Born term.

In the above procedure the closure amplitude is used to gauge how “effectively” complete the pseudostate basis is. However, even though a basis may be “effectively” complete its energy spectrum (4.26) may still not be satisfactory. Thus, in general, having obtained a good basis from the closure point of view, it may be necessary to add more functions to the basis in order to improve the energy distribution (4.26), this step is a matter of judgement. It should also be pointed out that, in general, the basis will be impact energy dependent, i.e., a basis which is good at one energy may not be satisfactory at another.

The approximation resulting from the above is a pure pseudostate approximation. This should not be confused with a mixed pseudostate-closure approximation such as that of Byron and Joachain [51] (see

also [37]). Their approximation is analogous to (4.23) but where the states 0 to M can be eigenstates or pseudostates.

From a practical point of view it is desirable to have a pure pseudostate approximation rather than a mixed pseudostate-closure approximation if one is to go beyond the plane-wave second Born term f_{f0}^{B2} to, for example, a distorted-wave second Born term (section 5.3).

4.2.3. Basic integrals

In calculating the second Born term one encounters the integrals

$$I(\lambda; m_1, \mathbf{k}_1, \mu_1; m_2, \mathbf{k}_2, \mu_2) = \int \frac{d\mathbf{k}}{(k^2 + \lambda^2)(|\mathbf{k} - \mathbf{k}_1|^2 + \mu_1^2)^{m_1}(|\mathbf{k} - \mathbf{k}_2|^2 + \mu_2^2)^{m_2}}, \quad (4.27)$$

or integrals related to this type. Usually these integrals are required for

$$\lambda^2 = -k_n^2 - i\eta, \quad (4.28)$$

where k_n^2 is positive and the limit $\eta \rightarrow 0+$ is to be taken (see (4.3)). An analytic formula for $I(\lambda; 1, \mathbf{k}_1, \mu_1; 1, \mathbf{k}_2, \mu_2)$ was given long ago by Lewis [56]. The more general integral (4.27) may be obtained from this formula by differentiating with respect to μ_1^2 and μ_2^2 . Holt [57] has described a computer program for calculating (4.27), under condition (4.28), from Lewis' formula; however, the computer program itself does not appear to have been published.

4.3. Exact calculations on atomic hydrogen

Consider elastic scattering of an e^\pm with incident momentum \mathbf{k}_0 off an atom in an S-state ψ_0 . Woollings [58] has shown that the real part of the second Born term at zero scattering angle $\text{Re } f_{00}^{B2}(\theta = 0)$, then satisfies the dispersion relation

$$\text{Re } f_{00}^{B2}(\theta = 0) = \frac{P}{2\pi^2} \int_0^\infty \frac{k^2 \sigma_{\text{total}}^{B1}(k) dk}{k^2 - k_0^2}, \quad (4.29)$$

where P stands for principal value and $\sigma_{\text{total}}^{B1}(k)$ is the first Born total cross section (4.6) at impact momentum k .

For scattering off the 1s-state of atomic hydrogen $\sigma_{\text{total}}^{B1}$ is easily calculated. Thus the cross section for exciting the discrete level with principal quantum number n is given by the simple expression (this can be deduced from equation (22) of reference [17] using (4.6))

$$\sigma_{n, 1s}^{B1} = \frac{2^{11} \pi n^7}{3k_0^5} \int_{q_{\min}}^{q_{\max}} \frac{dq [(n^2 - 1) + 3n^2 q^2][(n - 1)^2 + n^2 q^2]^{n-3}}{q[(n + 1)^2 + n^2 q^2]^{n+3}}, \quad (4.30a)$$

$$q_{\min} = k_0 \mp [k_0^2 - (n^2 - 1)/n^2]^{1/2}, \quad (4.30b)$$

while a simple formula also exists for the ionization cross section [59]. The ease with which $\sigma_{\text{total}}^{\text{B}1}(k)$ can be calculated means that it is feasible to do the infinite integration in (4.29). Kingston and Walters [32] have used this method to calculate exact values for $f_{1s, 1s}^{\text{B}2}(\theta = 0)$; note that $\text{Im } f_{00}^{\text{B}2}(\theta = 0)$ is determined by the optical theorem (4.6) once $\sigma_{\text{total}}^{\text{B}1}(k_0)$ is given. Their results are in agreement with an earlier calculation of Holt [60] which itself was an improvement upon a yet earlier calculation of Prasad [61]. More recently Byron and Joachain [51] have also calculated exact values for $\text{Re } f_{1s, 1s}^{\text{B}2}(\theta = 0)$.

Examination of the argument of Woollings indicates that (4.29) can be generalized to inelastic $S \rightarrow S$ transitions to give a dispersion relation for $\text{Re } f_{f0}^{\text{B}2}$, not at zero scattering angle but at (unphysical) zero momentum transfer. Byron and Joachain claim to have calculated exact values of $\text{Re } f_{2s, 1s}^{\text{B}2}(q = 0)$ for H , although not by the dispersion method; they do not give any results.

The exact calculation of $f_{f0}^{\text{B}2}$ at non-zero momentum transfer is a more formidable task. This has only been attempted by Ermolaev and Walters [43, 49, 54, 62] who have calculated $f_{1s, 1s}^{\text{B}2}$, $f_{2s, 1s}^{\text{B}2}$ and the second-order exchange amplitude for elastic electron scattering off H(1s) (section 8.2).

Before describing the procedure of Ermolaev and Walters it is useful to adapt the notation to atomic hydrogen. In the usual way the bound states of H will be written

$$\psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_{lm}(\hat{\mathbf{r}}) \quad (4.31a)$$

and, similarly, the continuum states

$$\psi_{\kappa lm}(\mathbf{r}) = R_{\kappa l}(r) Y_{lm}(\hat{\mathbf{r}}), \quad (4.31b)$$

where κ is the magnitude of the continuum electron momentum. The radial continuum functions are real and such that [10]

$$R_{\kappa l}(r) \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} \frac{\sin(\kappa r - \frac{1}{2}l\pi + (1/\kappa) \ln 2\kappa r + \eta_l)}{\kappa r}, \quad (4.32a)$$

$$\eta_l \equiv \arg \Gamma(l + 1 - i/\kappa), \quad (4.32b)$$

$$\int_0^\infty R_{\kappa l}(r) R_{\kappa' l}(r) r^2 dr = \delta(\kappa - \kappa')/\kappa^2, \quad (4.32c)$$

In the above notation the second Born term (4.3) becomes

$$f_{f0}^{\text{B}2} = -\frac{1}{8\pi^4} \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} \int \frac{dk \langle k_f \psi_{nl00} | V | k \psi_{nlm} \rangle \langle k \psi_{nlm} | V | k_0 \psi_{n000} \rangle}{k_n^2 - k^2 + i\eta} \quad (4.33a)$$

$$-\frac{1}{8\pi^4} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \int_0^\infty dk \kappa^2 \int \frac{dk \langle k_f \psi_{nl00} | V | k \psi_{\kappa lm} \rangle \langle k \psi_{\kappa lm} | V | k_0 \psi_{n000} \rangle}{k_\kappa^2 - k^2 + i\eta}, \quad (4.33a)$$

$$k_n^2 = k_0^2 - 1/n_0^2 + 1/n^2, \quad (4.33b)$$

$$k_\kappa^2 = k_0^2 - 1/n_0^2 - \kappa^2, \quad (4.33c)$$

where it is assumed that the initial and final states ψ_{n000} and ψ_{n_f00} , are s-states and where the limit $\eta \rightarrow 0+$ is understood.

It is convenient at this stage to remove the contributions of the initial and final states as intermediate states from f_{f0}^{B2} ; these are easily calculated in terms of Lewis integrals (4.27). The resulting second Born term will be denoted as \tilde{f}_{f0}^{B2} and the omission of ψ_{n000} and ψ_{n_f00} from the first sum in (4.33a) will be acknowledged by a prime on the summation symbol. Working in partial waves, \tilde{f}_{f0}^{B2} can be cast in two different forms. In the first form

$$\tilde{f}_{f0}^{B2} = \sum_{L=0}^{\infty} A_L P_L(\hat{k}_0 \cdot \hat{k}_f), \quad (4.34a)$$

$$A_L = \sum_{l=0}^{\infty} B_L^l, \quad (4.34b)$$

$$B_L^l = \sum_{n=l+1}^{\infty} C_L^l(n) + \int_0^{\infty} d\kappa \kappa^2 C_L^l(\kappa), \quad (4.34c)$$

$$C_L^l(x) = \frac{1}{\pi} \sum_{\lambda=|l-L|}^{l+L} (2\lambda+1)(2l+1)[C(\lambda, l, L, 0, 0, 0)]^2 D_{L\lambda}^l(x), \quad (4.34d)$$

$$x = n \quad \text{or} \quad \kappa, \quad (4.34e)$$

$$D_{L\lambda}^l(x) = \int_0^{\infty} \int_0^{\infty} dr dr' r^2 r'^2 j_L(k_f r) V_{fx}^l(r) h_{\lambda x}(r, r') V_{0x}^l(r') j_L(k_0 r'), \quad (4.34f)$$

$$V_{ix}^l(r) = \frac{\sqrt{4\pi}}{(2l+1)} \int_0^{\infty} R_i(r') \frac{r_{<}^l}{r_{>}^{l+1}} R_x(r') r'^2 dr', \quad i = 0 \quad \text{or} \quad f, \quad (4.34g)$$

$$r_{\geq} = \max_{\min} (r, r'), \quad (4.34h)$$

$$h_{\lambda x}(r, r') = k_x [-j_{\lambda}(k_x r_{<}) y_{\lambda}(k_x r_{>}) + i j_{\lambda}(k_x r_{<}) j_{\lambda}(k_x r_{>})], \quad \text{for } k_x^2 \geq 0, \quad (4.34i)$$

$$= \frac{1}{\sqrt{r_{>} r_{<}}} I_{\lambda+1/2}(|k_x|r_{<}) K_{\lambda+1/2}(|k_x|r_{>}), \quad \text{for } k_x^2 < 0, \quad (4.34j)$$

where P_L is a Legendre polynomial, $C(l_1, l_2, l_3, m_1, m_2, m_3)$ is a Clebsch-Gordan coefficient [12], $\max(\min)(r, r')$ means the greater (lesser) of r and r' , j_L and y_L are regular and irregular spherical Bessel functions [63] and $I_{\lambda+1/2}$, $K_{\lambda+1/2}$ are modified Bessel functions [63].

The second form of \tilde{f}_{f0}^{B2} is also given by (4.34a-e) but with $D_{L\lambda}^l(x)$ defined by

$$D_{L\lambda}^l(x) = -\frac{2}{\pi} \int_0^\infty dk k^2 \langle\langle j_L(k_f r) | V_{fx}^l | j_\lambda(kr) \rangle\rangle \frac{\langle\langle j_\lambda(kr) | V_{0x}^l | j_L(k_0 r) \rangle\rangle}{k_x^2 - k^2 + i\eta}, \quad (4.35a)$$

$$\langle\langle j_L(k_f r) | V_{fx}^l | j_\lambda(kr) \rangle\rangle = \int_0^\infty dr r^2 j_L(k_f r) V_{fx}^l(r) j_\lambda(kr), \quad \text{etc.} \quad (4.35b)$$

The difference between (4.34) and (4.35) lies only in the treatment of the Green's function

$$\frac{1}{(2\pi)^3} \int \frac{d\mathbf{k} |\mathbf{k}\rangle\langle\mathbf{k}|}{k_x^2 - k^2 + i\eta}. \quad (4.36)$$

In (4.34) the coordinate space form of (4.36) is used, i.e.,

$$-\frac{1}{4\pi} \frac{\exp(i k_x |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}, \quad (4.37)$$

while in (4.35) the momentum space version (4.36) is retained.

For open channels ($k_n^2 \geq 0, k_\kappa^2 \geq 0$) Ermolaev and Walters have used the form (4.34), while for closed channels ($k_n^2 < 0, k_\kappa^2 < 0$) they have adopted the form (4.35). The reason for this change-over lies in the structures of (4.34) and (4.35). Thus for closed channels the function $I_{\lambda+1/2}(|k_x|r_-)$ in (4.34j) grows exponentially with increasing r_- . It was judged that this behaviour might cause trouble in doing the integrations in (4.34f) numerically, hence (4.35) was chosen for closed channels. However, it should be pointed out that other authors [64] appear not to have experienced difficulties in using (4.34j). For closed channels the denominators in (4.35a), i.e., $k_x^2 - k^2 + i\eta$ do not go to zero so that the integrals over k in (4.35a) are well behaved. When the channels are open these integrals must be treated as a pole contribution and a principal value term (see (4.4)). Ermolaev and Walters judged that (4.34) might be a better way to treat open channels.

From (4.34) and (4.35) it is clear that the exact evaluation of the second Born term requires integrations over r, r', κ and k and summations over n, l and L . The integrals are done numerically, except for (4.34g) when R_x is a bound state. The sum over the principal quantum number n in (4.34c) converges fairly rapidly, at the larger n showing a $1/n^3$ behaviour which can be used to estimate the sum to infinity. The sum over l is a sum over the angular momenta of the intermediate target states. One does not have to go far in l to obtain reasonable convergence at the impact energies which have been studied, e.g., l up to about 7. The quantities A_L are just the partial wave components of the second Born term. These have to be calculated far enough for asymptotic behaviour in L to set in. Once the asymptotic (in L) region has been reached there are procedures for completing the summation on L to infinity.

Difficulties which arise in the calculation are: (i) long-range potentials (at worst $1/r^2$); (ii) getting accurate enough partial waves A_L to reproduce \tilde{f}_{f0}^{B2} over the full angular range 0° to 180° ; (iii) making sure that enough partial waves A_L are calculated to accurately reach the asymptotic L region.

Sample results of exact values of $f_{1s, 1s}^{B^2}$ and $f_{2s, 1s}^{B^2}$ have been given in tables 2 and 3; other numbers may be found in references [43, 49, 62]. Numbers are already, or soon will be, available for $f_{1s, 1s}^{B^2}$ at 3.4 [62], 12, 20 and 30 eV [43], and for $f_{2s, 1s}^{B^2}$ at 11, 19.6, 30 and 54.4 eV [49].

The exact calculation of the corresponding second order exchange terms can be carried out along lines similar to those described in (4.34) and (4.35). Exact numbers for the second order exchange term for elastic scattering off H(1s) at 30 eV are given in reference [54] and table 6.

It is not suggested that the technique of Ermolaev and Walters is the best way to calculate $f_{f0}^{B^2}$, rather it is a method which has been successfully put into practice.

5. The distorted-wave Born series

If the e^\pm -atom interaction V of (2.2c) is split into two pieces:

$$V = V_1 + V_2, \quad (5.1)$$

the two-potential formula [65]* may be used to write the scattering amplitude (2.7) in the form

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -\frac{1}{2\pi} \langle \mathbf{k}_f \psi_f | V_1 | \Phi_0^+(\mathbf{k}_0) \rangle - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 | \Psi^+ \rangle, \quad (5.2)$$

where

$$\Phi_n^\pm(\mathbf{k}) = \exp(i\mathbf{k} \cdot \mathbf{r}_0) \psi_n(\mathbf{X}) + G_0^\pm V_1 \Phi_n^\pm(\mathbf{k}), \quad (5.3a)$$

$$G_0^\pm = \lim_{\eta \rightarrow 0^+} (E - H_0 \pm i\eta)^{-1}, \quad (5.3b)$$

$$E = \frac{1}{2}k_0^2 + \epsilon_0 = \frac{1}{2}k_f^2 + \epsilon_f. \quad (5.3c)$$

Further, the Lippmann–Schwinger equation (3.1a) for Ψ^+ can be recast as

$$\Psi^+ = \Phi_0^+(\mathbf{k}_0) + G_1^+ V_2 \Psi^+, \quad (5.4a)$$

$$G_1^\pm = \lim_{\eta \rightarrow 0^+} (E - H_0 - V_1 \pm i\eta)^{-1}. \quad (5.4b)$$

Using (5.4) the scattering amplitude (5.2) can be expanded as a power series in V_2 :

$$\begin{aligned} f_{f0}(\mathbf{k}_f, \mathbf{k}_0) &= -\frac{1}{2\pi} \langle \mathbf{k}_f \psi_f | V_1 | \Phi_0^+(\mathbf{k}_0) \rangle - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | (V_2 + V_2 G_1^+ V_2 \\ &\quad + V_2 G_1^+ V_2 G_1^+ V_2 + \cdots + V_2 (G_1^+ V_2)^n + \cdots) | \Phi_0^+(\mathbf{k}_0) \rangle. \end{aligned} \quad (5.5)$$

* There is a more general form of two-potential formula which also appears in the literature [48, 66, 67]. This form allows for different decompositions of the Hamiltonian H in the initial and final channels.

The expression (5.5) is the distorted-wave Born series for the scattering amplitude.

The great virtue of (5.5) is that, although it treats V_2 perturbatively, it handles V_1 non-perturbatively. Truncating (5.5) to a finite number of terms one obtains a distorted-wave approximation. It is clear that the precise nature of this approximation depends upon the choice of V_1 . The choice $V_1 = 0$ gives the ordinary Born series (3.3).

In section 3.2 it was remarked that a primary cause of the slow convergence of the ordinary Born series was the singular e^\pm -nucleus potential, $\bar{Q}N/r_0$. Obviously, therefore, V_1 should be selected so that V_2 does not contain this interaction. In practice it is usually not convenient to place all of $\bar{Q}N/r_0$ in V_1 so a compromise results. Drawing again upon previous observations, it was seen in section 4.1.2 that the nuclear interaction appears most naturally ‘clothed’ as a static potential, $V_{nn}(r_0)$ (3.7b), and, in section 3.1 (ii), that such potentials spelt disaster for the ordinary Born series for the heavier atoms. All of this points to a choice of V_1 based upon the static potentials V_{nn} of the system.

It should perhaps be emphasized at this point that the distorted-wave approximation is very flexible; there is no obligation to restrict V_1 to static potentials. By suitably choosing V_1 we are able to take as much physics as we can, or want to, exactly into account, leaving the rest, i.e., V_2 , to be handled perturbatively. It is also important for the reader to note that once V_1 is given V_2 is fixed by $V_2 = V - V_1$.

5.1. The zeroth-order approximation

This is given by the first term of (5.5), which is of zero order in V_2 . This term is merely the amplitude for scattering by the potential V_1 alone.

5.2. The distorted-wave (first) Born approximation (DWBA)

This is

$$f_{f0}^{\text{DW Born } 1}(\mathbf{k}_f, \mathbf{k}_0) = -\frac{1}{2\pi} \langle \mathbf{k}_f \psi_f | V_1 | \Phi_0^+(\mathbf{k}_0) \rangle - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 | \Phi_0^+(\mathbf{k}_0) \rangle. \quad (5.6)$$

Formula (5.6) is not really suited to elastic scattering and has only ever been used for excitations where the choice of V_1 is usually such that the first term is zero:

$$f_{f0}^{\text{DW Born } 1}(\mathbf{k}_f, \mathbf{k}_0) = -\frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 | \Phi_0^+(\mathbf{k}_0) \rangle. \quad (5.7)$$

I shall not give a detailed account of the DWBA here but rather refer the reader to [48, 67–70] and references therein. However, before passing on to the distorted-wave second Born approximation I would like to highlight a few points.

The simplest reasonable choice of V_1 in (5.7) consistent with previously stated principles is

$$\begin{aligned} V_1 &= P_0 V P_0 + P_f V P_f \\ &= V_{00}(\mathbf{r}_0) P_0 + V_{ff}(\mathbf{r}_0) P_f, \end{aligned} \quad (5.8)$$

where P_i is the projection operator

$$P_i = |\psi_i(\mathbf{X})\rangle\langle\psi_i(\mathbf{X})|. \quad (5.9)$$

Although this choice does not remove the whole of the interaction $\bar{Q}N/r_0$ from V , the nuclear term is absent from V_2 in so far as (5.7) is concerned. This is easily seen. With the choice (5.8) the amplitude (5.7) reduces to

$$f_{f0}^{\text{DW Born 1}} = -\frac{1}{2\pi} \langle F_f^-(\mathbf{r}_0) | V_{f0}(\mathbf{r}_0) | F_0^+(\mathbf{r}_0) \rangle, \quad (5.10)$$

where

$$(\nabla_0^2 + k_0^2 - 2V_{00}(\mathbf{r}_0))F_0^+(\mathbf{r}_0) = 0, \quad (5.11a)$$

$$(\nabla_0^2 + k_f^2 - 2V_{ff}(\mathbf{r}_0))F_f^-(\mathbf{r}_0) = 0, \quad (5.11b)$$

$$V_{f0}(\mathbf{r}_0) \equiv \langle \psi_f(\mathbf{X}) | V | \psi_0(\mathbf{X}) \rangle, \quad (5.11c)$$

and the boundary conditions on F_0^+ and F_f^- are fixed by (5.3a)*. The term $\bar{Q}N/r_0$ is not present in the potential V_{f0} due to orthogonality of ψ_0 and ψ_f .

In (5.10) the failure of the ordinary first Born approximation for high energy large angle inelastic scattering (section 3.1 (i)) is corrected; scattering by the nuclear potential $\bar{Q}N/r_0$ is taken into account through the distorted waves F_0^+ and F_f^- . If (5.10) is expanded in powers of V it is easily found that

$$f_{f0}^{\text{DW Born 1}} = f_{f0}^{\text{B1}} + f_{f0}^{\text{B2},0} + f_{f0}^{\text{B2},f} + \text{third and higher order terms in } V, \quad (5.12)$$

where f_{f0}^{B1} , $f_{f0}^{\text{B2},0}$ and $f_{f0}^{\text{B2},f}$ are given in (3.5) and (4.14). Thus (5.10) contains the leading terms, $f_{f0}^{\text{B2},0}$ and $f_{f0}^{\text{B2},f}$, for high energy large angle scattering (section 4.1.2). The Born series analysis of an approximation, i.e., expansion in powers of V , is a method strongly recommended for gaining insight [18, 69].

In connection with the above it is worthwhile to mention one irregularity which has crept into the application of the DWBA [69]. This is a lop-sided use of the approximation resulting either from a bad choice of V_1 or from its deliberate neglect in either the final or initial channels. For example, (5.10) might be simplified to

$$-\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_0) | V_{f0}(\mathbf{r}_0) | F_0^+(\mathbf{r}_0) \rangle. \quad (5.13)$$

This may be viewed as a neglect of V_{ff} in (5.11b) or as a choice

$$V_1 = V_{00}(\mathbf{r}_0)P_0. \quad (5.14)$$

Expanding the amplitude (5.13) according to (5.12) it will be found that the term $f_{f0}^{\text{B2},f}$ is missing,

* Note from (5.3) that Φ_n^\pm satisfies the Schrödinger equation $(H_0 + V_1 - E)\Phi_n^\pm = 0$. Also, for the potential (5.8) $\Phi_0^+ = F_0^+(\mathbf{r}_0)\psi_0(\mathbf{X})$ and $\Phi_f^- = F_f^-(\mathbf{r}_0)\psi_f(\mathbf{X})$.

although $f_{f0}^{B2;0}$ is present. The amplitude (5.13) will therefore be inadequate at high energies and large scattering angles – in fact it will then give a cross section roughly one quarter of the correct size [69]. The choice (5.14), or the neglect of V_{ff} , amounts to an insufficient removal of the nuclear term $\bar{Q}N/r_0$ into V_1 .

When V_{00} and/or V_{ff} are not spherically symmetric it is customary to take a spherical average of these potentials [71, 72], otherwise (5.11) would have to be solved with non-spherical potentials – a considerable escalation in computational difficulty. Spherical averaging does not remove any part of the e^\pm -nucleus interaction from V_{00} and V_{ff} ; it corresponds to the choice

$$\begin{aligned} V_1 &= P_0 V^{\text{SA}} P_0 + P_f V^{\text{SA}} P_f \\ &= V_{00}^{\text{SA}}(\mathbf{r}_0) P_0 + V_{ff}^{\text{SA}}(\mathbf{r}_0) P_f \end{aligned} \quad (5.15\text{a})$$

where V^{SA} is the spherically symmetric part of (2.2c), i.e.,

$$V^{\text{SA}}(\mathbf{r}_0, \mathbf{X}) \equiv \bar{Q} \left(N/r_0 - \sum_{i=1}^N 1/r_{i>} \right) \quad (5.15\text{b})$$

$$r_{i>} = \max(r_i, r_0) \quad (5.15\text{c})$$

$\max(a, b)$ meaning the greater of a and b , and where

$$V_{nn}^{\text{SA}}(\mathbf{r}_0) \equiv \langle \psi_n(\mathbf{X}) | V^{\text{SA}}(\mathbf{r}_0, \mathbf{X}) | \psi_n(\mathbf{X}) \rangle. \quad (5.15\text{d})$$

As far as retaining the e^\pm -nucleus interaction in the initial and final channels is concerned (5.15) is as good a candidate for V_1 as (5.8). When ψ_0 and ψ_f are S-states (5.15) is identically equal to (5.8).

Calculations which allow for polarization and absorption effects as well as static field scattering in the initial and/or final channels have also been carried out ([69, 72–77], also the DWPO models of McDowell and collaborators, see [67]). Usually they correspond to a choice*

$$V_1 = P_0 \tilde{V}_0 P_0 + P_f \tilde{V}_f P_f, \quad (5.16)$$

where \tilde{V}_0 (\tilde{V}_f) contains the static field V_{00} (V_{ff}) as well as polarization and/or absorption. The potentials \tilde{V}_0 and \tilde{V}_f need not be local potentials. Apart from low energies and special circumstances [76] results with (5.16) tend not to be a lot different from those obtained from the simple static choice, i.e., (5.8) and (5.15), [69, 72, 73, 75, 77]. It is more important to go to second order in the distorted-wave approximation (section 5.3) than to improve upon the static potentials (5.8) and (5.15) in the way that (5.16) does.

5.3. The distorted-wave second Born approximation (DWSBA)

With the usual choices of V_1 that are made, e.g., (5.8), the distorted-wave first Born amplitude (5.6) does not contain the important physical effects of target polarization and flux loss which were

* As far as the DWPO models are concerned this statement is true only for DWPOI, not for DWPOII and DWPOIII.

mentioned in section 4.1. To build these effects into the scattering amplitude, second-order distorted-wave theory is required*:

$$\begin{aligned} f_{f0}^{\text{DW Born} 2}(\mathbf{k}_f, \mathbf{k}_0) = & -\frac{1}{2\pi} \langle \mathbf{k}_f \psi_f | V_1 | \Phi_0^+(\mathbf{k}_0) \rangle - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 | \Phi_0^+(\mathbf{k}_0) \rangle \\ & - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 G_1^+ V_2 | \Phi_0^+(\mathbf{k}_0) \rangle. \end{aligned} \quad (5.17)$$

There have been a number of calculations in the DWSBA: on the elastic scattering of electrons, and sometimes positrons, by H(1s), He(1^1S), Ne [32, 37]; on electron impact excitation of the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions in H [32, 69] and of the $2s \rightarrow 3s$ transition in Li [76]; on the electron and positron impact excitation of the $1^1S \rightarrow 2^1P$ transition in He [23, 70]. In addition earlier works on the elastic scattering of electrons (and in one case positrons) by H(1s), He(1^1S) and H(2s) [34, 36, 39, 40, 42] and on the electron and positron impact excitation of the $1^1S \rightarrow 2^1S$ transition in He [18] can be considered as forms of the DWSBA, although they have not been named as such in the papers cited.

5.3.1. Elastic scattering

In all of the calculations on elastic scattering [32, 34, 36, 37, 39, 40, 42] V_1 has been chosen to be

$$V_1 = P_0 V P_0 = V_{00}(\mathbf{r}_0) P_0, \quad (5.18a)$$

$$P_0 = |\psi_0(\mathbf{X})\rangle\langle\psi_0(\mathbf{X})|. \quad (5.18b)$$

Again it should be noted that (5.18) is a compromise in that the nuclear term $\bar{Q}N/r_0$ is not wholly removed from V_2 by this choice; however, it is eliminated from V_2 in so far as the final DWSBA amplitude (5.21) is concerned. The potential (5.18) results in

$$\Phi_0^\pm = F^\pm(\mathbf{r}_0) \psi_0(\mathbf{X}), \quad (5.19a)$$

where

$$(\nabla_0^2 - 2V_{00}(\mathbf{r}_0) + k_0^2)F^\pm(\mathbf{r}_0) = 0, \quad (5.19b)$$

and it is understood that F^+ and F^- are associated with incident plane waves $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)$ and $\exp(i\mathbf{k}_f \cdot \mathbf{r}_0)$ respectively (see (5.3a)) and (5.17)). Since Φ_0^\pm is merely the wave-function for scattering by the static field V_{00} , the first term in (5.17) is just the static-field scattering amplitude

$$f_{\text{st}}(\mathbf{k}_f, \mathbf{k}_0) \equiv -\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_0) | V_{00}(\mathbf{r}_0) | F^+(\mathbf{r}_0) \rangle. \quad (5.20)$$

Also, the second term in (5.17) is zero, while in the third term $V_2 G_1^+ V_2$ can be replaced by $V_2 G_0^+ V_2$.

* I would emphasize again the flexibility of the distorted-wave method. By a suitable choice of V_1 polarization and flux loss could be built into the zeroth-order amplitude, let alone the first-order one. In actual practice V_1 is chosen in a simple way, as in (5.8). Here it is assumed that such a simple choice of V_1 has been made.

With the choice (5.18) therefore

$$f_{00}^{\text{DW Born}^2}(\mathbf{k}_f, \mathbf{k}_0) = f_{\text{st}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \langle F^-(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | F^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle. \quad (5.21)$$

Making a spectral resolution of G_0^+ as in (4.1), the second term in (5.21) can be written

$$-\frac{1}{8\pi^4} \sum_{n \neq 0} \lim_{\eta \rightarrow 0^+} \int \frac{d\mathbf{k} \langle F^-(\mathbf{r}_0)\psi_0(\mathbf{X}) | V | \mathbf{k}(\mathbf{r}_0)\psi_n(\mathbf{X}) \rangle \langle \mathbf{k}(\mathbf{r}_0)\psi_n(\mathbf{X}) | V | F_0^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle}{k_n^2 - k^2 + i\eta}. \quad (5.22)$$

Note the replacement of V_2 by V and the consequent omission of the $n = 0$ intermediate state. Comparing (5.22) with (4.3) it is immediately seen that (5.22) is just the ordinary second Born term (4.3) but with plane waves $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)$ and $\exp(i\mathbf{k}_f \cdot \mathbf{r}_0)$ replaced by distorted waves F^+ and F^- respectively and the $n = 0$ intermediate state eliminated (here the $n = 0$ contribution is transferred to f_{st}). It therefore follows that (5.22) contains essentially the same physics as (4.3); in particular, the dipole polarizability α_{00} of the state ψ_0 and allowance for flux loss from the elastic channel (section 4.1.1). Note that, since $n = 0$ is not an intermediate state, the nuclear term $\bar{Q}N/r_0$ of V cannot survive in (5.22) due to the orthogonality of ψ_0 and ψ_n ; this proves the assertion made earlier that V_2 does not contain the nuclear potential in so far as (5.21) is concerned.

As with (4.3) the sum over intermediate states n in (5.22) is usually performed in a closure or pseudostate approximation (section 4.2). There are at present no exact evaluations of (5.22) even for atomic hydrogen, although such a calculation is under consideration.

In the early work [34, 36, 39, 40, 42] plane waves, rather than distorted waves, were used in (5.22), the effect of V_1 thereby being confined to f_{st} . This gives an approximate amplitude (see (5.21))

$$f_{\text{st}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | \mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle, \quad (5.23)$$

in which the second term is just the ordinary second Born term (4.3) with the $n = 0$ intermediate state contribution missing (5.22). In addition it was realized that, for electron scattering, some attempt should be made to include exchange even at high energies; this resulted in the cavalier prescription of replacing f_{st} by the static-exchange amplitude f_{se} [39, 40, 42]. Thus, for electron scattering, (5.23) was converted to

$$f_{\text{se}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | \mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle \quad (5.24)$$

(the SESSBA approximation of Buckley and Walters [42]).

The approximation (5.24) is a very considerable improvement upon the ordinary SBA (3.10) (or (3.12)) but yet it does not give really good agreement with experimental data [42]. This lack of accord led Dewangan and Walters [37] to the distorted-wave viewpoint of this section and the realization that the amplitude (5.23) was only an approximation to the more consistent formula (5.21). The latter is more consistent in that correct to second order in the “weak” potential V_2 , (5.21) treats the “strong” potential V_1 to all orders; this is not true of (5.23) or (5.24) where the effect of the strong potential in the second term is treated perturbatively, i.e., totally neglected.

The problem with using (5.21) rather than (5.23) is that the distorted-wave second-order term (5.22) is

much more difficult to evaluate than the corresponding plane-wave term (4.3) (with $n = 0$ removed). This is because (5.22), unlike (4.3), cannot be reduced to a set of Lewis integrals (4.27) for which analytic formulae exist; the evaluation of (5.22) is very much a numerical problem. It was therefore appropriate that first attempts to calculate (5.22) should try and relate this amplitude in an easy way to the simpler second Born term (4.3). Such a connection was successfully established, at least for H (1s) and He(¹S), by Dewangan and Walters [37]. The precise form of their approximation for scattering off an S-state ψ_0 is

$$\begin{aligned} & -\frac{1}{2\pi} \langle F^-(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | F^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle \\ & \triangleq \tilde{f}_{00}^{B2}(\mathbf{k}_f, \mathbf{k}_0) + \frac{1}{2} \sum_{l=0}^{\infty} (2l+1)i k_0 f_{st,l}(1 + \frac{1}{4}ik_0 f_{st,l}) \tilde{f}_l^{B2} P_l(\hat{\mathbf{k}}_0 \cdot \hat{\mathbf{k}}_f), \end{aligned} \quad (5.25a)$$

where

$$\tilde{f}_{00}^{B2}(\mathbf{k}_f, \mathbf{k}_0) \equiv -\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | \mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle \quad (5.25b)$$

(\tilde{f}_{00}^{B2} is just (4.3a) with the intermediate $n = 0$ state removed) and the partial wave amplitudes $f_{st,l}$ and \tilde{f}_l^{B2} are obtained from f_{st} and \tilde{f}_{00}^{B2} according to

$$g(\mathbf{k}_f, \mathbf{k}_0) = \frac{1}{2} \sum_{l=0}^{\infty} (2l+1) g_l P_l(\hat{\mathbf{k}}_0 \cdot \hat{\mathbf{k}}_f), \quad g = f_{st} \quad \text{or} \quad \tilde{f}_{00}^{B2}. \quad (5.25c)$$

Since $V_{00}(\mathbf{r}_0)$ is a short-range potential only a few partial waves have to be summed in (5.25a). The reader is referred to [37] for further details.

Another simple procedure for approximating (5.22) involves the generation of a local impact energy dependent potential by the Fourier transforming of the plane-wave second Born term:

$$\tilde{V}_{00}^{L2}(E, \mathbf{r}_0) = -\frac{1}{4\pi^2} \int \exp(-i\mathbf{q} \cdot \mathbf{r}_0) \tilde{f}_{00}^{B2}(\mathbf{k}_f, \mathbf{k}_0) d\mathbf{q} \quad (5.26a)$$

$$= -\frac{1}{\pi r_0} \int dq \sin qr_0 \tilde{f}_{00}^{B2}(\mathbf{k}_f, \mathbf{k}_0) dq, \quad (5.26b)$$

$$\mathbf{q} \equiv \mathbf{k}_0 - \mathbf{k}_f, \quad (5.26c)$$

where it is assumed that ψ_0 is an S-state. The distorted-wave term (5.22) is then calculated according to

$$-\frac{1}{2\pi} \langle F^-(\mathbf{r}_0)\psi_0(\mathbf{X}) | V_2 G_0^+ V_2 | F^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle \triangleq -\frac{1}{2\pi} \int F^{-*}(\mathbf{r}_0) \tilde{V}_{00}^{L2}(E, \mathbf{r}_0) F^+(\mathbf{r}_0) d\mathbf{r}_0. \quad (5.27)$$

When F^+ and F^- are plane waves $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)$ and $\exp(i\mathbf{k}_f \cdot \mathbf{r}_0)$ respectively, it is clear from (5.26a) that (5.27) gives the exact answer, i.e., $\tilde{f}_{00}^{B2}(\mathbf{k}_f, \mathbf{k}_0)$. References and a full description of local potential approximations are given in section 7.2.2.

The approximations (5.25) and (5.27) have now been justified for elastic electron-H (1s) and electron-He (1^1S) scattering at energies of interest [32, 78]. Of the two methods (5.27) appears to be the better [32].

The first DWSBA calculations of elastic scattering employing the full second-order amplitude (5.21) were made by Dewangan and Walters [37] who used the approximation (5.25). To allow for exchange in electron scattering they replaced f_{st} in (5.21) and (5.25) by the static-exchange amplitude f_{se} (as in (5.24)). Their results for electron-He (1^1S) elastic scattering at 500 eV are shown in fig. 10 where they are compared with the accurate experimental data of Bromberg [15]. The agreement with experiment is excellent [3]. It should be noted that the exchange contribution to the DWSBA cross section of fig. 10 is not negligible, it amounts to about 10% on average.

In the agreement between the DWSBA cross section and experiment illustrated in fig. 10 we see the vindication of the philosophy advanced in section 3.2, namely, that the singular nature of the nuclear interaction, $\bar{Q}N/r_0$, is a primary cause of the slow convergence of the ordinary Born series (3.3).

Dewangan and Walters went on to apply their DWSBA to e^\pm scattering by Ne. Compared with He, Ne is a heavy atom. In section 3.1(iii) and fig. 2 the disastrous performance of the ordinary Born series (3.3) for scattering by the heavier atoms was highlighted. It is therefore of some interest to see how the distorted-wave version of perturbation theory works in such cases. In fig. 11 the DWSBA and the FBA are compared with the experimental data of Bromberg for electron-Ne elastic scattering at 700 eV. The

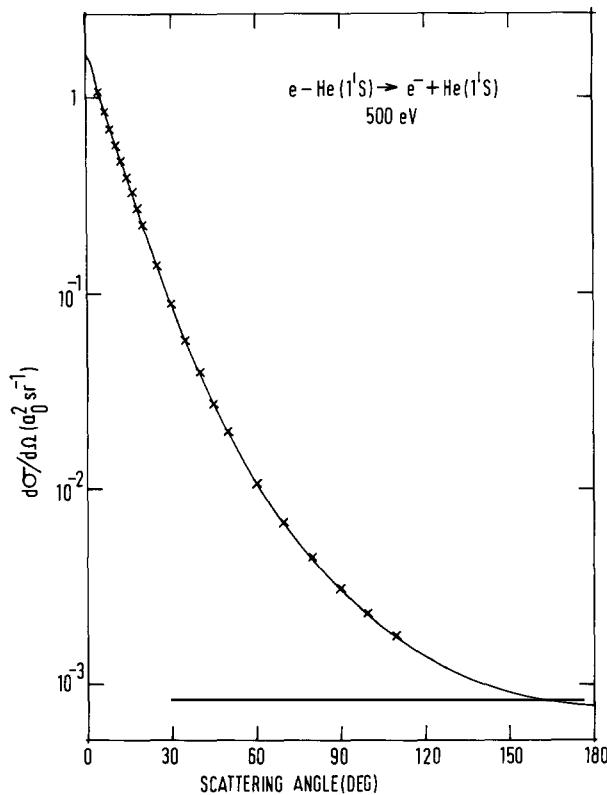


Fig. 10. Differential cross section for elastic scattering of electrons by He (1^1S) at 500 eV: (—) DWSBA cross section of [37]; (x) experimental data of Bromberg [15].

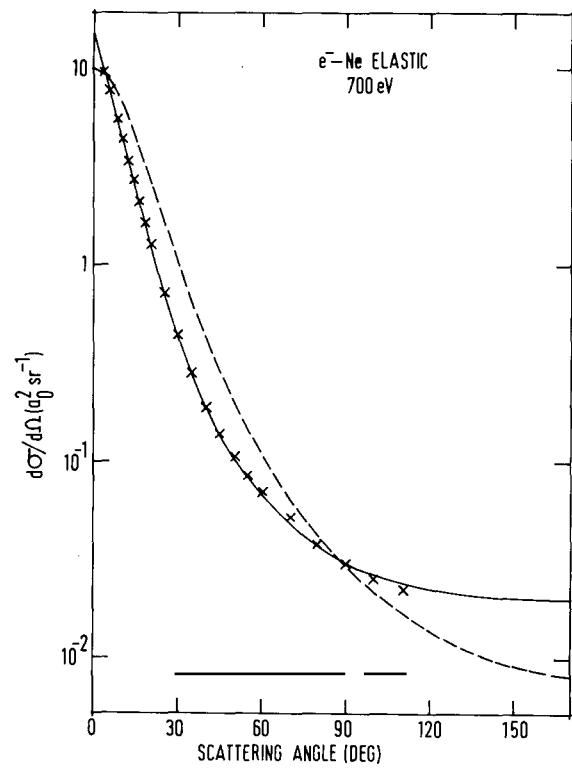


Fig. 11. Differential cross section for elastic scattering of electrons by Ne at 700 eV. Curves: (—) DWSBA cross section of [37]; (---) first Born approximation [37]. Experimental data: (x) Bromberg [15].

agreement between the DWSBA and experiment is again very good [3]. By contrast the FBA is generally much too large at those angles which contribute most to the integrated cross section (i.e. the smaller angles). The results on He and Ne indicate that the DWSBA is a viable approximation for atoms of varying size.

The most recent DWSBA calculations on elastic scattering are those of Kingston and Walters [32] on electron-H (1s) scattering. In these calculations neither of the approximations (5.25) and (5.27) are used, an exact evaluation of (5.22), in the closure approximation, being made. It is from this work that the conclusions concerning the viability of (5.25) and (5.27) for elastic electron-H (1s) and electron-He (1^1S) scattering are mainly drawn.

With decreasing impact energy the excellent agreement between the DWSBA and experiment shown in figs. 10 and 11 is lost, although slowly. It is thought that the primary cause of this breakdown lies in the inadequate treatment of exchange effects (section 8).

5.3.2. Inelastic scattering

In this section I shall assume for simplicity that ψ_0 and ψ_f are both S-states. Variations on the development given below when this is not so will be found in [32, 70].

Three different forms of V_1 have been used.

(i) The choice (5.8) [69, 76] (this becomes (5.15) when ψ_0 and ψ_f are not both S-states [23, 70]):

$$V_1 = V_{00}(\mathbf{r}_0)P_0 + V_{ff}(\mathbf{r}_0)P_f. \quad (5.28)$$

(ii) The form used by Walters and co-workers [18, 32]:

$$V_1 = (P_0 + P_f)V(P_0 + P_f) \quad (5.29a)$$

$$= V_{00}(\mathbf{r}_0)P_0 + V_{ff}(\mathbf{r}_0)P_f + |\psi_0(\mathbf{X})\rangle V_{0f}(\mathbf{r}_0)\langle\psi_f(\mathbf{X})| + |\psi_f(\mathbf{X})\rangle V_{f0}(\mathbf{r}_0)\langle\psi_0(\mathbf{X})|. \quad (5.29b)$$

(iii) The form (5.16) [69, 76]:

$$V_1 = P_0 \tilde{V}_0 P_0 + P_f \tilde{V}_f P_f, \quad (5.30a)$$

where

$$\tilde{V}_n = V_{nn}(\mathbf{r}_0) + \text{terms not containing } \bar{Q}N/r_0, \quad n = 0 \text{ or } f. \quad (5.30b)$$

In (5.30) the idea is that V_1 should go beyond the simple static potentials and include polarization, absorption, etc. in the initial and final channels.

All of the choices (i) to (iii) satisfy the requirement that V_2 should not contain the nuclear interaction in so far as the DWSBA is concerned.

When the potential (5.28) is used in (5.17) the first term vanishes and the resulting DWSBA amplitude is

$$f_{f0}^{\text{DW Born}^2}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle F_f^-(\mathbf{r}_0)|V_{f0}(\mathbf{r}_0)|F_0^+(\mathbf{r}_0)\rangle - (1/2\pi)\langle F_f^-(\mathbf{r}_0)\psi_f(\mathbf{X})|V_2 G_0^+ V_2 |F_0^+(\mathbf{r}_0)\psi_0(\mathbf{X})\rangle, \quad (5.31)$$

where F_0^+ and F_f^- satisfy (5.11). The first term on the right of (5.31) is easily recognized as $f_{f0}^{\text{DW Born} 1}$ of (5.10).

The use of the potential (5.29) in (5.17) causes the second term to disappear and gives

$$f_{f0}^{\text{DW Born} 2}(\mathbf{k}_f, \mathbf{k}_0) = f_{f0}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0) - 1/2\pi \langle \Phi_f^-(\mathbf{k}_f) | V_2 G_0^+ V_2 | \Phi_0^+(\mathbf{k}_0) \rangle. \quad (5.32)$$

Solution of the Schrödinger equation with the potential (5.29) is equivalent to solving a two-state, ψ_0 and ψ_f , close-coupling approximation. Thus $\Phi_{0,f}^\pm$ have the form

$$\Phi_n^\pm = F_{n0}^\pm(\mathbf{r}_0)\psi_0(\mathbf{X}) + F_{nf}^\pm(\mathbf{r}_0)\psi_f(\mathbf{X}_0), \quad n = 0 \quad \text{or} \quad f, \quad (5.33)$$

where

$$(\nabla_0^2 - 2V_{00}(\mathbf{r}_0) + k_0^2)F_{n0}^\pm = 2V_{0f}(\mathbf{r}_0)F_{nf}^\pm, \quad (\nabla_0^2 - 2V_{ff}(\mathbf{r}_0) + k_f^2)F_{nf}^\pm = 2V_{f0}(\mathbf{r}_0)F_{n0}^\pm, \quad (5.34)$$

f_{f0}^{cc} is the amplitude for the transition $\psi_0 \rightarrow \psi_f$ in the two-state close-coupling approximation (5.34). Substituting (5.33) in (5.32) gives

$$f_{f0}^{\text{DW Born} 2}(\mathbf{k}_f, \mathbf{k}_0) = f_{f0}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \sum_{n=0,f} \sum_{m=0,f} \langle F_f^-(\mathbf{r}_0)\psi_n(\mathbf{X}) | V_2 G_0^+ V_2 | F_{0m}^+(\mathbf{r}_0)\psi_m(\mathbf{X}) \rangle. \quad (5.35)$$

Kingston and Walters [32] have argued that the term with $n = f$ and $m = 0$ will be much more important than the remaining three. If so, it is reasonable to drop the latter, so that (5.35) becomes

$$f_{f0}^{\text{DW Born} 2}(\mathbf{k}_f, \mathbf{k}_0) = f_{f0}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0) - (1/2\pi) \langle F_f^-(\mathbf{r}_0)\psi_f(\mathbf{X}) | V_2 G_0^+ V_2 | F_{00}^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle, \quad (5.36)$$

a form very similar to (5.31).

The potential (5.30) gives

$$f_{f0}^{\text{DW Born} 2}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi) \langle F_f^-(\mathbf{r}_0) | V_{f0}(\mathbf{r}_0) | F_0^+(\mathbf{r}_0) \rangle - (1/2\pi) \langle F_f^-(\mathbf{r}_0)\psi_f(\mathbf{X}) | V_2 G_1^+ V_2 | F_0^+(\mathbf{r}_0)\psi_0(\mathbf{X}) \rangle, \quad (5.37)$$

where F_0^+ and F_f^- are determined by (5.11) but with V_{00} and V_{ff} replaced by \tilde{V}_0 and \tilde{V}_f respectively. The amplitude (5.37) is of exactly the same structure as (5.31) except that G_1^+ (see (5.4b)) appears instead of G_0^+ (3.1b). In (5.31) it was possible to replace G_1^+ by G_0^+ since

$$\langle \psi_0 | V_2 | \psi_0 \rangle = \langle \psi_f | V_2 | \psi_f \rangle = 0 \quad (5.38)$$

in that case. However, with the potential (5.30) this is not so. Nevertheless, the condition (5.38) is imposed on (5.37) [69, 76] with the result that (5.37) becomes identical with (5.31) except that F_0^+ and F_f^- are calculated in the fields of \tilde{V}_0 and \tilde{V}_f rather than V_{00} and V_{ff} . Where there is a marked difference between using (5.28) and (5.30) [76] this simplification will probably have a pronounced effect!

Making a spectral resolution of G_0^+ according to (4.1) it is easily seen that the three cases (5.31), (5.36) and (5.37) ((5.38) imposed) all have the structure

$$\begin{aligned}
f_{f0}^{\text{DW Born}^2}(\mathbf{k}_f, \mathbf{k}_0) &= f'_{f0}(\mathbf{k}_f, \mathbf{k}_0) \\
&- \frac{1}{8\pi^4} \sum_{n \neq 0, f} \lim_{\eta \rightarrow 0+} \int \frac{d\mathbf{k} \langle F_f^-(\mathbf{r}_0)\psi_f(\mathbf{X})|V|\mathbf{k}(\mathbf{r}_0)\psi_n(\mathbf{X})\rangle \langle \mathbf{k}(\mathbf{r}_0)\psi_n(\mathbf{X})|V|F_0^+(\mathbf{r}_0)\psi_0(\mathbf{X})\rangle}{k_n^2 - k^2 + i\eta}
\end{aligned} \tag{5.39}$$

where f'_{f0} is an amplitude which contains the direct transition from ψ_0 to ψ_f ; indirect transitions through an intermediate state ψ_n ($n \neq 0, f$) are represented by the second term. The only difference between the three cases lies in the precise form of f'_{f0} and in how the distorted waves F_0^+ and F_f^- are calculated. Since the second term in (5.39) is just a distorted-wave version of (4.3) it incorporates such physics as the non-diagonal dipole polarizability (section 4.1.2). To calculate this term a closure or pseudostate approximation is usually adopted (section 4.2).

To make a proper calculation of electron scattering it is necessary also to make allowance for exchange. The same cavalier approach has been adopted as in elastic scattering (section 5.3.1). Thus in the calculations which have been performed exchange has been included in (5.31) and (5.37) by merely antisymmetrizing the first term, while for (5.36) the procedure has been to replace f_{f0}^{cc} by $f_{f0}^{\text{cc,ex}}$ where the latter is the scattering amplitude in the same close-coupling approximation but with exchange included. In all cases the distorted waves which appear in (5.31), (5.36) and (5.37) have always been calculated without allowance for exchange; this has been justified by Kingston and Walters [32] for the calculations they have done.

Work on inelastic scattering has followed more or less the same pattern as that on elastic scattering. The first calculation [18] tried to ignore the distorted waves in the second term of (5.36), replacing them with plane waves. As with elastic scattering it is now known that this is not really a good approximation [32]. The inelastic analogues of the Dewangan-Walters prescription (5.25) and of the local potential approximation (5.26) have been tried, but, unlike the elastic case, have been found to be unreliable [32]. Apparently, nothing short of a proper evaluation of the distorted-wave second-order term would seem to be acceptable. It is an unfortunate fact that of the inelastic calculations carried out only those of Kingston and Walters [32], on the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation of H, have made a proper evaluation of the distorted-wave second-order term. The results of other works [18, 23, 69, 70, 76] must be treated with caution. At present there is no precise description of why (5.25) and (5.26) work for elastic scattering but not for inelastic scattering.

In fig. 12 the DWSBA calculations of Kingston and Walters [32] for the sum of the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ cross sections for electron impact excitation of H are compared with the experimental data of Williams and Willis [79] at 54.4, 100 and 200 eV. Generally speaking the agreement between theory and experiment is not too good.

More recent measurements by Williams [80] at 54.4 eV have been able to separate the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ cross sections. These data, which also include the ratio, $\sigma(2s)/\sigma(2p)$, of the 2s cross section to the 2p cross section, are compared with the DWSBA in fig. 13. Agreement is not satisfactory.

Also shown in fig. 13 are the results of a pseudostate close-coupling calculation [81] employing the nine states of Fon et al. [82]; this calculation takes exchange into account and also applies a correction for the incompleteness of the pseudostate set. For the $1s \rightarrow 2p$ excitation the pseudostate calculation improves agreement with experiment at angles above 30° but leads to a deterioration at lower angles. For $1s \rightarrow 2s$ the pseudostate numbers support the DWSBA except in the “shoulder” region from 30° to 60° . As far as $\sigma(2s)/\sigma(2p)$ is concerned the pseudostate approximation and the DWSBA are in reasonable accord up to 90° .

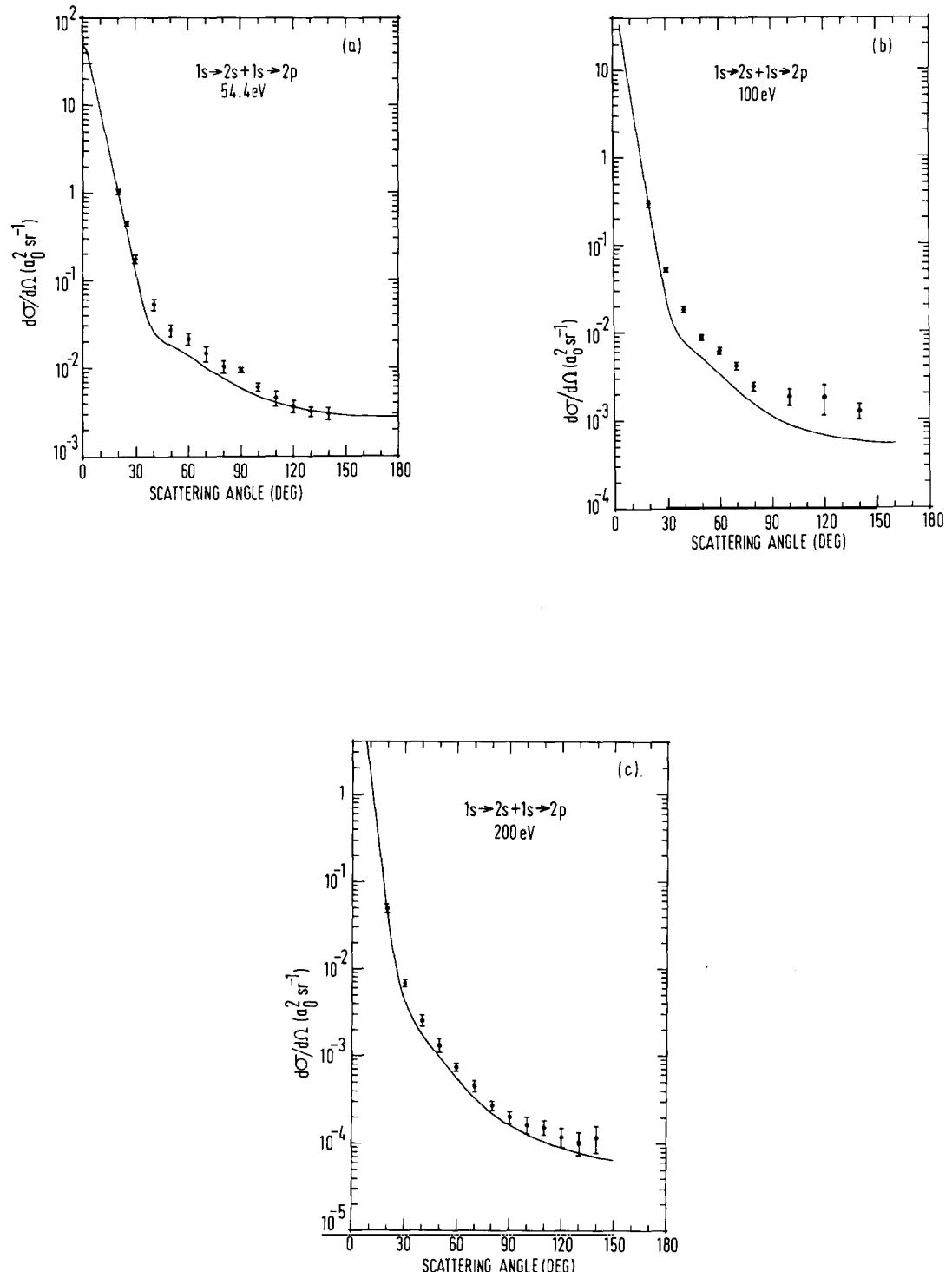


Fig. 12. Differential cross sections for $e^- + H(1s) \rightarrow e^- + H(2s + 2p)$ at (a) 54.4 eV, (b) 100 eV, (c) 200 eV. (—) DWSBA cross section of [32]; (●) experimental data of [79].

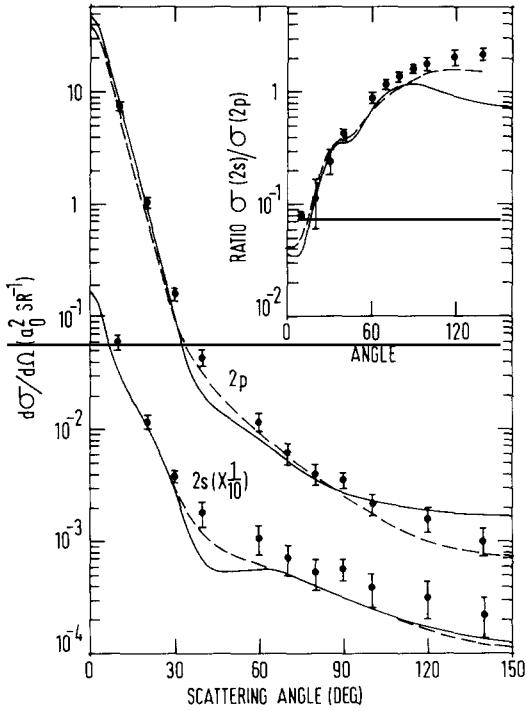


Fig. 13. Differential cross sections for $e^- + H(1s) \rightarrow e^- + H(2s)$ and $e^- + H(1s) \rightarrow e^- + H(2p)$ at 54.4 eV. Curves: (—) DWSBA cross section of [32]; (---) pseudostate close-coupling cross section of [81]. Experimental data: (●) Williams [80]. Inset: ratio, $\sigma(2s)/\sigma(2p)$, of 2s and 2p differential cross sections.

The pseudostate calculation is presently the most sophisticated calculation of the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions at this energy. The fact that it does not produce a significant improvement in agreement with experiment suggests that in the comparisons of figs. 12 and 13 it is not necessarily the DWSBA which is at fault. To be fair to the DWSBA it should be emphasized that to compare it with experiment at as low an energy as 54.4 eV is to assess it under adverse conditions – the higher the energy the better should be the DWSBA.

Concerning the data at 54.4 eV, it is ironical that a simple three-state, $1s-2p-2p$, close-coupling approximation [83] gives very good agreement with the measurements of Williams [9, 80]. Such an approximation should be inferior to the pseudostate calculation mentioned above. It is this author's opinion that the seemingly good agreement is fortuitous.

Inelastic scattering provides a wider range of tests for approximations than elastic scattering; in particular, those tests arising from electron-photon coincidence measurements. Such measurements have been carried out by Williams [80] on the $1s \rightarrow 2p$ excitation of H at 54.4 eV. The results are conveniently given in terms of two parameters λ and R :

$$\lambda \equiv \frac{\langle |f_0|^2 \rangle}{\langle |f_0|^2 + 2|f_1|^2 \rangle} = \frac{\sigma_0}{\sigma_0 + 2\sigma_1}, \quad (5.40)$$

$$R \equiv \text{Real } \langle f_0^* f_1 \rangle / \langle |f_0|^2 + 2|f_1|^2 \rangle, \quad (5.41)$$

$$\sigma_m \equiv (k_f/k_0) \langle |f_m|^2 \rangle, \quad (5.42)$$

where f_0 and f_1 are the scattering amplitudes for exciting the $m = 0$ and $m = +1$ magnetic substates of the 2p state[†], atomic quantization being along the direction of incidence, i.e., k_0 , $\langle \rangle$ stands for an average over initial spin states and a sum over final spin states, and σ_m is a differential cross section (2.9).

In figs. 14 and 15 the experimental results for (5.40) and (5.41) are compared with the DWSBA values of Kingston and Walters. Agreement is poor. Also shown are the pseudostate close-coupling numbers, these support the experiment in the angular range up to 60° thereby suggesting that the error lies with the DWSBA.

Madison and Winters [70] have been more successful in the application of their DWSBA to electron-photon coincidence parameters for the $1^1S \rightarrow 2^1P$ excitation of He. However, since they use a local second-order potential (see (5.26)) to evaluate the distorted-wave second-order term caution should be urged in interpreting these results.

As in the case of the first-order distorted-wave approximation (section 5.2), and barring low energies and special circumstances [76], there is reason to believe [69, 70] that results calculated with the potential (5.30) will not be a lot different from those obtained from the simple static potential (5.28).

It is difficult at this time to make precise comment upon the accuracy of the DWSBA for inelastic scattering. There are several reasons:

- (i) the lack of really high quality experimental measurements at the higher energies;

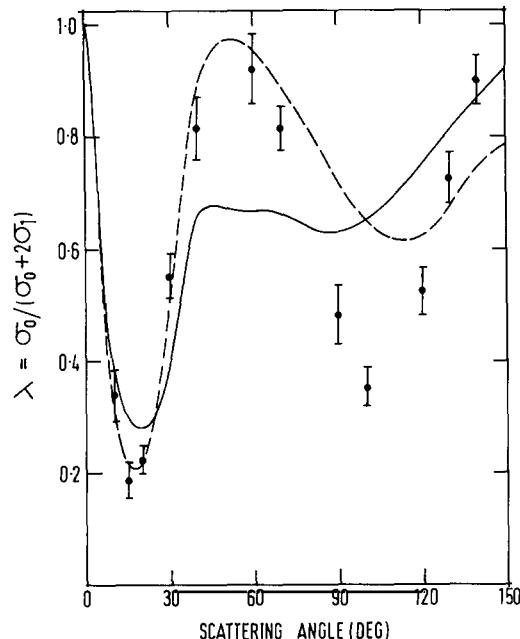


Fig. 14. The parameter λ of (5.40) for $e^- + H(1s) \rightarrow e^- + H(2p)$ at 54.4 eV. Curves: (—) DWSBA of [32]; (---) pseudostate close-coupling approximation of [81]. Experimental data: (●) Williams [80].

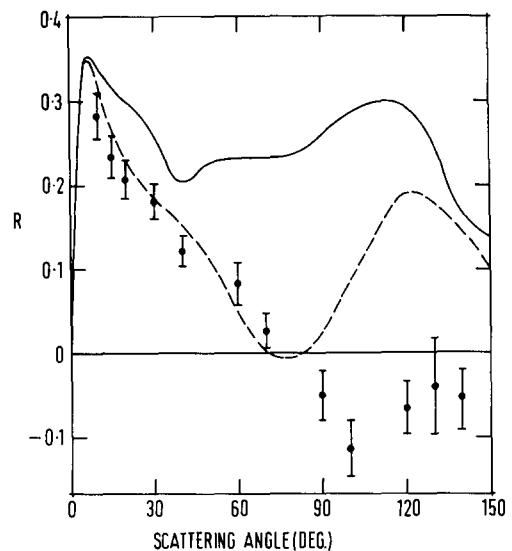


Fig. 15. The parameter R of (5.41) for $e^- + H(1s) \rightarrow e^- + H(2p)$ at 54.4 eV. Curves: (—) DWSBA of [32]; (---) pseudostate close-coupling approximation of [81]. Experimental data: (●) Williams [80].

[†]A factor of $e^{-i\phi}$ has been assumed removed from f_1 , where ϕ is the azimuthal angle of k_f about k_0 as z -axis.

- (ii) limited application of the DWSBA to inelastic transitions;
- (iii) the need to include the distorted waves properly in the second terms of (5.31), (5.36) and (5.37); only the calculations of Kingston and Walters [32] are free from criticism on this score.

5.4. A slightly different viewpoint

In this section I would like to reconcile the notation, viewpoint and terminology of Winters and co-authors [7, 23, 69, 70, 76, 84] with that used in the previous sections where I have described their work in my own terms, i.e., from (5.5).

In the development of the distorted-wave Born series which has been given I have emphasized the fact that the expansion (5.5) is a power series in the “weak” potential V_2 which, to each order in V_2 , treats the “strong” potential V_1 exactly. In the work of Winters et al. this emphasis is absent.

The viewpoint of Winters et al. is developed as follows. (This section is best read in conjunction with section 2.1 of reference [84]). Firstly, they allow for different decompositions of V in the initial (0) and final (f) channels:

$$V = U_0 + W_0, \quad (5.43a)$$

$$V = U_f + W_f. \quad (5.43b)$$

The correspondence with (5.1) is $V_1 = U_0$, $V_2 = W_0$ with the assumption that $U_0 = U_f$ and $W_0 = W_f$. Thus U is the strong potential and W is the weak potential.

Using (5.43b) in the two-potential formula (5.2) gives

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi) \langle \chi_f^- | W_f | \Psi^+ \rangle, \quad (5.44)$$

where it is assumed that U_0 and U_f cannot cause a transition between ψ_0 and ψ_f (Winters et al. consider only inelastic scattering) and where

$$\chi_n^\pm = \exp(i\mathbf{k}_n \cdot \mathbf{r}_0) \psi_n(\mathbf{X}) + G_0^\pm U_n \chi_n^\pm, \quad n = 0 \quad \text{or} \quad f \quad (5.45)$$

(χ_n^\pm is Φ_n^\pm of (5.3a)). Analogous to (5.4a)

$$\Psi^+ = \chi_0^+ + G_{U_0}^+ W_0 \Psi^+, \quad (5.46a)$$

$$G_{U_0}^\pm = \lim_{\eta \rightarrow 0^+} (E - H_0 - U_0 \pm i\eta)^{-1}. \quad (5.46b)$$

This can be rewritten as

$$\Psi^+ = \chi_0^+ + G^+ W_0 \chi_0^+, \quad (5.47a)$$

$$G^\pm = \lim_{\eta \rightarrow 0^+} (E - H_0 - V \pm i\eta)^{-1}. \quad (5.47b)$$

Substituting (5.47) in (5.44) gives

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle \chi_f^- | W_f (1 + G^+ W_0) | \chi_0^+ \rangle. \quad (5.48)$$

It is easily verified that

$$G^\pm = G_0^\pm + G_0^\pm V G^\pm. \quad (5.49)$$

This is an operator analogue of the Lippmann–Schwinger equation (3.1a) for the wavefunction. Solving (5.49) by iteration starting with $G^\pm = G_0^\pm$ (i.e., making a Born series expansion) gives

$$G^\pm = G_0^\pm \sum_{i=0}^{\infty} (V G_0^\pm)^i. \quad (5.50)$$

Employing (5.50) in (5.48) yields

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle \chi_f^- | (W_f + W_f G_0^+ W_0 + W_f G_0^+ V G_0^+ W_0 + \cdots + W_f G_0^+ (V G_0^+)^i W_0 + \cdots) | \chi_0^+ \rangle. \quad (5.51)$$

In the terminology of Winters et al. the first, second and n th distorted-wave Born terms are then:

$$f_{f0}^{DWB1} = -(1/2\pi)\langle \chi_f^- | W_f | \chi_0^+ \rangle, \quad (5.52a)$$

$$f_{f0}^{DWB2} = -(1/2\pi)\langle \chi_f^- | W_f G_0^+ W_0 | \chi_0^+ \rangle, \quad (5.52b)$$

$$f_{f0}^{DWBn} = -(1/2\pi)\langle \chi_f^- | W_f G_0^+ (V G_0^+)^{n-2} W_0 | \chi_0^+ \rangle, \quad n \geq 3. \quad (5.52c)$$

(Note that Winters et al. usually write W_n as $V - U_n$, see (5.43)).

In (5.52) an important divergence between the philosophy of Winters et al. and that of (5.5) is seen, namely, the appearance in (5.52c) of the full potential V in third and higher orders. Having taken the trouble to split V into weak and strong potentials, W and U respectively, Winters et al. go on to ignore this distinction when it comes to the expansion (5.50). The result is that (5.51) is a power series in the strong potential V which is precisely what we were trying to avoid in making the expansion (5.5). It is noteworthy that the first- and second-order distorted-wave terms, (5.52a) and (5.52b), contain only the weak potentials W_0 and W_f . In practice Winters et al. have only performed calculations to second order.

If instead of (5.49) the equally trivial identity

$$G^\pm = G_{U_0}^\pm + G_{U_0}^\pm W_0 G^\pm \quad (5.53)$$

is adopted, then iterative solution of (5.53) gives

$$G^\pm = G_{U_0}^\pm \sum_{i=0}^{\infty} (W_0 G_{U_0}^\pm)^i. \quad (5.54)$$

This is a “distorted-wave” expansion of G^\pm , as opposed to a “plane-wave” expansion (5.50). Using (5.54) in (5.48) produces

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi) \langle \chi_f^- | (W_f + W_f G_{U_0}^+ W_0 + W_f G_{U_0}^+ W_0 G_{U_0}^+ W_0 + \cdots + W_f G_{U_0}^+ (W_0 G_{U_0}^+)^i W_0 + \cdots) | \chi_0^+ \rangle, \quad (5.55)$$

which is a power series only in the weak potential W . On making the translation $U_0 \rightarrow V_1$, $W_0 \rightarrow W_f \rightarrow V_2$, (5.55) is seen to be (5.5).

For $U_0(U_f)$ Winters et al. recommend the one-channel optical potential in the initial (final) channel (optical potentials are discussed in section 7), i.e.,

$$U_n = P_n V P_n + P_n V Q_n [Q_n (E - H_0 - V + i\eta) Q_n]^{-1} Q_n V P_n, \quad (5.56a)$$

$$Q_n \equiv 1 - P_n, \quad n = 0 \quad \text{or} \quad f, \quad (5.56b)$$

where it is assumed that the limit $\eta \rightarrow 0+$ is to be taken. Expanding this potential in powers of V gives (see (5.47b) and (5.50))

$$U_n = P_n V P_n + P_n V G_0^+ Q_n V P_n + P_n V G_0^+ Q_n V G_0^+ Q_n V P_n + \cdots. \quad (5.57)$$

The first order term, $P_n V P_n$, is just the static potential

$$P_n V P_n = V_{nn}(\mathbf{r}_0) P_n. \quad (5.58)$$

It is easily verified that if U_n is taken to be (5.58) then (5.52a) and (5.52b) yield the same results to second order as when (5.8) is used in (5.5).

The second and higher terms in (5.57) allow for polarization, flux loss, etc., in elastic scattering in channel n . In the preceding sections the work of Winters et al. using higher-order versions of U_n has been described in terms of the potential (5.16). In section 5.3.2 it is shown that further approximations, i.e., imposition of (5.38), are required in order to arrive at the DWSBA amplitude (5.39) actually used by Winters et al.

Multiple counting, which may not be important, can arise when higher orders of U_n than (5.58) are used. Sometimes this is remedied by making a small change in the form of U_n [76]. The reader is referred to [84] for details.

Finally, Winters et al. usually describe their calculations as being of N th order in the transition potential (or in target distortion) and containing M th order (projectile) distortion in a particular channel [7, 70]. By this they mean that terms of (5.52) up to $n = N$ are included with the distorting potential (5.57) being calculated up to power M in V .

5.5. Perturbative philosophy

In the perturbative philosophy developed in this article the e^\pm -nucleus interaction has been identified as a primary, if not the primary, cause of trouble for perturbation theory. It has been seen that in matrix elements $\langle \psi_m(\mathbf{X}) | V | \psi_n(\mathbf{X}) \rangle$ the e^\pm -nucleus potential survives only in the diagonal terms, $m = n$, i.e., in the static fields. Put another way, therefore, the perturbative principle is that it is reasonable to do perturbation theory in the non-diagonal elements of V but not in the diagonal elements. This principle is very clear in the forms (5.21), (5.22) and (5.39) of the distorted-wave second Born approximation.

One of the unsatisfactory features about sections 5.2 and 5.3 was that the choices of the potential V_1 did not totally remove the e^\pm -nucleus interaction from $V_2 (= V - V_1)$. Indeed, it was a bit unfair to

criticize the formulation of Winters et al. (section 5.4) for retaining the full potential V in third and higher orders (5.52) when the choices of V_1 that are actually used in (5.5) would lead to the appearance of the nuclear potential in V_2 in third and higher orders.

Dewangan and Walters [37] have voiced concern over the inconsistency in the choice of V_1 . They have suggested the choice

$$V_1 = \sum_n V_{nn}(\mathbf{r}_0) P_n, \quad (5.59)$$

where the sum is over all atomic states n . This indeed removes all of the nuclear potential from V_2 . Although the idea embodied in (5.59) is right, the potential is unsatisfactory from a practical viewpoint in that it does not conserve the total orbital angular momentum of the system. A better choice would be the spherically symmetric potential (5.15) which does conserve angular momentum, i.e.,

$$V_1 = \bar{Q} \left\{ N/r_0 - \sum_{i=1}^N 1/r_{i>} \right\}. \quad (5.60)$$

It is clear from (2.2c) and (5.60) that $V_2 = V - V_1$ does not contain the nuclear interaction.

Of course, the real trouble with (5.59) and (5.60) is that they are considerably more difficult to handle than the choices of sections 5.2 and 5.3. However, it may be possible to make some reasonable progress with (5.60) if an independent particle model of the atom is adopted.

6. The Glauber, eikonal-Born Series, modified Glauber, Wallace and unitarized eikonal-Born series approximations

6.1. The Glauber approximation

In this section I give a simple-minded derivation of the Glauber approximation [85]; the intent is to catch the spirit of the approximation rather than to give a technically perfect account. Readers interested in further details should consult the review articles [2, 4, 86, 87].

Starting from the Schrödinger equation (2.5)

$$\left(-\frac{1}{2}\nabla_0^2 + H_a + V(\mathbf{r}_0, \mathbf{X}) - \frac{1}{2}k_0^2 - \varepsilon_0 \right) \Psi^+ = 0, \quad (6.1)$$

the first approximation is to set H_a equal to a constant, in fact equal to ε_0 . Then

$$\left(-\frac{1}{2}\nabla_0^2 + V(\mathbf{r}_0, \mathbf{X}) - \frac{1}{2}k_0^2 \right) \Psi^+ = 0. \quad (6.2)$$

The next step is to write $-\frac{1}{2}\nabla_0^2$ as

$$\frac{1}{2}[(-i\nabla_0 - \mathbf{k}_0) + \mathbf{k}_0]^2 = \frac{1}{2}[(-i\nabla_0 - \mathbf{k}_0)^2 + 2\mathbf{k}_0 \cdot (-i\nabla_0 - \mathbf{k}_0) + \mathbf{k}_0^2]. \quad (6.3)$$

It is now assumed that the scattering does not cause the momentum of the incident particle, $-i\nabla_0$, to differ much from \mathbf{k}_0 so that the first term on the right-hand side of (6.3) can be neglected in comparison

with the others. This gives the second approximation

$$-\frac{1}{2}\nabla_0^2 \rightarrow -i\mathbf{k}_0 \cdot \nabla_0 - \frac{1}{2}k_0^2. \quad (6.4)$$

Implementing (6.4) in (6.2) leads to the differential equation

$$(-ik_0 \partial/\partial z_0 + V(\mathbf{r}_0, \mathbf{X}) - k_0^2)\Psi^+ = 0, \quad (6.5)$$

where the z -axis is in the direction of \mathbf{k}_0 . Solving (6.5) subject to the incoming boundary condition

$$\Psi^+ \xrightarrow{z_0 \rightarrow -\infty} \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)\psi_0(\mathbf{X}), \quad (6.6)$$

and substituting the result in the formula (2.7) gives the scattering amplitude

$$\begin{aligned} f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = & -\frac{1}{2\pi} \int d\mathbf{r}_0 d\mathbf{X} \exp(-i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_f^*(\mathbf{X}) V(\mathbf{r}_0, \mathbf{X}) \\ & \times \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0) \psi_0(\mathbf{X}) \exp \left[-i/k_0 \int_{-\infty}^{z_0} V(x_0, y_0, z'_0, \mathbf{X}) dz'_0 \right], \end{aligned} \quad (6.7)$$

the term on the second line is the wavefunction from (6.5). If the momentum transfer, $\mathbf{q} \equiv \mathbf{k}_0 - \mathbf{k}_f$, is perpendicular to the direction of \mathbf{k}_0 , which is true for near forward elastic scattering, then the integral over z_0 in (6.7) may be performed to give

$$f_{f0}^G(\mathbf{k}_f, \mathbf{k}_0) = \frac{ik_0}{2\pi} \int d^2\mathbf{b}_0 d\mathbf{X} \exp(i\mathbf{q} \cdot \mathbf{b}_0) \psi_f^*(\mathbf{X}) \left(1 - \exp \left[-i/k_0 \int_{-\infty}^{+\infty} V(x_0, y_0, z_0, \mathbf{X}) dz_0 \right] \right) \psi_0(\mathbf{X}), \quad (6.8a)$$

$$\mathbf{r}_0 = x_0 \mathbf{i} + y_0 \mathbf{j} + z_0 \mathbf{k}, \quad (6.8b)$$

$$\mathbf{b}_0 \equiv x_0 \mathbf{i} + y_0 \mathbf{j}, \quad (6.8c)$$

where \mathbf{i} , \mathbf{j} and \mathbf{k} are the usual Cartesian unit vectors. Arguments have been advanced [85, 86] for accepting (6.8) even when \mathbf{q} is not perpendicular to \mathbf{k}_0 , as, for example, occurs for large angle scattering and forward inelastic scattering. In this case the z -axis is to be chosen to lie in the same plane as \mathbf{k}_0 and \mathbf{k}_f and to be perpendicular to \mathbf{q} . The amplitude (6.8), with this choice of z -axis, is the standard Glauber approximation studied here.

It is clear from the above derivation that the two main assumptions behind the Glauber approximation are:

- (i) all (important) atomic states $\psi_n(\mathbf{X})$ have the same energy, i.e., $H_a = \varepsilon_0$;
- (ii) forward scattering, i.e., $-i\nabla_0 \approx \mathbf{k}_0$.

The angular range in which the Glauber approximation is valid is a much more subtle question than

my derivation or bare statement (ii) would suggest [4, 86, and below]. Suffice it to say that (ii) is correct in the sense that one should not be surprised if the Glauber approximation gives poor results away from the forward scattering region.

The first assumption is really just the closure approximation of Massey and Mohr which was studied in section 4.2.1. In that section it was seen that the Massey-Mohr closure approximation gives an infinite second Born term for forward elastic scattering, one that diverges as $\ln q$. The same is true for f_{00}^G and for the same reason. Further, this result can be trivially extended to inelastic scattering when ψ_0 and ψ_f have the same total orbital angular momentum. Here, however, if $\varepsilon_0 \neq \varepsilon_f$, which is usually the case, the $\ln q$ divergence of f_{00}^G does not occur in the physical region where $q > 0$.

An interesting contrast is provided by the Glauber results for elastic scattering of electrons by H (1s) and K (4s) at 50 and 54.4 eV respectively, i.e., much the same energy. These are illustrated in fig. 16 where they are compared with experimental data. For H the Glauber cross section lies well below the experimental points, by a factor of 2 to 3. For K there is good agreement up to 20° with less good, although reasonable, accord out to 50°. For elastic scattering by Li (2s) and Na (3s) it is also found that the Glauber approximation (6.8) is good at forward angles [88, 89], while for He (1^1S) the situation is the same as that for H (1s) [44, 87].

The obvious difference between the alkali metals on the one hand and H (1s) and He (1^1S) on the other lies in atomic energy differences. Thus, for example, the energy separation between the 1s state of H and the first excited state is 0.375 a.u. (for He (1^1S) it is 0.75 a.u.). In K the first excited state is 4p which is a mere 0.06 a.u. above the ground state; furthermore the main coupling of the ground state is with the 4p level; the other alkalis, Li and Na, are similar. All of this points to assumption (i) as being the principal explanation behind the success of the Glauber approximation for the alkali metals and of its failure for H and He.

The above comparisons illustrate the point that in assessing the Glauber approximation it is important to be fair. It is unreasonable to expect the Glauber approximation to be satisfactory under circumstances where one or both of the main assumptions, (i) and (ii), are grossly violated. When the assumptions are respected reasonable results can be obtained.

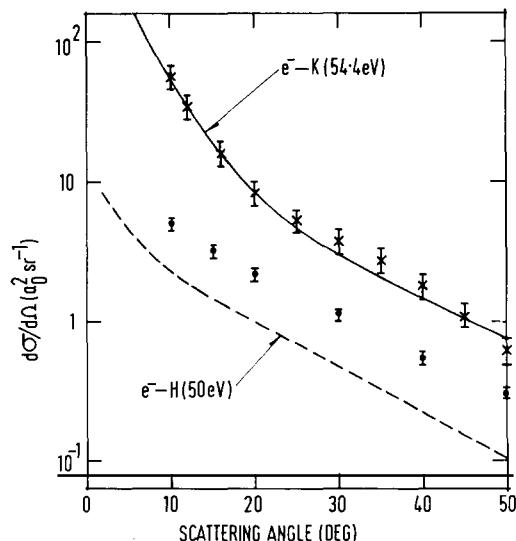


Fig. 16. Differential cross sections for elastic scattering of electrons by H (1s) at 50 eV and by K (4s) at 54.4 eV. The curves represent calculations in the Glauber approximation: (—) for H [50]; (—) for K (with core potential included) [13]. Experimental data: (●) for H [161], (x) for K [92].

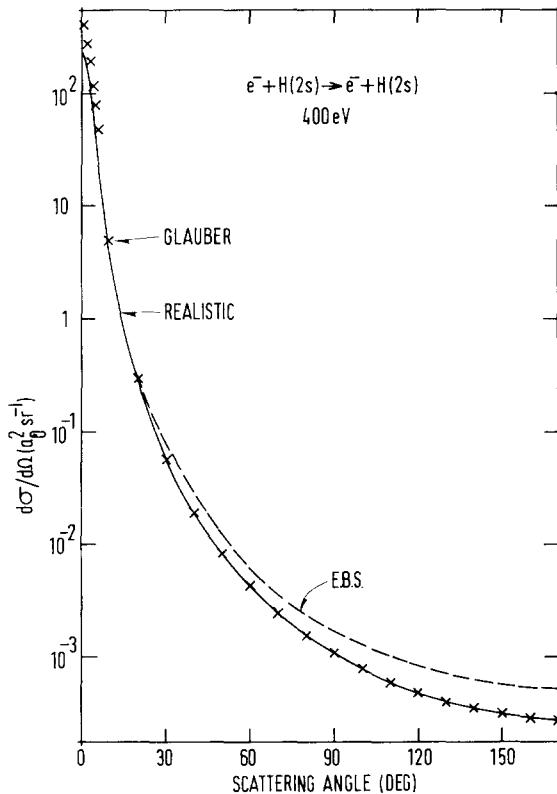


Fig. 17. Differential cross section for elastic scattering of electrons by H (2s) at 400 eV: (—) realistic estimate based upon the better approximations of [36, 118]; (---) EBS result [36]; (x) Glauber approximation [162].

There is one very important qualification of the above remarks which concerns assumption (ii). A very important property of the Glauber approximation is that it reproduces exactly the Coulomb scattering amplitude *at all angles* [85, 86]. Since large momentum transfer scattering is dominated by the e^\pm -nucleus interaction it follows that the Glauber approximation, at least for elastic scattering, will be good under these circumstances. This is illustrated in fig. 17 for elastic electron scattering by H (2s) at 400 eV. It is seen that for angles from about 10° right up to 180° the Glauber cross section is doing very well. This is a result of the dominance of the nuclear interaction at these angles – the 2s wavefunction is not very good at screening the nucleus.

Finally, it should be mentioned that the Glauber approximation predicts equal cross sections for electron and positron scattering. This is easily seen when ψ_0 and ψ_f are both S-states. In this case ψ_0 and ψ_f may both be chosen real; the effect of changing V to $-V$ in (6.8) is then merely to complex conjugate the amplitude without therefore affecting its modulus.

6.2. The eikonal-Born series

6.2.1. Born series analysis of the Glauber approximation

It is very instructive to make a Born series expansion of the Glauber amplitude (6.8), i.e., a series expansion in powers of V [44]. Then

$$f_{f0}^G = \sum_{n=1}^{\infty} f_{f0}^{Gn}, \quad (6.9a)$$

where

$$f_{f0}^{Gn} = \frac{1}{2\pi} \left(\frac{i}{k_0} \right)^{n-1} \frac{1}{n!} \int \exp(i\mathbf{q} \cdot \mathbf{b}_0) \psi_f^*(\mathbf{X}) [\chi_0(\mathbf{b}_0, \mathbf{X})]^n \psi_0(\mathbf{X}) d^2\mathbf{b}_0 d\mathbf{X}, \quad (6.9b)$$

$$\chi_0(\mathbf{b}_0, \mathbf{X}) \equiv - \int_{-\infty}^{+\infty} V(x_0, y_0, z_0, \mathbf{X}) dz_0. \quad (6.9c)$$

The term f_{f0}^{Gn} is of n th order in V . The series (6.9) is called the Glauber (or eikonal) series.

For the sake of simplicity I shall tacitly assume in this section, unless otherwise stated, that ψ_0 and ψ_f are S-states so that their wavefunctions may be taken to be purely real; the theory which follows is easily adapted to non-S-states [20]. When ψ_0 and ψ_f are S-states it can be seen from (2.2c) and (6.9) that the terms of the Glauber series are alternately real and imaginary:

$$f_{f0}^G = f_{f0}^{G1} + f_{f0}^{G2} + f_{f0}^{G3} + f_{f0}^{G4} + \dots, \quad (6.10)$$

the first, third and other odd terms are real; the second, fourth and other even terms are imaginary.

Let us now compare the series (6.10) with the proper Born series (3.3):

$$f_{f0} = f_{f0}^{B1} + f_{f0}^{B2} + f_{f0}^{B3} + f_{f0}^{B4} + \dots, \quad (6.11)$$

the first term is real, the other terms are complex. The first thing to note is that f_{f0}^{G1} is identically equal to f_{f0}^{B1} , remember that \mathbf{q} is perpendicular to the z -direction so $\mathbf{q} \cdot \mathbf{b}_0 = \mathbf{q} \cdot \mathbf{r}_0$ in (6.9b). Here the resemblance between (6.10) and (6.11) stops, for, unlike (6.10), the higher terms in the Born series do not alternate between real and imaginary values, they are, in general, complex.

Let us look at the second term in both series. In section 4.1 it was seen that the second Born term f_{f0}^{B2} contains some very important physics. In particular, for elastic scattering f_{00}^{B2} contains the dipole polarizability of the state ψ_0 and also allowance for flux loss from the elastic channel. The former appears in $\text{Re } f_{00}^{B2}$ while flux loss is represented in $\text{Im } f_{00}^{B2}$. Since f_{00}^{G2} is pure imaginary the dipole polarizability is missing from the Glauber approximation but flux loss is retained.

Previously it was indicated that f_{00}^G is infinite for forward scattering and this infinity was connected with the Massey–Mohr closure approximation (section 4.2.1). In the Massey–Mohr closure approximation to the second Born term f_{00}^{B2} the infinity arises in $\text{Im } f_{00}^{B2}$, as shown in section 4.2.1. It is therefore not surprising to find that the infinity in f_{00}^G is associated with, and only with, f_{00}^{G2} [2, 44, 90, 91]. The same is true for those inelastic transitions (i.e. ψ_0 and ψ_f both have the same total orbital angular momentum) where f_{f0}^G possesses a $\ln q$ divergence at (usually unphysical) $q = 0$.

I hope that by now the reader will be beginning to see the importance of the second Born term f_{f0}^{B2} in e^\pm –atom scattering – some very important physics is contained in it. It is time, therefore, to enunciate another important principle, namely, that any good approximation to the scattering amplitude when expanded in powers of V , i.e., Born series analyzed, should contain in second order a good representation of f_{f0}^{B2} . How well the Glauber approximation performs depends very much, although not entirely, upon how well f_{f0}^{G2} represents f_{f0}^{B2} . Let us look at some examples.

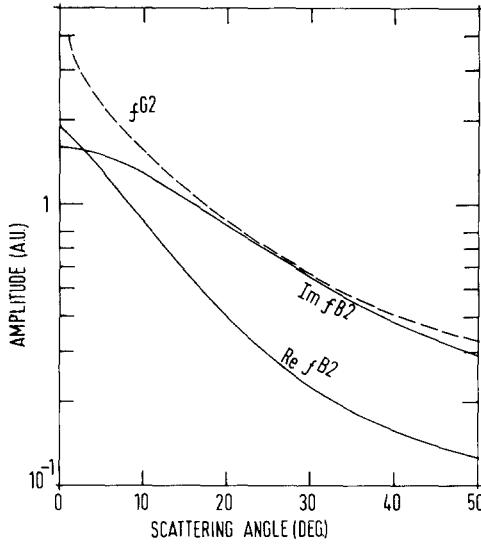


Fig. 18. Second-order Born and Glauber terms for electron-H (1s) elastic scattering at 50 eV. Curves: (—) second Born term f_{00}^{B2} (calculated in the closure approximation of [32]); (---) Glauber term f_{00}^{G2} (this is pure imaginary).

(a) *Electron-H (1s) elastic scattering.* In fig. 18 f_{00}^{B2} is illustrated for scattering at 50 eV. Also shown is f_{00}^{G2} . Except at small momentum transfers, where it diverges as $\ln q$, f_{00}^{G2} is in fairly good agreement with $i \operatorname{Im} f_{00}^{B2}$. However, $\operatorname{Re} f_{00}^{B2}$ is comparable with $\operatorname{Im} f_{00}^{B2}$ at the angles of fig. 18 – it is this, and the omission of exchange which also further enhances the real part of the scattering amplitude, which lies behind the pronounced failure of the Glauber approximation for H (1s) seen in fig. 16.

(b) *Electron-K (4s) elastic scattering.* Since K is a large atom f_{00}^{B2} will be dominated by $f_{00}^{B2;0}$, however, this term will be cut down to size, through unitarity, by cancellation with higher terms in the Born series. What is really important in f_{00}^{B2} for K, at least as far as the forward peak is concerned, is the contribution of intermediate states (primarily 4p) other than 4s, i.e.,

$$\tilde{f}_{00}^{B2} = \sum_{n \neq 0} f_{00}^{B2; n}. \quad (6.12)$$

There are no proper calculations of \tilde{f}_{00}^{B2} for K. However, there is little doubt [88, 89, 92] that \tilde{f}_{00}^{B2} is predominantly imaginary at all but the lowest energies. Now, in fig. 18 it was seen that f_{00}^{G2} can give a good approximation to $i \operatorname{Im} f_{00}^{B2}$ (indeed below it will be argued that this is generally true for S-S transitions). If the same is true for $i \operatorname{Im} \tilde{f}_{00}^{B2}$ and \tilde{f}_{00}^{G2} for K then the Glauber amplitude should contain a good representation of \tilde{f}_{00}^{B2} . This, coupled with the fact that electron exchange is not very significant in the overall scattering amplitude [88, 89] “explains” the agreement between theory and experiment in fig. 16.

The pronounced dominance of the imaginary part of \tilde{f}_{00}^{B2} is connected with atomic energy differences, the smaller and energy differences the more dominant is the imaginary part (after all for zero energy difference the Massey-Mohr closure approximation is exact and $\operatorname{Im} f_{00}^{B2}$ is infinite at the forward direction). Here then is the contact with assumption (i) of the Glauber approximation.

For electron scattering by alkali atoms at energies below the first excitation threshold the very large

dipole polarizability, α_{00} , of the alkali plays an extremely important part. Here \tilde{f}_{00}^{B2} is purely real (recall that α_{00} appears in $\text{Re } \tilde{f}_{00}^{B2}$, section 4.1.1). With increasing energy beyond the first excitation threshold the real part of \tilde{f}_{00}^{B2} rapidly declines while the imaginary part grows, becoming ultimately dominant. This reflects a change-over from a situation where polarization is dominant to one in which flux loss has the upper hand. Calculations which ignore this change run rapidly and disastrously into trouble [30]. The alkali metals provide a stark example of the importance of treating second-order effects in a dynamical way, through f_{00}^{B2} , rather than in an adiabatic way through (4.7) (or an equivalent) [30].

(c) $e^- + He (1^1S) \rightarrow e^- + He (2^1S)$. In fig. 19 the Glauber approximation for the 2^1S excitation of He (1^1S) at 200 eV is compared with experimental data. Agreement between theory and experiment at angles up to about 30° is quite good, although beyond 30° the Glauber cross section appears to be too small. Unfortunately no values of $f_{2s, 1s}^{B2}$ and $f_{2s, 1s}^{G2}$ have been published for He, but they are available for the analogous transition, $1s \rightarrow 2s$, in H; these numbers for H are shown in fig. 9, also at an impact energy of 200 eV. It is seen that $\text{Im } f_{2s, 1s}^{B2}$ is very much larger (by a factor of about 10) than $\text{Re } f_{2s, 1s}^{B2}$ at most angles, and that $f_{2s, 1s}^{G2}$ is quite close to $i \text{Im } f_{2s, 1s}^{B2}$; in other words $f_{2s, 1s}^{G2}$ is a good representation of $f_{2s, 1s}^{B2}$. The same is almost certainly true for the He transition in fig. 19 and therefore "explains" the measure of agreement that is obtained.

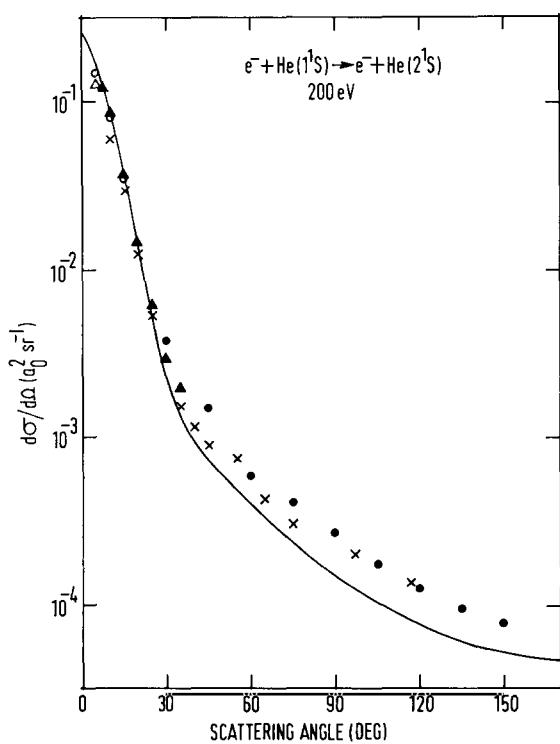


Fig. 19. Differential cross section for $e^- + He (1^1S) \rightarrow e^- + He (2^1S)$ at 200 eV. The curve is the Glauber cross section of [96]. Experimental data [163]: (▲) Dillon and Lassettre; (×) Suzuki and Takayanagi; (●) Opal and Beaty; (○) Vriens et al.; (Δ) Chamberlain et al.

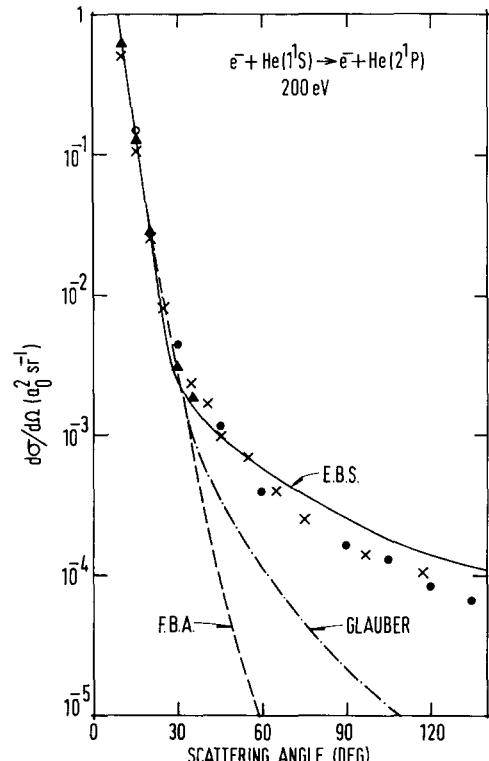


Fig. 20. Differential cross section for $e^- + He (1^1S) \rightarrow e^- + He (2^1P)$ at 200 eV. Curves [47]: (—) EBS approximation; (— · —) Glauber approximation; (— - -) first Born approximation. Experimental data [163]: (▲) Dillon and Lassettre; (×) Suzuki and Takayanagi; (●) Opal and Beaty; (○) Vriens et al. (Taken from Joachain and Winters [47], fig. 1a.)

Previously assumption (i) was used to explain failure of the Glauber approximation in electron-He (1^1S) elastic scattering. For elastic scattering this was indeed correct, however, assumption (i) is equally invalid for the $1^1S \rightarrow 2^1S$ excitation, yet the Glauber approximation works here. The fact is that assumptions (i) and (ii) are sufficient but not necessary conditions for the Glauber approximation to succeed; the effect of the assumptions depends very much upon the scattering process being considered.

(d) $e^- + He (1^1S) \rightarrow e^- + He (2^1P)$. In fig. 20 the FBA, Glauber and experimental cross sections for the 2^1P excitation are shown at an energy of 200 eV. Since this excitation is optically allowed it is not surprising to see that all three are in agreement at small angles. At large angles the FBA is poor as expected (section 3.1(i)), but the Glauber approximation is also very bad, much worse than in the 2^1S case of fig. 19! It was seen in section 4.1.2 that the second Born term f_{f0}^{B2} gives the leading behaviour for large momentum transfer inelastic scattering. The pronounced failure of the Glauber approximation in fig. 20 results from the fact that* $f_{2^1P_m, 1^1S}^{G2}$ is not a good representation of $f_{2^1P_m, 1^1S}^{B2}$ for large momentum transfers.

With the usual conventions and with the omission of an unimportant azimuthal phase factor the eikonal series (6.9a) for 2^1P excitation still alternates real and imaginary values, but starts off with a pure imaginary term, i.e., $f_{2^1P_m, 1^1S}^{G1}$; the second term, $f_{2^1P_m, 1^1S}^{G2}$, is therefore purely real. It is found [20] that for large momentum transfers $\text{Im } f_{2^1P_m, 1^1S}^{B2}$ dominates $\text{Re } f_{2^1P_m, 1^1S}^{B2}$ so that the purely real second-order Glauber term, $f_{2^1P_m, 1^1S}^{G2}$, cannot give the leading behaviour of the large momentum transfer scattering amplitude – hence the failure. The same is true for the $1s \rightarrow 2p$ excitation of H [20].

The situations in figs. 19 and 20 should be contrasted. Although the Glauber approximation is not good for the large angle 2^1S excitation, it is very much worse in the 2^1P case. For 2^1S we saw that f^{G2} was a good representation of f^{B2} at nearly all angles, for 2^1P it is an extremely poor representation at large momentum transfers.

The agreement between $i \text{Im } f_{f0}^{B2}$ and f_{f0}^{G2} seen in figs. 9 and 18 is thought to be part of a much wider measure of accord between the eikonal and Born series (6.10) and (6.11) for $S \rightarrow S$ transitions. Thus it is conjectured that

$$f_{f0}^{Gn} \approx \text{Re } f_{f0}^{Bn}, \quad n \text{ odd}, \quad (6.13a)$$

$$f_{f0}^{Gn} \approx i \text{Im } f_{f0}^{Bn}, \quad n \text{ even}, \quad (6.13b)$$

are fairly good approximations. If this is so then the Glauber approximation gives fairly accurate information on half of the Born series. The relations (6.13) were first brought to light in a study of scattering by Yukawa potentials [4, 93, 94] where it was shown that they are exact for all q at asymptotically large k_0 – this is the so-called “all angle property” of the eikonal series.

However, the results (6.13) do not seem to generalize to $S \rightarrow P$ transitions, as has been remarked in the case of $\text{He} (1^1S) \rightarrow \text{He} (2^1P)$. Nevertheless, there is still some measure of agreement between f^{B2} and f^{G2} at least at small angles; the reader is referred to [20] for details.

6.2.2. High energy behaviour of Born and Glauber terms

Byron and Joachain [50, 95, 96] have analyzed the leading behaviour (in k_0) of the terms of the Glauber and Born series (6.10) and (6.11) for e^\pm scattering off the ground states of H and He. Their results, which apply only to $S \rightarrow S$ transitions, are summarized in table 4. The behaviour obtained

* m labels the magnetic substates, i.e., $m = 0, \pm 1$.

Table 4

Leading behaviour in k_0 of the terms f_{f0}^{Bn} and f_{f0}^{Gn} of the Born and Glauber series (6.11) and (6.10) respectively. It is assumed that ψ_0 and ψ_f are S-states. For large q the results quoted are to leading order in k_0 , q and $\ln q$

Term	Elastic and inelastic scattering		Elastic scattering, $\psi_0 = \psi_f$	Inelastic scattering, $\psi_0 \neq \psi_f$
	Small q ($q < k_0^{-1}$)	Intermediate q ($k_0^{-1} < q < 1$)	Large q ($q > k_0$)	Large q ($q > k_0$)
$f^{B1} = f^{G1}$	1	1	q^{-2}	q^{-6}
$\text{Re } f^{B2}$	k_0^{-1}	k_0^{-2}	$k_0^{-2}q^{-2}$	$k_0^{-2}q^{-2}$
$\text{Re } f^{G2}$	0	0	0	0
$\text{Im } f^{B2}$	$k_0^{-1}\ln k_0$	k_0^{-1}	$k_0^{-1}q^{-2}\ln q$	$k_0^{-1}q^{-2}$
$\text{Im } f^{G2}$	$k_0^{-1}\ln q$	k_0^{-1}	$k_0^{-1}q^{-2}\ln q$	$k_0^{-1}q^{-2}$
$\text{Re } f^{B3}$	k_0^{-2}	k_0^{-2}	$k_0^{-2}q^{-2}\ln^2 q$	$k_0^{-2}q^{-2}\ln q$
$\text{Re } f^{G3}$	k_0^{-2}	k_0^{-2}	$k_0^{-2}q^{-2}\ln^2 q$	$k_0^{-2}q^{-2}\ln q$
$\text{Im } f^{B3}$	k_0^{-3}	k_0^{-3}	$k_0^{-3}q^{-2}\ln q$	$k_0^{-3}q^{-2}$
$\text{Im } f^{G3}$	0	0	0	0
f^{Bn}	$(ik_0)^{1-n}$	$(ik_0)^{1-n}$	$(ik_0)^{1-n}q^{-2}\ln^{n-1} q$	$(ik_0)^{1-n}q^{-2}\ln^{n-2} q$
f^{Gn} $n \geq 4$	$(ik_0)^{1-n}$	$(ik_0)^{1-n}$	$(ik_0)^{1-n}q^{-2}\ln^{n-1} q$	$(ik_0)^{1-n}q^{-2}\ln^{n-2} q$

depends upon whether the momentum transfer q is small ($q < k_0^{-1}$), of intermediate size ($k_0^{-1} < q < 1$), or large ($q > k_0$). Some points worth noting are the following.

(i) For elastic scattering f^{B1} is the dominant term for all q . However, for inelastic scattering f^{B2} is dominant at large q ; this is because, as previously remarked (section 3.1(i)), f^{B1} does not contain the e^\pm -nucleus interaction for inelastic scattering; f^{B2} is the first term in the Born series to contain this interaction for inelastic scattering.

(ii) The q^{-2} behaviour and the $\ln q$ factors which appear at large q are signatures of the e^\pm -nucleus interaction (see (3.13)).

(iii) Note that because of the $\ln q$ factors perturbation theory converges more slowly at large q than at small and intermediate q , i.e., the singular nature of the e^\pm -nucleus interaction slows the convergence of perturbation theory (section 3.2).

(iv) Except for f^{B2} , the Born terms f^{Bn} have the same behaviour at small and intermediate q . This “anomalous” behaviour of f^{B2} at small q is associated with the intermediate P-states.

(v) The Glauber terms f^{Gn} give in each order the leading piece of f^{Bn} at all q . The only exception is in second order at small q where f^{G2} diverges as $\ln q$ as $q \rightarrow 0$. As pointed out earlier this divergence is associated with the Massey-Mohr closure approximation, i.e. $H_a = \epsilon_0$, and arises from the intermediate P-states (section 4.2.1). Note that the infinity in the Glauber amplitude at $q = 0$ comes only from the second-order term.

6.2.3. The eikonal-Born series approximation (EBS)

It is clear from table 4 that the sum of the three terms

$$f_{f0}^{B1} + f_{f0}^{B2} + \text{Re } f_{f0}^{B3} \quad (6.14)$$

gives the scattering amplitude for S → S transitions correct through order k_0^{-2} . Now, f_{f0}^{B2} is difficult to calculate (sections 4.2, 4.3) but $\text{Re } f_{f0}^{B3}$ will be much worse. However, in (6.13), we saw, also for S → S transitions, that $\text{Re } f_{f0}^{B3}$ is probably well approximated by f_{f0}^{G3} ; indeed, from table 4, f_{f0}^{G3} gives the leading piece, of order k_0^{-2} , of $\text{Re } f_{f0}^{B3}$; f_{f0}^{G3} is not too difficult to evaluate. On the above reasoning Byron and Joachain [44] have suggested the practical approximation

$$f_{f0}^{\text{EBS}} = f_{f0}^{B1} + f_{f0}^{B2} + f_{f0}^{G3} \quad (6.15)$$

(6.15) is known as the eikonal-Born series approximation (EBS).

The virtue of (6.15) compared with the ordinary second Born approximation (3.9) is that it is correct to a higher order in k_0^{-1} , see table 4. Compared with the Glauber approximation (6.8) the advantage of (6.15) is that it contains the full second Born term f_{f0}^{B2} . Because f_{f0}^{G2} is pure imaginary it is clear from table 4 that the Glauber amplitude is not even correct to order k_0^{-1} .

For electron scattering the direct amplitude (6.15) should be combined with an exchange term. Since (6.15) is correct through order k_0^{-2} it is necessary, for consistency, to require that the exchange amplitude also be correct to this order. A good enough exchange amplitude is provided in first order by the Ochkur approximation [5, 97] (see section 8.2).

In fig. 21 the EBS cross section, calculated from (6.15) and including exchange through the Ochkur approximation, is compared with the accurate experimental data of Bromberg [15] and the ordinary

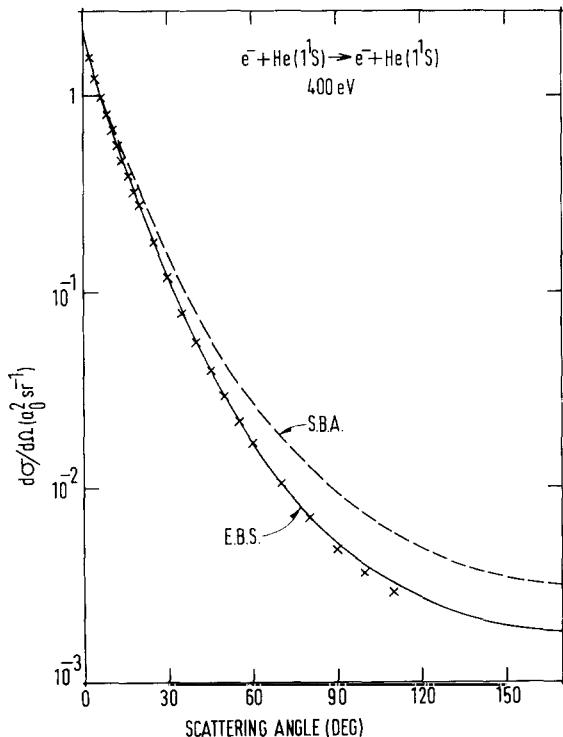


Fig. 21. Differential cross section for elastic scattering of electrons by He(1S) at 400 eV. Curves: (—) EBS approximation [50]; (---) second Born approximation (3.10) (the FSSB1 numbers of [42]). Experimental data: (x) Bromberg [15].

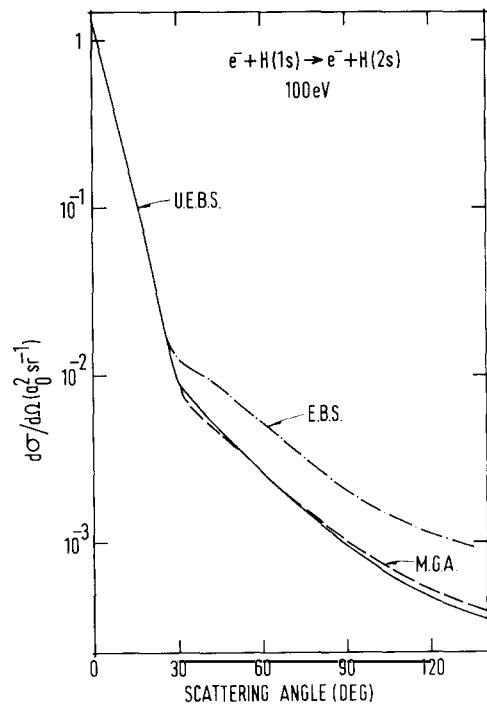


Fig. 22. Differential cross section for $e^- + H(1s) \rightarrow e^- + H(2s)$ at 100 eV. Theoretical curves: (—) Unitarized eikonal Born Series (UEBS); (---) Modified Glauber Approximation (MGA); (—·—) eikonal Born Series (EBS). (Taken from Byron et al. [98], fig. 2.)

second Born approximation (3.10) for electron-He (1^1S) elastic scattering at 400 eV. Agreement between the EBS and experiment is very good. As seen previously, fig. 3, the second Born cross section is in quite good agreement with experiment at small angles but is much too big at large angles. It is also interesting to note that the EBS cross section at 500 eV is indistinguishable from the DWSBA cross section on the scale of fig. 10, i.e., both theories agree closely with each other and with the experimental data at this energy.

The EBS approximation (6.15) may be viewed as a form of third Born approximation. What fig. 21 shows is that perturbation theory is more slowly convergent at large momentum transfers (i.e. large angles) than at small momentum transfers: while second-order perturbation theory is acceptable at small angles, large angles require at least third order, i.e., EBS – this is a measure of the difficulty perturbation theory has in handling the singular electron-nucleus interaction (section 3.2).

A beautiful example of the failure of even third-order perturbation theory, i.e., EBS, for large momentum transfer scattering is provided in fig. 17 for electron-H (2s) elastic scattering at 400 eV. Here it is seen that the EBS cross section is too large beyond about 20° ; by 180° it is a factor of two too big. The effect of the electron-nucleus interaction in electron-H (2s) scattering is more pronounced than in electron-H (1s) or electron-He (1^1S) collisions since the 2s wavefunction does not screen the nucleus as well as the 1s function. This result emphasises the correctness of the diagnosis given in section 3.2 and of the approach adopted in section 5, namely, that the e^\pm -nucleus interaction is a, if not the, primary cause of trouble for perturbation theory and that it would be best if this interaction could be treated non-perturbatively.

The failure pattern of the EBS cross section in fig. 17 is to become too big at large momentum transfers. In section 6.5 the same failure pattern for elastic scattering will be seen again. Indeed, even in fig. 21 it is noticeable that the EBS cross section starts to exceed the experimental data at angles beyond 80° .

Let us now consider inelastic $S \rightarrow S$ transitions. Although there are several EBS-type calculations on the $1s \rightarrow 2s$ excitation of H and the $1^1S \rightarrow 2^1S$ excitation of He there is only one published cross section using the pure EBS approximation (6.15). This cross section is shown in fig. 22; it relates to the electron impact excitation of the $1s \rightarrow 2s$ transition in H at 100 eV. Exchange has been included in this calculation. Also shown in the figure are the more accurate MGA and UEBS cross sections (see sections 6.3 and 6.4). At small angles the EBS cross section agrees well with the more accurate results but at large angles, above about 25° , it is much too large – once more third-order perturbation theory, in the form of the EBS amplitude, is not working at large angles.

This is perhaps not surprising in view of what has been seen in the case of elastic scattering. The EBS amplitude (6.15) can only take account of elastic scattering within the initial 1s and final 2s-states partially to *second order* (it would be fully to second order if (6.15) included $\text{Im } f_{f0}^{B3}$). Since this elastic scattering is important for large momentum transfer inelastic collisions (section 4.1.2) and since second-order perturbation theory works so badly for large momentum transfer elastic scattering, see figs. 3 and 21, the large angle failure of the EBS cross section of fig. 22 is understandable.

The demise of the large angle EBS inelastic cross section may be looked at another way. From table 4 we see that for fixed large angle the leading (in k_0) contribution to the inelastic scattering amplitude comes from $\text{Im } f^{B2}$; this term varies as $k_0^{-1}q^{-2}$ (remember that for fixed non-zero angle $q \propto k_0$, (2.15) (2.10)). The Glauber term f^{G3} which varies as $k_0^{-2}q^{-2}\ln q$ corrects this leading term essentially to order k_0^{-1} ; f^{B1} which varies as q^{-6} can be ignored. Thus although the EBS amplitude (6.15) is correct to *relative* order k_0^{-2} at *fixed* q , it is correct only to *relative* order k_0^{-1} at *fixed angle*. To get a fixed angle cross section correct to *relative* order k_0^{-2} one needs to go as far as f^{B4} (table 4). For elastic scattering

this argument does not go through since $f^{B1} \propto q^{-2}$; (6.15) is then correct to relative order k_0^{-2} at both fixed q and fixed angle. This reasoning suggests that the EBS large angle inelastic cross section will be of lower quality than that for elastic scattering. Note that going to fourth order in the Born series would be equivalent to treating elastic scattering in the 1s and 2s states correct to third order.

Byron and Latour [20] who first applied the EBS approximation to inelastic scattering realized that the amplitude (6.15) was defective for large angle collisions. They tried to patch up the $1s \rightarrow 2s$ differential cross sections by including a term in $\text{Im } f^{B4}$. Byron and Joachain [96] forsook the simple EBS approximation (6.15) for the more sophisticated EBS' approximation (section 6.3) for the $1^1S \rightarrow 2^1S$ excitation of He. A yet more complicated approximation, the unitarized EBS approximation (section 6.5), has recently been used by Byron et al. [98] on the $1s \rightarrow 2s$ transition in H.

So far I have just considered S \rightarrow S inelastic transitions. The only other inelastic transitions which have been studied by the EBS method are of the S \rightarrow P type [20, 47]. The EBS approximation for the S \rightarrow P case is open to the same criticisms which apply to S \rightarrow S but there is one further important problem.

Firstly, it should be noted that with the usual phase conventions* for S \rightarrow P transitions f^{B1} ($= f^{G1}$) and f^{G3} are pure imaginary. The analogue of (6.14) is then

$$f_{f0}^{B1} + f_{f0}^{B2} + i \text{Im } f_{f0}^{B3}, \quad (6.16)$$

where the EBS amplitude is still given by (6.15). The problem centres upon whether the EBS replacement $i \text{Im } f_{f0}^{B3} \rightarrow f_{f0}^{G3}$ is a good one in the S \rightarrow P case. Evidence that this may not be so is provided in second order where it is found that, unlike the S \rightarrow S case, f_{f0}^{G2} does not generally give a good representation of $\text{Re } f_{f0}^{B2}$ [20]. In other words the property (6.13) does not go over very well to the S \rightarrow P case – this makes the replacement $i \text{Im } f_{f0}^{B3} \rightarrow f_{f0}^{G3}$ doubtful.

Nevertheless, calculations using (6.15) have been carried out for electron impact excitation of the $1s \rightarrow 2p$ and $1^1S \rightarrow 2^1P$ transitions in H and He respectively, exchange being included via the Ochkur approximation [20, 47]. A good measure of agreement is obtained with available experimental data, although doubts have been cast upon the situation in hydrogen [32]. The $1^1S \rightarrow 2^1P$ EBS cross section for He at 200 eV is shown in fig. 20, where it is seen that the EBS cross section is a big improvement upon the ordinary Glauber approximation, the reasons for this have already been discussed in section 6.2.1(d) above.

Finally, since the EBS approximation (6.15) is essentially just a form of third Born approximation, it will be unsuitable for the heavier atoms where the appearance of large first Born elastic matrix elements (section 3.1(iii)) in the second- and third-order terms for inelastic scattering, and also in the first-order term for elastic scattering, will cause the EBS amplitude to grow uncontrollably in magnitude as the size of the atom is increased. Combining this result with the large angle problems of the EBS approximation mentioned previously, it is to be concluded that the EBS method is really suitable only for e $^\pm$ scattering by light atoms at not too large angles.

6.3. The modified Glauber approximation (MGA) (or EBS' approximation)

In section 6.2.1 I enunciated the principle that any good approximation should contain a realistic representation of the second Born term f_{f0}^{B2} . I then went on to analyze the successes and failures of the

* See section 6.2.1(d) above.

Glauber approximation f_{f0}^G , on the basis of how well its second order term, f_{f0}^{G2} , reproduced f_{f0}^{B2} . There is, however, a simple way in which the defects of the Glauber approximation in second order can be removed, i.e.,

$$f_{f0}^{MG} = f_{f0}^G + f_{f0}^{B2} - f_{f0}^{G2}. \quad (6.17)$$

The amplitude (6.17) is known as the modified Glauber approximation (MGA).

Byron and Joachain [96] were the first to suggest the approximation (6.17); they were, however, followed closely by Gien [99]. Preferring to regard (6.17) as an extension of the eikonal-Born series (EBS) method (section 6.2.3), Byron and Joachain refer to (6.17) as the EBS' approximation.

Expanded in powers of V , the amplitude f_{f0}^{MG} has the structure

$$f_{f0}^{MG} = f_{f0}^{B1} + f_{f0}^{B2} + f_{f0}^{G3} + \sum_{n=4}^{\infty} f_{f0}^{Gn}. \quad (6.18)$$

The first three terms in (6.18) are recognized as the EBS approximation (6.15). In (6.18) the EBS amplitude is extended to infinite order by the addition of Born terms of orders $n \geq 4$ calculated in the Glauber approximation. In this way (6.18) incorporates the successful features of the EBS method and, *perhaps*, largely eliminates one of its main defects, i.e., being of too low an order in the Born series for large momentum transfer scattering – of course, the success of the extra terms in (6.18) depends upon how well $\sum_{n=3}^{\infty} f_{f0}^{Gn}$ approximates $\sum_{n=3}^{\infty} f_{f0}^{Bn}$.

The MGA and EBS cross sections (including exchange) for the $1s \rightarrow 2s$ electron impact excitation of H at 100 eV have already been compared in fig. 22. It is clear from (6.18) that the difference between these cross sections reflects the importance of terms of order greater than 3 in the Born series. The conclusion to be drawn from fig. 22 is that such terms are unimportant at small angles but very significant at large angles. The same conclusion results from a study of elastic electron scattering by He (1^1S) [100].

For positron scattering [50, 101] the difference between the MGA and EBS cross sections is more significant than in the case of electron scattering, i.e. higher order ($n \geq 4$) terms are more important for positron scattering than electron scattering. Further, experimental data on the positron-He (1^1S) total cross section clearly prefer the MGA to the EBS approximation.

That the MGA (6.17) rectifies the most serious defects of the ordinary Glauber approximation is shown very clearly in the papers of Gien [99–102]. This rectification takes place at both small and large angles which indicates, as emphasized by Gien, that correcting the Glauber approximation in second order relaxes both of the main assumptions of the Glauber method, i.e., all atomic states have equal energies ε_0 and scattering is mainly in the forward direction (i) and (ii) of section 6.1).

One criticism of Gien's calculations is his use of a rather drastic closure approximation in evaluating f_{f0}^{B2} . Usually he uses the Massey-Mohr closure approximation (4.20), although with $\bar{\varepsilon} \neq \varepsilon_0$. Amongst other things, see [98], this leads to the undesirable feature that when ψ_0 and ψ_f appear as intermediate states in f_{f0}^{B2} they are assigned a different energy, i.e. $\bar{\varepsilon}$, than elsewhere in the calculation (see section 4.2.1). An interesting feature of his papers is the use, in many cases, of the Glauber approximation for the exchange amplitude in electron scattering.

To summarize. The MGA shows the importance of including higher terms ($n \geq 4$) in the Born series for large momentum transfer electron-atom scattering and also, more generally, for positron scattering.

In this respect the MGA is to be preferred to the EBS approximation. The importance of these higher terms, I would suggest, derives mainly from the singular e^\pm –nucleus interaction, a theme which I have emphasized over and over again in this review. The MGA is a very substantial improvement upon the ordinary Glauber approximation; thus correcting the Glauber approximation in second order eliminates many of its serious defects [99].

6.4. The (first-order) Wallace approximation

Some time ago Wallace suggested a way of systematically improving upon the Glauber approximation for potential scattering [103–105]. His ideas are readily generalized to scattering by composite particles if a “frozen” target approximation is made [28, 98, 104–107]. This latter is none other than the approximation $H_a = \varepsilon_0$ of the Glauber method (see section 6.1), or, in other words, the Massey–Mohr closure approximation (section 4.2). The frozen target nature of the Glauber amplitude is easily perceived. Thus, see (6.8),

$$\frac{ik_0}{2\pi} \int d^2 b_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \left\{ 1 - \exp \left[-\frac{i}{k_0} \int_{-\infty}^{+\infty} V(x_0, y_0, z_0, \mathbf{X}) dz_0 \right] \right\} \quad (6.19)$$

is the Glauber amplitude for scattering by the target atom when its electrons are frozen at the positions \mathbf{X} ; the Glauber approximation (6.8) is obtained by averaging (6.19) over the configurations \mathbf{X} using the weight function $\psi_f^*(\mathbf{X})\psi_0(\mathbf{X})$.

The (first-order) Wallace approximation for e^\pm –atom scattering is given by [28]

$$f_{f0}^W = \frac{ik_0}{2\pi} \int d^2 b_0 d\mathbf{X} \exp(i\mathbf{q} \cdot \mathbf{b}_0) \psi_f^*(\mathbf{X}) \left\{ 1 - \exp \left[i \left(\frac{1}{k_0} \chi_0(\mathbf{b}_0, \mathbf{X}) + \frac{1}{k_0^3} \chi_1(\mathbf{b}_0, \mathbf{X}) \right) \right] \right\} \psi_0(\mathbf{X}), \quad (6.20a)$$

where

$$\chi_0(\mathbf{b}_0, \mathbf{X}) \equiv - \int_{-\infty}^{+\infty} V(x_0, y_0, z_0, \mathbf{X}) dz_0, \quad (6.20b)$$

$$\chi_1(\mathbf{b}_0, \mathbf{X}) \equiv \frac{1}{2} \int_{-\infty}^{+\infty} (\nabla_0 \chi_+) \cdot (\nabla_0 \chi_-) dz_0, \quad (6.20c)$$

$$\chi_+(\mathbf{b}_0, z_0, \mathbf{X}) \equiv - \int_{-\infty}^{z_0} V(x_0, y_0, z'_0, \mathbf{X}) dz'_0, \quad (6.20d)$$

$$\chi_-(\mathbf{b}_0, z_0, \mathbf{X}) \equiv - \int_{z_0}^{\infty} V(x_0, y_0, z'_0, \mathbf{X}) dz'_0, \quad (6.20e)$$

$$\nabla_0 \equiv \mathbf{i} \frac{\partial}{\partial x_0} + \mathbf{j} \frac{\partial}{\partial y_0} + \mathbf{k} \frac{\partial}{\partial z_0}. \quad (6.20f)$$

The notation and conventions of (6.20) are the same as in the Glauber approximation (6.8); in particular, the z -axis is to be taken perpendicular to \mathbf{q} .

Comparing (6.20) with the Glauber approximation (6.8) it is easy to recognize the same basic structure. The Wallace approximation (6.20) amounts to a correction of the Glauber phase χ_0 by a term of relative order k_0^{-2} , i.e. χ_1/k_0^3 ; this is the leading (in powers of k_0) correction to the Glauber phase. The Wallace approximation partially relaxes the forward scattering assumption (ii) (section 6.1) of the Glauber approximation; however, it still retains the zero excitation energy assumption (i) – as a result f_{f0}^W still exhibits the unsatisfactory $\ln q$ divergence, as $q \rightarrow 0$, of the Glauber approximation and also still lacks polarization (setting $\varepsilon_n = \varepsilon_0$ in (4.12) and (4.15) makes the polarization term zero).

Following section 6.2.1 it is interesting to make a Born series analysis of the Wallace amplitude (6.20). Remembering that χ_0 is of first order in V while χ_1 is of second order, it is found that

$$f_{f0}^W = \sum_{n=1}^{\infty} f_{f0}^{Wn}, \quad (6.21)$$

where

$$f_{f0}^{W1} = f_{f0}^{B1}, \quad (6.22a)$$

and, for $n \geq 2$,

$$\begin{aligned} f_{f0}^{Wn} &= \frac{1}{2\pi} \left(\frac{i}{k_0} \right)^{n-1} \frac{1}{n!} \int \exp(i\mathbf{q} \cdot \mathbf{b}_0) \psi_f^*(\mathbf{X}) \\ &\times \{ \chi_0^n(\mathbf{b}_0, \mathbf{X}) - n(n-1) \frac{i}{k_0} \chi_0^{n-2}(\mathbf{b}_0, \mathbf{X}) \chi_1(\mathbf{b}_0, \mathbf{X}) + \text{terms containing higher powers of } \chi_1 \\ &\text{if } n \geq 4 \} \psi_0(\mathbf{X}) d^2\mathbf{b}_0 d\mathbf{X}. \end{aligned} \quad (6.22b)$$

Note that the first-order term is just the first Born amplitude.

Let us now examine the higher-order terms in (6.21). For simplicity I shall assume that ψ_0 and ψ_f are both S-states and therefore real. A close comparison between (6.22b) and (6.9b) reveals that

$$\text{Im } f_{f0}^{W2} = \text{Im } f_{f0}^{G2}, \quad (6.23a)$$

$$\text{Re } f_{f0}^{W3} = \text{Re } f_{f0}^{G3}. \quad (6.23b)$$

As in the Glauber approximation (section 6.2.1) the $\ln q$ divergence of f_{f0}^W for small q comes from $\text{Im } f_{f0}^{W2}$. However, unlike the Glauber approximation, $\text{Re } f_{f0}^{W2}$ and $\text{Im } f_{f0}^{W3}$ are non-zero. On the basis of studies in potential scattering [94, 104, 108] these latter are expected to give the leading (in k_0) parts of $\text{Re } f_{f0}^{B2}$ and $\text{Im } f_{f0}^{B3}$ calculated in the closure approximation (since (6.20) is derived using $H_a = \varepsilon_0$). Byron et al. [28] explicitly demonstrate that this is so for $\text{Re } f_{f0}^{W2}$ in elastic $e^\pm-H$ (1s) scattering.

For $n \geq 4$ the integrand in (6.22b) contains higher powers of χ_1 than the first. As $b_0 \rightarrow 0$ the phase χ_1

is singular in such a way that the integrals over b_0 for $n \geq 4$ are divergent, i.e., f_{f0}^{Wn} ($n \geq 4$) is not defined, or, in other words, the Born series expansion (6.21) of the Wallace amplitude does not exist! Since χ_1 appears in a phase factor the full Wallace amplitude (6.20) is, however, all right. The non-existence of the Wallace Born series is interesting but appears to be an artefact of the Wallace approximation – it must not be concluded that the true Born series (3.3) does not exist.

Calculations in the Wallace approximation have been performed for $e^\pm\text{-H}$ (1s) elastic scattering by Byron et al. [28, 98] and by Franco and Iwinski [106], for 1s–2s excitation by Byron et al. [98] and for 1s–2s and 1s–2p excitation by Unnikrishnan and Prasad [107]. With the exception of Byron et al. [28, 98] exchange has been included in all electron calculations. Comparisons with experiments on electron scattering suggest that the Wallace amplitude is an improvement over the Glauber approximation. However, the elastic scattering results also reveal the weakness of the Wallace approximation. Thus at 50 eV [106] the Wallace cross section, although a lot better than the Glauber cross section of fig. 16 (for electron–H) is still far from being in agreement with experiment; by contrast DWSBA [32] and EBS [50] calculations give fairly good accord with experiment at this energy. This failure of the Wallace approximation is almost certainly due, in the main, to $f_{1s,1s}^{W2}$ not giving a good enough representation of $f_{1s,1s}^{B2}$. It should be noted that the DWSBA and EBS calculations cited above explicitly contain $f_{1s,1s}^{B2}$.

6.5. The unitarized eikonal-Born series approximation (or modified Wallace approximation)

Following the logic of section 6.3, the Wallace approximation (6.20) should be significantly improved by correcting it in second order. This leads to the Unitarized Eikonal Born Series approximation (UEBS) of Byron et al. [28, 98]:

$$f_{f0}^{\text{UEBS}} = f_{f0}^W + (f_{f0}^{B2} - f_{f0}^{W2}). \quad (6.24)$$

In the opinion of this author (6.24) might be better called the modified Wallace approximation (MWA). However, Byron et al. like to view (6.24) as an extension of the EBS amplitude (6.15). Thus, see (6.22a) and (6.23b), (6.24) contains the three terms of the EBS approximation (6.15) and therefore all of the virtues of this approximation. Like the MGA (6.17), the UEBS amplitude may be regarded as extending the third-order perturbative EBS amplitude to infinite order.

The description “unitarized” as applied to (6.24) arises as follows. The amplitude f_{f0}^W , and also f_{f0}^G , is unitary; The sense in which this is so needs, however, to be carefully specified [4, 86]. A crude, but perhaps better, way of seeing that f_{f0}^W and f_{f0}^G are “unitary” is to realize that, since the potential V occurs in a phase factor in both amplitudes, they cannot grow indefinitely in size as the strength of V is increased; this is perhaps the most important hallmark of a unitary approximation.

By adding correction terms, as in (6.17) and (6.24) the unitarity of f_{f0}^W and f_{f0}^G is disturbed – the correction terms scale as V^2 . The degree to which unitarity is lost depends upon the balance between f_{f0}^{B2} on the one hand and f_{f0}^{W2} and f_{f0}^{G2} on the other. Since f_{f0}^{G2} is purely imaginary/real while f_{f0}^{B2} is complex there is obviously a lack of balance in the real/imaginary part of the MGA (6.17). However, the second-order Wallace term f_{f0}^{W2} has both real and imaginary parts and should therefore better balance f_{f0}^{B2} . Of the three amplitudes EBS (which is most definitely not unitary), EBS' (i.e. MGA) and (6.24) the latter is the most unitary. It is for this reason that, of the three, it has earned the accolade “unitarized”.

The degree to which an approximation is unitary, at least in so far as static field scattering is concerned, is most important if the approximation is to be extended to the heavier atoms. At the end of

section 6.2.3 it was mentioned that the EBS method is restricted to light atoms because, being non-unitary, the EBS amplitude grows too large as the static field of the atom is increased. The UEBS approximation (6.24) should be a better candidate for extension to the heavier atoms although since it is not strictly unitary, because of the correction term ($f_{f0}^{B2} - f_{f0}^{W2}$), it is a question of how heavy.

In fig. 23 the EBS approximation (6.15), the Wallace approximation (6.20) and the UEBS approximation (6.24) are compared with one another for electron-H (1s) elastic scattering at 100 eV [28] (these calculations do *not* include exchange). Firstly, it is seen that the EBS cross section is about a factor of two larger than the UEBS numbers at large angles, this further confirms the conclusion, drawn on the basis of other evidence (section 6.2.3), that the EBS method gives too large a cross section at large angles. At small angles the EBS and UEBS cross sections are in fairly good agreement – perturbation theory (i.e. EBS) converges more rapidly at small angles than at large. At small angles the Wallace approximation is poor in comparison with UEBS – for electron-H (1s) elastic scattering $f_{1s, 1s}^{W2}$ is a poor representation of $f_{1s, 1s}^{B2}$ at small angles. At large angles the Wallace and UEBS curves merge – $f_{1s, 1s}^{W2}$ is a good representation of $f_{1s, 1s}^{B2}$ at large momentum transfers.

Byron et al. [28] have developed an exchange amplitude based upon the UEBS approximation (which will be discussed in section 8) to go with their direct UEBS amplitude (6.24). They have combined the two amplitudes to calculate electron-H (1s) elastic cross sections at energies of 100, 200, 300 and 400 eV. UEBS positron-H (1s) elastic cross sections are also given at these energies.

In reference [98] Byron et al. also report UEBS cross sections for exciting the $1s \rightarrow 2s$ transition in e^\pm -H (1s) collisions at 100 eV. The electron cross section, which includes exchange, is shown in fig. 22. An interesting point to note from this figure is how well the UEBS result is approximated by the MGA cross section (which is calculated under identical conditions). It would be very interesting to see how these two approximations compared for elastic scattering; even though MGA cross sections for e^\pm -H (1s) elastic scattering exist [99, 102] the fact that they are not calculated under identically the same

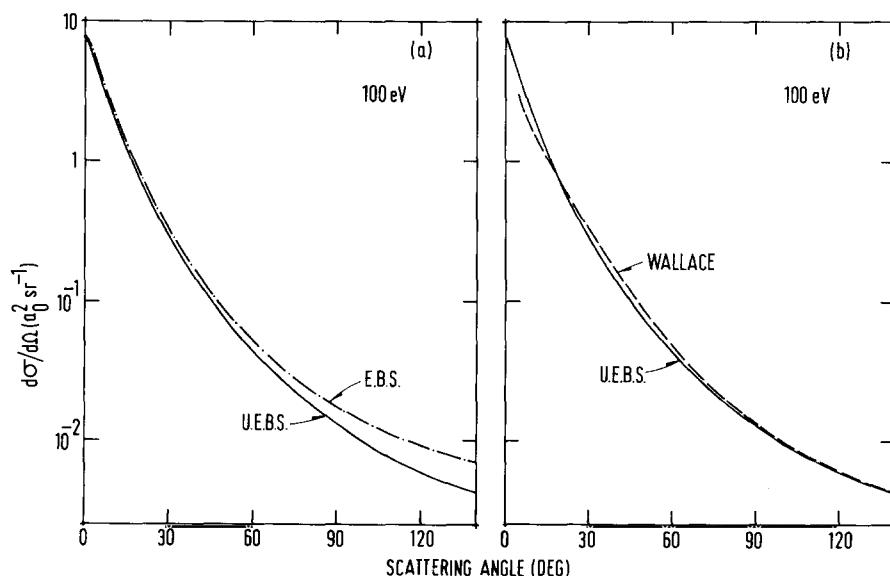


Fig. 23. Comparison of theoretical differential cross sections for electron-H (1s) elastic scattering at 100 eV: (a) comparison of UEBS with EBS; (b) comparison of UEBS with Wallace approximation. The theoretical curves do *not* include exchange. Curves [28]: (—) UEBS; (- · - · -) EBS; (— —) Wallace approximation.

conditions as the UEBS numbers of Byron et al. [28] makes a valid comparison between the two impossible. In view of Byron et al.'s comment that [28] "the many-body Wallace amplitude is vastly more difficult to evaluate than . . . the many-body Glauber amplitude" it is important to establish how significant is the difference between the MGA and the UEBS methods.

7. Optical potentials

In theory, at least, the Schrödinger equation (2.5)

$$(H_0 + V - E)\Psi^+ = 0 \quad (7.1)$$

may be solved by expanding Ψ^+ in atomic eigenstates

$$\Psi^+ = \sum_n F_n^+(\mathbf{r}_0) \psi_n(\mathbf{X}), \quad (7.2)$$

where I have ignored exchange when the projectile is an electron. Substituting (7.2) in (7.1) gives the infinity of coupled equations

$$(\nabla_0^2 + k_n^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^{\infty} \langle \psi_n(\mathbf{X}) | V | \psi_m(\mathbf{X}) \rangle F_m^+(\mathbf{r}_0), \quad n = 0, 1, 2, \dots \quad (7.3)$$

If we want to look at the transition $\psi_0 \rightarrow \psi_f$ then, ultimately, all we are interested in are the asymptotic forms of F_0^+ and F_f^+ . The optical potential formalism is a way of re-writing (7.3) to look like a finite set of equations which contains only channels of interest.

Let us suppose that we are interested in the channels which involve the eigenstates $\psi_0, \psi_1, \dots, \psi_M$. Then, we require only that part of Ψ^+ which contains these states, Ψ^{P+} say. This component may be extracted from Ψ^+ by using the projection operator

$$P \equiv \sum_{n=0}^M |\psi_n(\mathbf{X})\rangle \langle \psi_n(\mathbf{X})|, \quad (7.4)$$

i.e.,

$$\Psi^{P+} = P\Psi^+ \quad (7.5a)$$

$$= \sum_{n=0}^M F_n^+(\mathbf{r}_0) \psi_n(\mathbf{X}). \quad (7.5b)$$

It is easily shown [10] that Ψ^{P+} satisfies the equation

$$(H_0 + V^{\text{OPT}} - E)\Psi^{P+} = 0, \quad (7.6)$$

where*

* Note that P and Q commute with H_0 and that $Q^2 = Q$, $P^2 = P$, $PQ = QP = 0$.

$$V^{\text{OPT}} \equiv PVP + PVQ[Q(E + i\eta - H_0 - V)Q]^{-1}QVP, \quad (7.7)$$

$$Q \equiv 1 - P, \quad (7.8)$$

and the limit $\eta \rightarrow 0+$ is implied in (7.7). V^{OPT} is the optical potential for the P-space (7.4). Using (7.5b), the eq. (7.6) may be written in the coupled form

$$(\nabla_0^2 + k_n^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^M \langle \psi_n(\mathbf{X}) | V^{\text{OPT}} | \psi_m(\mathbf{X}) \rangle F_m^+(\mathbf{r}_0), \quad n = 0, 1, \dots, M, \quad (7.9)$$

thereby explicitly demonstrating that (7.3) has been formally reduced to a finite set of coupled equations involving only the states of interest. The price paid for this reduction is the appearance of the complicated object (7.7). Unlike V which is real, local and impact energy independent, the optical potential (7.7) is complex, non-local and energy dependent.

For basic references to the optical potential the reader is directed to [109].

7.1. Perturbative expansion

It is interesting, and useful, to make a perturbative expansion of (7.7) in powers of V :*

$$V^{\text{OPT}} = PVP + PVQ(E + i\eta - H_0)^{-1}QVP + PVQ(E + i\eta - H_0)^{-1}QVQ(E + i\eta - H_0)^{-1}QVP + \dots \quad (7.10)$$

The first-order term

$$V^{\text{OPT1}} = PVP \quad (7.11)$$

is just the ordinary potential V acting in the P-space. The second-order term

$$V^{\text{OPT2}} = PVQ(E + i\eta - H_0)^{-1}QVP \quad (7.12)$$

will be the main consideration of this section 7. The third-order term

$$V^{\text{OPT3}} = PVQ(E + i\eta - H_0)^{-1}QVQ(E + i\eta - H_0)^{-1}QVP \quad (7.13)$$

will be the subject of section 7.3.

It is worth noting that the DWSBA (5.17) with the choice of potential

$$V_1 = PVP, \quad (7.14)$$

where P is given by (7.4) (this includes the cases (5.18) and (5.29)) may be considered as an approximation resulting from a perturbative solution of (7.9) where V^{OPT} is treated only to second order [3, 37]. Thus to second order (7.9) is (this is the SOPM approximation, see section 7.4)

* Note that P and Q commute with H_0 and that $Q^2 = Q$, $P^2 = P$, $PQ = QP = 0$.

$$(\nabla_0^2 + k_n^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^M \{\langle \psi_n | V | \psi_m \rangle + \langle \psi_n | PVQ(E + i\eta - H_0)^{-1} QVP | \psi_m \rangle\} F_m^+(\mathbf{r}_0). \quad (7.15)$$

Solving equations (7.15) to first order in* $\langle \psi_n | PVQ(E + i\eta - H_0)^{-1} QVP | \psi_m \rangle$ results in the amplitude (5.17)**. In so far as comparison is possible it would appear that the DWSBA is a good approximation to (7.15) for the systems and at the energies for which it has been used. It has been suggested [37] that in situations where the DWSBA does not give a good approximation to (7.15) third and higher order terms in the optical potential will probably be important. A different view has been expressed in [110]. For further discussion see the end of section 8.3.

7.2. The second-order optical potential

Using (3.1b), (4.1), (7.4) and (7.8) the matrix elements of the second-order optical potential (7.12) may be written

$$\begin{aligned} V_{ab}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) &\equiv \langle \psi_a(\mathbf{X}) | V^{\text{OPT2}} | \psi_b(\mathbf{X}) \rangle, \\ &= \frac{1}{4\pi^3} \sum_{n=M+1}^{\infty} \lim_{\eta \rightarrow 0^+} \int d\mathbf{k} \langle \psi_a | V | \mathbf{k}, \psi_n \rangle \frac{\langle \mathbf{k}, \psi_n | V | \psi_b \rangle}{k_n^2 - k^2 + i\eta}, \end{aligned} \quad (7.16)$$

where

$$\langle \psi_a | V | \mathbf{k}, \psi_n \rangle \equiv \int \psi_a^*(\mathbf{X}) V(\mathbf{r}_0, \mathbf{X}) \exp(i\mathbf{k} \cdot \mathbf{r}_0) \psi_n(\mathbf{X}) d\mathbf{X}, \quad (7.17a)$$

$$\langle \mathbf{k}, \psi_n | V | \psi_b \rangle \equiv \int \exp(-i\mathbf{k} \cdot \mathbf{r}'_0) \psi_n^*(\mathbf{X}) V(\mathbf{r}'_0, \mathbf{X}) \psi_b(\mathbf{X}) d\mathbf{X}, \quad (7.17b)$$

$$k_n^2 = 2(E - \varepsilon_n). \quad (7.17c)$$

Firstly, note that V^{OPT2} , like the full potential V^{OPT} , is non-local, i.e.,

$$V_{ab}^{\text{OPT2}} F(\mathbf{r}_0) = \int V_{ab}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) F(\mathbf{r}'_0) d\mathbf{r}'_0. \quad (7.18)$$

Secondly, comparing (7.16) with the second Born term (4.3) we see that

$$-\frac{1}{2\pi} \langle \mathbf{k}_a | V_{ab}^{\text{OPT2}} | \mathbf{k}_b \rangle, \quad (7.19a)$$

where

$$\frac{1}{2} k_a^2 + \varepsilon_a = E = \frac{1}{2} k_b^2 + \varepsilon_b \quad (7.19b)$$

* Note that $\langle \psi_n | PVQ(E + i\eta - H_0)^{-1} QVP | \psi_m \rangle = \langle \psi_n | V_2 G_0^\dagger V_2 | \psi_m \rangle$.

** Note that when V_1 is given by (7.14) the second term in (5.17) is zero and G_1^\dagger in the third term can be replaced by G_0^\dagger .

is just that part of the second Born term f_{ab}^{B2} coming from intermediate states $n > M$. The second-order optical potential therefore contains, not surprisingly, the same physics (from states $n > M$) as the corresponding second Born term.

7.2.1. Physical content

Two very important physical effects contained in f_{00}^{B2} for elastic scattering* are the dipole polarizability α_{00} of the state ψ_0 (in $\text{Re } f_{00}^{B2}$) and flux loss (in $\text{Im } f_{00}^{B2}$) (section 4.1.1). These two effects also appear in V_{00}^{OPT2} . The former is associated with $\text{Re } V_{00}^{\text{OPT2}}$, which is often written as V_{pol} , while the latter is responsible for $\text{Im } V_{00}^{\text{OPT2}}$, often written as V_{abs} (abs = absorptive):

$$V_{00}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) = V_{\text{pol}}(E, \mathbf{r}_0, \mathbf{r}'_0) + iV_{\text{abs}}(E, \mathbf{r}_0, \mathbf{r}'_0). \quad (7.20)$$

Note from (7.16) that V_{00}^{OPT2} can only have an imaginary part if $k_n^2 > 0$, i.e., if flux can be lost from the ψ_0 channel to the ψ_n channel.

Intuitively, V_{00}^{OPT2} is expected to behave, *in effect*, like the local adiabatic polarization potential $-\alpha_{00}/r_0^4$ for distant collisions (see reasoning in section 4.1.1). Recently McCarthy et al. [111, 112] have disputed this fact. In section 7.2.2.2 I shall show that their argument is erroneous and results from a local approximation to V_{00}^{OPT2} which does not reproduce the correct effective long-range behaviour of V_{00}^{OPT2} .

For small k_0 , when only the elastic channel is open, V_{00}^{OPT2} is purely real. It might be thought that in the adiabatic limit ($k_0 \rightarrow 0$) V_{00}^{OPT2} would go over to the “adiabatic” potential (4.7). This is not so. V_{00}^{OPT2} is the correct *dynamical* expression of second-order potential effects at all energies.

Non-diagonal components of V^{OPT2} , i.e., V_{pq}^{OPT2} ($p \neq q$), contain non-diagonal polarizabilities – such as were discussed in section 4.1.2.

7.2.2. Approximate methods of calculation

7.2.2.1. The sum over intermediate states. In the infinite sum over intermediate states ψ_n in (7.16) we are confronted with the same problem that was encountered with the second Born term. The approximate solution is the same, i.e., use closure and/or pseudostates (section 4.2).

7.2.2.2. Localization. From a computational point of view the non-locality of optical potentials is very inconvenient; local approximations have therefore been sought; in this section I shall describe the main methods.

Consider a non-local potential $V_{ab}^{\text{NL}}(E, \mathbf{r}_0, \mathbf{r}'_0)$ connecting the states ψ_a and ψ_b , e.g. $V_{ab}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0)$. In the first method the local approximation $\bar{V}_{ab}^L(E, \mathbf{r}_0)$ is defined by demanding that its *on-energy-shell* plane wave matrix elements reproduce exactly those of the non-local potential, i.e.,

$$\int \exp(-ik \cdot \mathbf{r}_0) \bar{V}_{ab}^L(E, \mathbf{r}_0) \exp(ik' \cdot \mathbf{r}_0) d\mathbf{r}_0 = \langle \mathbf{k} | V_{ab}^{\text{NL}} | \mathbf{k}' \rangle, \quad (7.21a)$$

when

$$\frac{1}{2}k^2 + \varepsilon_a = E = \frac{1}{2}k'^2 + \varepsilon_b. \quad (7.21b)$$

* For simplicity I shall tacitly assume that ψ_0 is an S-state and that $P = |\psi_0\rangle\langle\psi_0|$; this is the case in most elastic scattering calculations.

Recognizing the left-hand side of (7.21a) as a Fourier transform, inversion of this transform gives

$$\bar{V}_{ab}^L(E, \mathbf{r}_0) = \frac{1}{(2\pi)^3} \int \exp(-i\mathbf{q} \cdot \mathbf{r}_0) \langle \mathbf{k} | V_{ab}^{NL} | \mathbf{k}' \rangle d\mathbf{q}, \quad (7.22a)$$

$$\mathbf{q} \equiv \mathbf{k}' - \mathbf{k}, \quad (7.22b)$$

where the precise manner in which one performs the \mathbf{q} integration in (7.22a) still remains to be specified (see below, following (7.27)).

Another method, which, as far as I can see, has only been applied to elastic scattering, demands that the local potential, \tilde{V}_{00}^L , operating upon the incident plane wave produce the same result as the non-local potential

$$\tilde{V}_{00}^L(E, \mathbf{r}_0) \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0) = \int V_{00}^{NL}(E, \mathbf{r}_0, \mathbf{r}'_0) \exp(i\mathbf{k}_0 \cdot \mathbf{r}'_0) d\mathbf{r}'_0, \quad (7.23a)$$

$$\frac{1}{2}k_0^2 + \varepsilon_0 = E, \quad (7.23b)$$

Thus

$$\tilde{V}_{00}^L(E, \mathbf{r}_0) = \int \exp(-i\mathbf{k}_0 \cdot \mathbf{r}_0) V_{00}^{NL}(E, \mathbf{r}_0, \mathbf{r}'_0) \exp(i\mathbf{k}_0 \cdot \mathbf{r}'_0) d\mathbf{r}'_0. \quad (7.24)$$

Until very recently [70] localization methods were applied only to optical potentials which conserved the angular momentum of the incident electrons; such is the case if ψ_a and ψ_b are S-states and if P-space consists of complete sets of magnetic substates. It is interesting to enquire whether the local approximations \bar{V}^L and \tilde{V}^L also conserve angular momentum in this case. If they do then they must be spherically symmetric.

When $V_{ab}^{NL}(E, \mathbf{r}_0, \mathbf{r}'_0)$ conserves angular momentum it is a function only of the magnitudes E, r_0, r'_0 and of the angle θ between \mathbf{r}_0 and \mathbf{r}'_0 :

$$V_{ab}^{NL}(E, \mathbf{r}_0, \mathbf{r}'_0) \rightarrow V_{ab}^{NL}(E, r_0, r'_0, \theta). \quad (7.25)$$

It is easy then to see that $\langle \mathbf{k} | V_{ab}^{NL} | \mathbf{k}' \rangle$ depends only upon the magnitudes $k, k', E, |\mathbf{k} - \mathbf{k}'|$:

$$\langle \mathbf{k} | V_{ab}^{NL} | \mathbf{k}' \rangle = F_{ab}(E, k, k', |\mathbf{k} - \mathbf{k}'|). \quad (7.26)$$

Substituting (7.26) in (7.22) gives

$$\bar{V}_{ab}^L(E, \mathbf{r}_0) = \frac{1}{(2\pi)^3} \int \exp(-i\mathbf{q} \cdot \mathbf{r}_0) F_{ab}(E, k, k', q) d\mathbf{q}. \quad (7.27)$$

In order that (7.21) should hold k and k' in (7.27) are fixed according to (7.21b). However, for fixed k and k' the left-hand side of (7.26) is defined only for

$$|\mathbf{k} - \mathbf{k}'| \leq q \leq (k + k'). \quad (7.28)$$

Since it is intended that the integral over \mathbf{q} in (7.27) be over all vectors \mathbf{q} , an analytic continuation of the right-hand side of (7.26) outside the range (7.28) is required. When $V^{\text{NL}} = V^{\text{OPT2}}$ and when the latter is calculated in the closure approximation this analytic continuation is easily done. Since F_{ab} depends only upon the magnitude of q the angular integrals in (7.27) can be readily performed to yield

$$\tilde{V}_{ab}^L(E, r_0) = \frac{1}{2\pi^2} \frac{1}{r_0} \int_0^\infty q \sin qr_0 F_{ab}(E, k, k', q) dq, \quad (7.29)$$

a potential which is spherically symmetric and therefore conserves angular momentum.

Using the delta function representation

$$\frac{1}{(2\pi)^3} \int \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')] d\mathbf{q} = \delta(\mathbf{r} - \mathbf{r}') \quad (7.30)$$

(7.24) can be written

$$\begin{aligned} \tilde{V}_{00}^L(E, \mathbf{r}_0) &= \frac{1}{(2\pi)^3} \int \exp(-i\mathbf{q} \cdot \mathbf{r}_0) \exp[-i(\mathbf{k}_0 - \mathbf{q}) \cdot \mathbf{r}_0''] V_{00}^{\text{NL}}(E, \mathbf{r}_0'', \mathbf{r}_0') \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0') d\mathbf{r}_0' d\mathbf{r}_0'' d\mathbf{q} \\ &= \frac{1}{(2\pi)^3} \int \exp(-i\mathbf{q} \cdot \mathbf{r}_0) F_{00}(E, |\mathbf{k}_0 - \mathbf{q}|, k_0, q) d\mathbf{q}, \end{aligned} \quad (7.31)$$

where (7.26) has been employed in the last step. Since F_{00} in (7.31) has a non-trivial dependence upon the direction of \mathbf{q} the potential \tilde{V}_{00}^L will not be spherically symmetric and will therefore not conserve angular momentum. Thus \tilde{V}^L is superior to \tilde{V}^L in this very important respect.

McCarthy and Stelbovics [113] have proposed a spherical average of (7.31). This averaging is done at the momentum level by replacing $F_{00}(E, |\mathbf{k}_0 - \mathbf{q}|, k_0, q)$ by

$$V_{00}(E, q) \equiv \frac{1}{2} \int_{-1}^{+1} F_{00}(E, |\mathbf{k}_0 - \mathbf{q}|, k_0, q) du, \quad (7.32a)$$

$$u \equiv (\mathbf{k}_0 \cdot \mathbf{q})/k_0 q, \quad (7.32b)$$

and results in the spherically symmetric potential

$$V_{00}^{\text{MCL}}(E, r_0) = \frac{1}{2\pi^2} \frac{1}{r_0} \int_0^\infty q \sin qr_0 V_{00}(E, q) dq. \quad (7.33)$$

When $V^{\text{NL}} = V^{\text{OPT2}}$ the approximation (7.29) takes on a particularly nice form. From (4.3), (7.16), (7.21b) and (7.26) $F_{ab}(E, k, k', q)$ is then simply

$$-2\pi \sum_{n=M+1}^{\infty} f_{ab}^{\text{B2}; n}(\mathbf{k}, \mathbf{k}'), \quad (7.34)$$

i.e., that part of the second Born term f_{ab}^{B2} coming from intermediate states $n \geq M + 1$, let us write (7.34) as

$$-2\pi \tilde{f}_{ab}^{B2}(\mathbf{k}, \mathbf{k}') . \quad (7.35)$$

Thus

$$\bar{V}_{ab}^{L2}(E, r_0) = -\frac{1}{\pi} \frac{1}{r_0} \int_0^\infty q \sin qr_0 \tilde{f}_{ab}^{B2}(\mathbf{k}, \mathbf{k}') dq , \quad (7.36)$$

so that the local approximation is obtained by Fourier transforming the corresponding second Born term. This method is used in, for example, [7, 51, 69].

Recently McCarthy et al. [111, 112] have disputed the commonly held belief that V_{00}^{OPT2} behaves effectively as $-\alpha_{00}/2r_0^4$ for collisions at large distance. In section 4.1.1 it was argued that effective long-range behaviour could be examined by considering partial wave matrix elements at high angular momentum; in the case of V_{00}^{OPT2} this would be (see (4.10))

$$-4\langle j_l(k_0 r_0) Y_{l0}(\hat{\mathbf{r}}_0) | V_{00}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) | j_l(k_0 r'_0) Y_{l0}(\hat{\mathbf{r}}'_0) \rangle , \quad (7.37a)$$

$$\frac{1}{2}k_0^2 + \epsilon_0 = E . \quad (7.37b)$$

The conclusions of McCarthy et al. were based upon the local potential approximation (7.33) to V_{00}^{OPT2} . Taking on-energy-shell plane wave matrix elements of (7.33) and using (7.32) gives

$$\langle \mathbf{k} | V_{00}^{\text{MCL2}} | \mathbf{k}' \rangle = \frac{1}{2} \int_{-1}^{+1} F_{00}(E, |\mathbf{k}_0 - \mathbf{q}|, k_0, q) du , \quad (7.38a)$$

$$k = k' = k_0 . \quad (7.38b)$$

Thus,

$$\begin{aligned} \langle \mathbf{k} | V_{00}^{\text{MCL2}} | \mathbf{k}' \rangle &\neq \langle \mathbf{k} | V_{00}^{\text{OPT2}} | \mathbf{k}' \rangle \\ &\parallel \\ &F_{00}(E, k_0, k_0, q) , \end{aligned} \quad (7.39)$$

except when $\mathbf{q} = \mathbf{k}' - \mathbf{k} = \mathbf{0}$. The partial wave equivalent of (7.39) is

$$\langle j_l(k_0 r_0) Y_{l0}(\hat{\mathbf{r}}_0) | V_{00}^{\text{MCL2}}(E, \mathbf{r}_0) | j_l(k_0 r_0) Y_{l0}(\hat{\mathbf{r}}_0) \rangle \neq \langle j_l(k_0 r_0) Y_{l0}(\hat{\mathbf{r}}_0) | V_{00}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) | j_l(k_0 r'_0) Y_{l0}(\hat{\mathbf{r}}'_0) \rangle . \quad (7.40)$$

Since the inequality (7.40) holds even in the limit $l \rightarrow \infty$, it is to be concluded that V_{00}^{MCL2} does not give the effective behaviour of V_{00}^{OPT2} at large distance. What McCarthy et al. have shown is that at large r_0 the potential V_{00}^{MCL2} does not have the classic $-\alpha/2r_0^4$ polarization form; this result is correct. McCarthy et al. then go on to conclude that the effective behaviour of the exact optical potential V_{00}^{OPT2} is not

$-\alpha/2r_0^4$; it is this step which is wrong, since, as shown above, the long-range behaviour of V_{00}^{MCL2} at large r_0 does not coincide with the effective behaviour of V_{00}^{OPT2} [114].

From the on-shell requirement (7.21) it is easy to show that

$$-4\langle j_l(k_0 r_0) Y_{l0}(\hat{r}_0) | \bar{V}_{00}^{\text{L2}}(E, r_0) | j_l(k_0 r_0) Y_{l0}(\hat{r}_0) \rangle \quad (7.41)$$

is equal to (7.37) for all l ; in fact this equality is just the demand (7.21) in partial wave form. That (7.41) equals (7.37) implies that the long-range behaviour of \bar{V}_{00}^{L2} is the same as that of V_{00}^{OPT2} .

In the author's opinion the local approximation \bar{V}^{L} should always be preferred to \bar{V}^{L} and V^{MCL} .

That V_{00}^{OPT2} does behave effectively like the classic form $-\alpha/2r_0^4$ at large distance can be seen by combining (4.1), (4.10), (7.16) and (7.37) when it is observed that (7.37) is just $\tilde{f}_{00,l}^{\text{B2}}$ of (4.10) (\sim since only intermediate states $n \geq M + 1$ are included in (7.16), see (7.35)). In table 1 (and more convincingly in [114] vis-a-vis McCarthy et al.'s oscillatory asymptotic form [111, 112]) it was demonstrated that $f_{00,l}^{\text{B2}}$ converges to f_l^{AD2} (4.11) at large l . This implies that V_{00}^{OPT2} has the same effective behaviour as V_{00}^{AD2} of (4.7) at large distance, i.e., $-\alpha/2r_0^4$, as expected!

While the idea of replacing a non-local potential by a local potential is a nice one, the really important question is whether it is a good approximation. For elastic electron scattering by H (1s) and He (1¹S) it has been shown that (7.36) works very well indeed at impact energies of interest [32, 78]. It would be interesting to see how well it fared for elastic scattering by a heavier atom, like neon; here the scattered wave function should have a much larger off-energy-shell component than in the case of the light atoms H and He – remember that \bar{V}^{L} was only required to give correct results on-energy-shell (see (7.21)). The approximation (7.36) has also been tested on the 1s → 2s excitation of H [32]. Here, by contrast, it was found to be unacceptable. It is therefore to be *strongly* recommended that local potential approximations be used with caution, particularly for excitation.

7.2.2.3. Approximate local forms. Although the localization procedures described in the previous section considerably simplify V^{OPT2} they still require an evaluation of the second Born term (see (7.36)) which is a non-trivial task, particularly for the heavier atoms. Further simplifications of the local potentials, which may be readily extended to complex atoms, have therefore been sought. In the main this work has been directed towards elastic scattering where P-space consists only of the initial state ψ_0 and where this state is an S-state.

Perhaps the most successful form of ab-initio approximate local potential is that suggested by Byron and Joachain [115, 116]; the pedigree of this potential may be traced through ideas developed in [31, 117]. Writing the local approximation in the form (7.20):

$$V_{00}^{\text{L2}}(E, r_0) = V_{\text{pol}}(E, r_0) + i V_{\text{abs}}(E, r_0), \quad (7.42)$$

V_{pol} and V_{abs} are separately approximated.

The atomic polarizability α_{00} is the most important physical effect contained in V_{pol} . In (4.12) we saw the dynamical manifestation of α_{00} in the large k_0 small q limit of $\text{Re } f_{00}^{\text{B2}}$. Byron and Joachain have suggested that V_{pol} be generated from the asymptotic form (4.12) using (7.36). Further, since oscillator strengths will not generally be known for an arbitrary atom, (4.12) will usually have to be calculated in a closure approximation – this amounts to replacing k_n by* k_0 in (4.12) and ε_n by an average energy $\bar{\varepsilon}$.

* A less drastic approximation would be the replacement $k_n \rightarrow \bar{k} \equiv (k_0^2 - 2\Delta)^{1/2}$. Although this form has been mentioned in the literature [118] it does not seem to have been used in practice.

Thus Byron and Joachain's formula for V_{pol} is

$$V_{\text{pol}}(E, r_0) = -\frac{\langle \psi_0 | Z^2 | \psi_0 \rangle}{k_0 r_0} \int q \sin qr_0 \left(1 - \frac{qa}{(q^2 a^2 + 1)^{1/2}} \right) dq, \quad (7.43a)$$

$$a \equiv k_0/2\Delta, \quad (7.43b)$$

$$\Delta \equiv \bar{\epsilon} - \epsilon_0. \quad (7.43c)$$

Performing the integration over q yields

$$V_{\text{pol}}(E, r_0) = \frac{-\pi}{2k_0 a^3 \rho} \langle \psi_0 | Z^2 | \psi_0 \rangle \left([I_0(\rho) - L_0(\rho)] - \frac{1}{\rho} [I_1(\rho) - L_1(\rho)] \right), \quad (7.44a)$$

$$\rho \equiv r_0/a, \quad (7.44b)$$

where I_n and L_n are modified Bessel and modified Struve functions respectively [63].

For large r_0 the potential (7.44) has the asymptotic expansion

$$V_{\text{pol}}(E, r_0) \xrightarrow{r_0 \rightarrow \infty} -\frac{\bar{\alpha}}{2r_0^4} \left(1 + \frac{6a^2}{r_0^2} + \frac{135a^4}{r_0^4} + \dots \right), \quad (7.45a)$$

$$\bar{\alpha} \equiv 2\langle \psi_0 | Z^2 | \psi_0 \rangle / \Delta. \quad (7.45b)$$

The leading term in (7.45a) is of the classic polarization form, i.e., $-\bar{\alpha}/2r_0^4$, where the constant $\bar{\alpha}$ is easily recognized as the dipole polarizability of the state ψ_0 in the closure approximation (see (4.13)). This fixes the choice of $\bar{\epsilon}$, i.e., $\bar{\epsilon}$ is chosen so that (7.45b) agrees with the (assumed) known polarizability α_{00} .

An unsatisfactory feature of (7.44) is that it is singular as $1/r_0$ for small r_0 . However, in the cases that have been studied [116, 119], this singularity does not pose a problem since the static potential, which is also singular as $1/r_0$, is much larger than V_{pol} at small r_0 (see fig. 9 of [116]).

Starting from (4.15) rather than (4.12) Winters [69, also 76, 84] has made an obvious generalization of (7.44) to inelastic S \rightarrow S transitions. However, the reader should be reminded of the warning given at the end of section 7.2.2 concerning local approximations to non-diagonal elements of V^{OPT2} . Anyway, as it turns out, Winters [69] found that for the 1s \rightarrow 2s excitation of H the inelastic analogue of (7.44) did not give very satisfactory agreement even with the real part of the local potential (7.36) which it was supposed to be approximating.

In section 6.2.1 we saw that, except at small momentum transfers, the second order Glauber term, f_{00}^{G2} , could give a good representation of $i \text{Im} f_{00}^{\text{B2}}$ when ψ_0 is an S-state. Byron and Joachain's prescription* for V_{abs} amounts, in the first instance, to the replacement of $i \text{Im} \tilde{f}_{00}^{\text{B2}}$ by $\tilde{f}_{00}^{\text{G2}}$ in (7.36) to give

$$iV_{\text{abs}}^{\text{G}}(E, r_0) = -\frac{1}{\pi} \frac{1}{r_0} \int_0^\infty q \sin qr_0 \tilde{f}_{00}^{\text{G2}} dq. \quad (7.46)$$

* The description given here differs from that of Byron and Joachain [116] but amounts to the same thing. See section 7.3 for Byron and Joachain's approach.

From (6.9)

$$f_{00}^{G2} = \frac{i}{4\pi k_0} \int d^2 b_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \langle \psi_0 | \chi_0^2(\mathbf{b}_0, \mathbf{X}) | \psi_0 \rangle. \quad (7.47)$$

Since it is assumed that P-space consists only of the state ψ_0 the term \tilde{f}_{00}^{G2} is just f_{00}^{G2} with the ψ_0 intermediate state contribution subtracted out (see (7.34), (7.35)):

$$\tilde{f}_{00}^{G2} = \frac{i}{4\pi k_0} \int d^2 b_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \{ \langle \psi_0 | \chi_0^2(\mathbf{b}_0, \mathbf{X}) | \psi_0 \rangle - \langle \psi_0 | \chi_0(\mathbf{b}_0, \mathbf{X}) | \psi_0 \rangle^2 \}. \quad (7.48)$$

Since ψ_0 is an S-state the matrix elements in (7.48) are functions only of the magnitude of \mathbf{b}_0 . This enables us to integrate analytically over the angular part of \mathbf{b}_0 :

$$\tilde{f}_{00}^{G2} = \frac{i}{2k_0} \int_0^\infty db_0 b_0 J_0(qb_0) \chi_{\text{abs}}(b_0), \quad (7.49)$$

where $\chi_{\text{abs}}(b_0)$ stands for the curly bracket in (7.48) and J_0 is a Bessel function [63]. Employing (7.49) in (7.46) then gives

$$V_{\text{abs}}^G(E, r_0) = -\frac{1}{2\pi k_0 r_0} \int_0^\infty dq q \sin qr_0 \int_0^\infty db_0 b_0 J_0(qb_0) \chi_{\text{abs}}(b_0). \quad (7.50)$$

Integrating over b_0 by parts and using ([120] page 634)

$$\int x J_0(x) dx = x J_1(x) \quad (7.51)$$

gives

$$V_{\text{abs}}^G(E, r_0) = \frac{1}{2\pi k_0 r_0} \int_0^\infty dq \sin qr_0 \int_0^\infty db_0 b_0 J_1(qb_0) \frac{d\chi_{\text{abs}}(b_0)}{db_0}. \quad (7.52)$$

Finally, integrating over q and using ([120] p. 730)

$$\begin{aligned} \int \sin qr_0 J_1(qb_0) dq &= r_0/b_0(b_0^2 - r_0^2)^{1/2}, & r_0 < b_0, \\ &= 0, & r_0 > b_0, \end{aligned} \quad (7.53)$$

yields Byron and Joachain's formula

$$V_{\text{abs}}^G(E, r_0) = \frac{1}{2\pi k_0} \int_{r_0}^\infty db_0 \frac{1}{(b_0^2 - r_0^2)^{1/2}} \frac{d\chi_{\text{abs}}(b_0)}{db_0}. \quad (7.54)$$

For large b_0 the phase $\chi_{\text{abs}}(b_0)$ varies as $1/b_0^2$. This results in a $1/r_0^3$ behaviour of V_{abs}^G at large r_0 . Viewed another way, this long-range tail of V_{abs}^G arises from the (usually) unphysical divergence of f_{00}^{G2} at zero momentum transfer – large values of r_0 are associated with small values of q in (7.46) – which divergence, as shown in section 4.2.1, results from setting all atomic state energies, in particular those of P-states, equal to ε_0 in the Glauber approximation. Except in special cases (see below), therefore, the r_0^{-3} tail is an undesirable feature.

In order to get a satisfactory V_{abs} Byron and Joachain have added a correction term to (7.54):

$$V_{\text{abs}}(E, r_0) = V_{\text{abs}}^G(E, r_0) + V_{\text{abs}}^{\text{corr}}(E, r_0). \quad (7.55)$$

The correction term, $V_{\text{abs}}^{\text{corr}}$, is based upon a comparison between the leading, in $1/k_0$, part of f_{00}^{B2} , calculated in the Massey–Mohr closure approximation with an average energy $\bar{\varepsilon}$, and the Glauber term f_{00}^{G2} . I refer the reader to reference [116] for the precise details. Suffice it to say here that the effect of $V_{\text{abs}}^{\text{corr}}$ is to relax the Glauber assumption that all atomic states have energy ε_0 ; this is achieved by introducing an average energy $\bar{\varepsilon} \neq \varepsilon_0$; the spurious r_0^{-3} behaviour of V_{abs}^G is thereby cancelled. For $\bar{\varepsilon}$ we are instructed to take the same value as used for V_{pol} of (7.44).

Although the calculation of (7.55) is a little bit involved Byron and Joachain [116] claim that it is easier than starting with a closure approximation to $\text{Im } \tilde{f}_{00}^{B2}$ in (7.36).

When ψ_0 is a non-degenerate S-state a close inspection of V_{abs} of (7.55) shows that at large distance it falls off exponentially. This should be contrasted with the long-range $-\alpha/2r_0^4$ variation of V_{pol} (in this context note the pronounced difference between $\text{Re } f_{00,l}^{B2}$ and $\text{Im } f_{00,l}^{B2}$ with increasing l in table 1). This exponential fall-off is interesting in that it involves two distinct types of behaviour. The first is an exponential decrease whose scale is set by the size of the atom, i.e., terms involving $\exp(-Zr_0)$ where Z is a typical orbital exponent of ψ_0 . The second is a fall-off like

$$(1/ar_0)^{3/2} \exp(-r_0/a) \quad (7.56a)$$

$$a = k_0/2(\bar{\varepsilon} - \varepsilon_0). \quad (7.56b)$$

The scale of this exponential is obviously set by the incident momentum k_0 and the average energy $\bar{\varepsilon}$.

There is one example in the literature [118] where V_{abs} correctly displays a long-range r_0^{-3} tail. This is the case of elastic scattering off the 2s state of atomic hydrogen. Here the tail arises because the 2p state is degenerate in energy with the 2s state*; thus the Glauber assumption that all states have energy ε_0 is correct for this coupling. The formula (7.44) for V_{pol} must also be modified in this case to eliminate the contribution of the 2p state since, as (4.12) shows, the 2p state does not appear in the large k_0 small q form of $\text{Re } f_{2s,2s}^{B2}$.

In section 4.2.1 it was pointed out that in applying the closure approximation to “heavy” atoms different average energies should be associated with contributions from different atomic shells. In reference [38] the same kind of reasoning has been applied to (7.55). Here, however, the prescription is slightly more drastic – it is recommended that only the outer shells be taken into account in calculating (7.55) and that only a single average energy $\bar{\varepsilon}$ be used. For example, for Ar, only the 3s and 3p orbital contributions to (7.55) should be retained. For Ar the difference between this prescription and a calculation which allows all atomic orbitals to contribute to (7.55) with the same energy $\bar{\varepsilon}$ is found to be

* Assuming fine and hyperfine structure etc. are neglected.

significant, with the former giving better agreement with experiment. In earlier calculations on Ne and Ar [115, 116, 121] allowance was not made for shell structure in the evaluation of V_{abs} . For V_{pol} of (7.44) no attempt has been made to allow for shell structure, it is argued [38] that (7.44) is less sensitive to shell structure than (7.55).

Another form of approximate local ab-initio second-order potential for elastic scattering is that of Vanderpoorten [122]. Here the localization prescription (7.24) is used, i.e.,

$$\tilde{V}_{00}^{\text{L2}}(E, \mathbf{r}_0) = \int \exp(-i\mathbf{k}_0 \cdot \mathbf{r}_0) V_{00}^{\text{OPT2}}(E, \mathbf{r}_0, \mathbf{r}'_0) \exp(i\mathbf{k}_0 \cdot \mathbf{r}'_0) d\mathbf{r}'_0. \quad (7.57)$$

A Glauber-style approximation (section 6.1) is now made to the operator $(E + i\eta - H_0)$ appearing in (7.12), however, instead of taking $H_a = \varepsilon_0$, as in section 6.1, the atomic Hamiltonian is set equal to $\bar{\varepsilon}$ where $\bar{\varepsilon}$ may be different from ε_0 . The final result is the local potential

$$V_{00}^{\text{V2}}(E, \mathbf{r}_0) = \frac{-i}{\bar{k}} \int_{-\infty}^{z_0} \exp[-i(\mathbf{k}_0 - \bar{\mathbf{k}})(z_0 - z'_0)] A(\mathbf{r}_0, \mathbf{r}'_0) dz'_0, \quad (7.58a)$$

$$A(\mathbf{r}_0, \mathbf{r}'_0) = \langle \psi_0(\mathbf{X}) | V(\mathbf{r}_0, \mathbf{X}) V(\mathbf{r}'_0, \mathbf{X}) | \psi_0(\mathbf{X}) \rangle - \langle \psi_0(\mathbf{X}) | V(\mathbf{r}_0, \mathbf{X}) | \psi_0(\mathbf{X}) \rangle \langle \psi_0(\mathbf{X}) | V(\mathbf{r}'_0, \mathbf{X}) | \psi_0(\mathbf{X}) \rangle, \quad (7.58b)$$

$$\bar{k}^2 = k_0^2 + 2(\varepsilon_0 - \bar{\varepsilon}), \quad (7.58c)$$

where the z -direction is that of \mathbf{k}_0 . In (7.58) it has been assumed that $P = |\psi_0\rangle\langle\psi_0|$, hence the structure of (7.58b).

When ψ_0 is an S-state V_{00}^{V2} is not spherically symmetric as we would desire it to be (section 7.2.2.2). A close inspection of (7.58) shows that, in fact, V_{00}^{V2} is a function of z_0 and the magnitude of \mathbf{b}_0 ($\mathbf{r}_0 = \mathbf{b}_0 + z_0 \hat{\mathbf{k}}_0$, $\mathbf{b}_0 \cdot \hat{\mathbf{k}}_0 = 0$):

$$V_{00}^{\text{V2}}(E, \mathbf{r}_0) \rightarrow V_{00}^{\text{V2}}(E, z_0, b_0). \quad (7.59)$$

Vanderpoorten arbitrarily enforces spherical symmetry by defining the local approximation to be used, $V_{00}^{\text{VL2}}(E, \mathbf{r}_0)$ to be

$$V_{00}^{\text{VL2}}(E, \mathbf{r}_0) = V_{00}^{\text{V2}}(E, z_0 = 0, b_0 = r_0). \quad (7.60)$$

For large r_0 Vanderpoorten's local potential (7.60) has the form

$$V_{00}^{\text{VL2}}(E, \mathbf{r}_0) \xrightarrow{r_0 \rightarrow \infty} -\frac{\langle \psi_0 | Z^2 | \psi_0 \rangle}{\bar{k} \zeta r_0^4} \left[1 + \frac{3}{\zeta^2 r_0^2} + \dots \right], \quad (7.61a)$$

$$\zeta \equiv k_0 - \bar{k}. \quad (7.61b)$$

Thus V_{00}^{VL2} contains the long-range polarization term proportional to $1/r_0^4$. This, in fact, is how the

average energy $\bar{\varepsilon}$ is selected, by requiring that the first term in (7.61a) be of the form $-\alpha_{00}/r_0^4$ where α_{00} is the experimental polarizability. Note that $\bar{\varepsilon}$ determined in this way will be impact energy dependent.

It is interesting to compare (7.61) with Byron and Joachain's polarization potential (7.45). For large k_0

$$\bar{k} \rightarrow k_0, \quad (7.62a)$$

and

$$\zeta \rightarrow (\bar{\varepsilon} - \varepsilon_0)/k_0 = \Delta/k_0. \quad (7.62b)$$

The first term of (7.61a) then agrees with the first term of (7.45a) but the second terms ($\propto 1/r_0^6$) differ by a factor of two. In a later paper [88] Vanderpoorten has replaced \bar{k} and $(k_0 - \bar{k})$ in (7.58) by their high energy approximations (7.62), this makes the determination of $\bar{\varepsilon}$ impact energy independent.

Vanderpoorten and Winters [119] have made an acid test of the local approximations of Byron and Joachain ((7.44) and (7.55)) and of Vanderpoorten ((7.58) and (7.60)). It was concluded that the *Byron and Joachain potentials gave the best overall results*.

7.3. The third-order optical potential

In [31, 119, 122] some estimates were made of the effect of the third-order optical potential (7.13) in elastic electron-H (1s) scattering. These estimates suggested that the third-order contribution was not totally negligible even at an energy as high as 100 eV. Byron and Joachain [51] have since tried to make a more realistic evaluation of the third-order term.

Taking P-space to consist only of the 1s state, it is first assumed that $\langle \psi_{1s} | V^{\text{OPT}} | \psi_{1s} \rangle$ can be expanded to third order in local central potentials:

$$\langle \psi_{1s} | V^{\text{OPT}} | \psi_{1s} \rangle = V^{(1)}(E, r_0) + V^{(2)}(E, r_0) + V^{(3)}(E, r_0) + \dots, \quad (7.63)$$

where $V^{(1)}$, $V^{(2)}$ and $V^{(3)}$ are respectively of first, second and third order in V . Substituting (7.63) in (7.9) yields

$$(\nabla_0^2 - 2V^{(1)} - 2V^{(2)} - 2V^{(3)} + k_0^2)F_{1s}(\mathbf{r}_0) = 0. \quad (7.64)$$

If this equation is now solved in the eikonal approximation (i.e. (6.4)) one obtains the elastic amplitude

$$f_E = \frac{ik_0}{2\pi} \int d^2\mathbf{b}_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \left[1 - \exp\left\{ \frac{i}{k_0} (\chi_1 + \chi_2 + \chi_3) \right\} \right], \quad (7.65a)$$

$$\chi_i \equiv - \int_{-\infty}^{+\infty} V^{(i)}(E, \sqrt{b_0^2 + z_0^2}) dz_0. \quad (7.65b)$$

Expanding (7.65a) to third order in V gives

$$f_E = \frac{1}{2\pi} \int d^2 b_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \left[\chi_1 + \left(\chi_2 + \frac{i}{2k_0} \chi_1^2 \right) + \left(\chi_3 + \frac{i}{k_0} \chi_1 \chi_2 - \frac{1}{6k_0^2} \chi_1^3 \right) + \dots \right], \quad (7.66)$$

where terms in (7.66) have been grouped according to whether they are of first, second or third order. The expansion (7.66) is next compared with the expansion of the Glauber amplitude (6.8) to third order, i.e. (see (6.9)),

$$f_{1s,1s}^G = \frac{1}{2\pi} \int d^2 b_0 \exp(i\mathbf{q} \cdot \mathbf{b}_0) \left[\langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle + \frac{i}{2k_0} \langle \psi_{1s} | \chi_0^2 | \psi_{1s} \rangle - \frac{1}{6k_0^2} \langle \psi_{1s} | \chi_0^3 | \psi_{1s} \rangle + \dots \right]. \quad (7.67)$$

It is now demanded that (7.66) and (7.67) agree to third order, this gives

$$\chi_1 = \langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle, \quad (7.68a)$$

$$\chi_2 = \frac{i}{2k_0} \{ \langle \psi_{1s} | \chi_0^2 | \psi_{1s} \rangle - \langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle^2 \}, \quad (7.68b)$$

$$\chi_3 = -\frac{1}{6k_0^2} \{ \langle \psi_{1s} | \chi_0^3 | \psi_{1s} \rangle - 3 \langle \psi_{1s} | \chi_0^2 | \psi_{1s} \rangle \langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle + 2 \langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle^3 \}, \quad (7.68c)$$

With χ_1, χ_2, χ_3 determined by (7.68) the relationship (7.65b) can be inverted to give

$$V^{(i)}(E, r_0) = \frac{1}{\pi} \int_{r_0}^{\infty} \frac{1}{(b_0^2 - r_0^2)^{1/2}} \frac{d}{db_0} \chi_i(b_0) db_0. \quad (7.69)$$

The above procedure produces the exact first-order result, i.e. (see (7.11)),

$$V^{(1)}(E, r_0) = \langle \psi_{1s} | V | \psi_{1s} \rangle, \quad (7.70)$$

and the second-order Glauber result (7.54). The new feature is the local approximation $V^{(3)}$ to the third-order optical potential matrix element $\langle \psi_{1s} | V^{\text{OPT}3} | \psi_{1s} \rangle$.

There are two interesting observations to make about the local approximation $V^{(3)}$ of (7.69). The first concerns its structure. A characteristic feature of the structure of V^{OPT} is that matrix elements of the form $\langle \psi_a | V | \psi_b \rangle$ where ψ_a and ψ_b are states from P-space can occur only in the first-order term (7.11) but not in higher orders (see (7.10)). The absence of these matrix elements from second order is obvious from (7.16). In the present context P-space consists only of the 1s state, this implies that the matrix element $\langle \psi_{1s} | V | \psi_{1s} \rangle$ should not appear in second and higher orders. Thus inserting a complete set of target eigenstates between each V of (7.13),

$$\langle \psi_{1s} | V^{\text{OPT}3} | \psi_{1s} \rangle = \sum_{\substack{m \neq 1s \\ n \neq 1s}} \langle \psi_{1s} | V | \psi_m \rangle G_0^+(m) \langle \psi_m | V | \psi_n \rangle G_0^+(n) \langle \psi_n | V | \psi_{1s} \rangle. \quad (7.71a)$$

$$G_0^+(m) \equiv \langle \psi_m | (E + i\eta - H_0)^{-1} | \psi_m \rangle, \quad (7.71b)$$

from which it is clear that $\langle \psi_{1s} | V | \psi_{1s} \rangle$ is absent.

Consider next $V^{(3)}$. Placing a complete set of target eigenstates between each χ_0 in the powers χ_0^3 and χ_0^2 of (7.68c) gives

$$\begin{aligned}\chi_3 &= \frac{1}{6k_0^2} \sum_{\substack{n \neq 1s}} \langle \psi_{1s} | \chi_0 | \psi_n \rangle \langle \psi_n | \chi_0 | \psi_{1s} \rangle \langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle \\ &\quad - \frac{1}{6k_0^2} \sum_{\substack{m \neq 1s \\ n \neq 1s}} \langle \psi_{1s} | \chi_0 | \psi_m \rangle \langle \psi_m | \chi_0 | \psi_n \rangle \langle \psi_n | \chi_0 | \psi_{1s} \rangle.\end{aligned}\quad (7.72)$$

The matrix element $\langle \psi_{1s} | V | \psi_{1s} \rangle$ appears in the first sum of (7.72) through the last term $\langle \psi_{1s} | \chi_0 | \psi_{1s} \rangle$ (see (6.9c)). Since $V^{(3)}$ is obtained from χ_3 via (7.69) it follows that this local approximation incorporates the matrix element $\langle \psi_{1s} | V | \psi_{1s} \rangle$. $V^{(3)}$ therefore differs from the exact $\langle \psi_{1s} | V^{\text{OPT3}} | \psi_{1s} \rangle$ in an important structural respect. How this has come about sheds a very interesting light upon the nature of local potential approximations to the optical potential [55].

The second observation concerns the large r_0 behaviour of the local approximation $V^{(3)}$. In reference [51] it was pointed out that $V^{(3)}$ varies as r_0^{-5} at long range. In section 7.2.1 we saw that the long-range behaviour of the second-order optical potential $V_{1s, 1s}^{\text{OPT2}}$ is given by the adiabatic potential $V_{1s, 1s}^{\text{AD2}}$ of (4.7). Remembering that $V_{1s, 1s}^{\text{AD2}}$ is just the second-order perturbed energy of the atom in the presence of a fixed electron, it is not unreasonable to speculate that the effective long-range variation of $V_{1s, 1s}^{\text{OPT3}}$ may be given by the corresponding third-order potential energy:

$$V_{1s, 1s}^{\text{AD3}}(r_0) = \sum_{m \neq 1s} \sum_{n \neq 1s} \frac{\langle \psi_{1s} | V | \psi_m \rangle \langle \psi_m | V | \psi_n \rangle \langle \psi_n | V | \psi_{1s} \rangle}{(\varepsilon_{1s} - \varepsilon_m)(\varepsilon_{1s} - \varepsilon_n)}.\quad (7.73)$$

For large r_0 the potential (7.73) varies as* r_0^{-7} which is a much more rapid fall-off than that of the local approximation $V^{(3)}$.

In support of the above speculation I would make two points. The first is the example of table 5. In this table the values of (see (4.10) and (4.11))

Table 5
Contribution of 2p as an intermediate state to the partial wave amplitudes of the third-order optical and adiabatic potentials for electron-H (1s) elastic scattering. The amplitudes listed are defined according to (7.74) and (7.75), l is the angular momentum and $k_0 = 1$ a.u. is the impact momentum

l	Adiabatic Real	Optical potential Real	Imaginary
2	$+0.111 \times 10^{-1}$	$+0.938 \times 10^{-2}$	$+0.359 \times 10^{-1}$
4	-0.641×10^{-3}	-0.742×10^{-3}	-0.120×10^{-3}
6	-0.387×10^{-3}	-0.437×10^{-3}	-0.225×10^{-4}
8	-0.119×10^{-3}	-0.121×10^{-3}	-0.93×10^{-6}
10	-0.379×10^{-4}	-0.376×10^{-4}	-0.35×10^{-7}
14	-0.561×10^{-5}	-0.563×10^{-5}	about 1×10^{-9}

* To contribute to this leading term ψ_m and ψ_n must both be P-states or one a P-state and the other a D-state.

$$-4(j_l(k_0 r_0) Y_{l0}(\hat{r}_0) | V_{1s, 1s}^{\text{OPT3}}(2p) | j_l(k_0 r'_0) Y_{l0}(\hat{r}'_0) \rangle) \quad (7.74)$$

and

$$-4(j_l(k_0 r_0) Y_{l0}(\hat{r}_0) | V_{1s, 1s}^{\text{AD3}}(2p) | j_l(k_0 r_0) Y_{l0}(\hat{r}_0) \rangle) \quad (7.75)$$

are listed for an incident momentum $k_0 = 1$ a.u.; here $V_{1s, 1s}^{\text{AD3}}(2p)$ and $V_{1s, 1s}^{\text{OPT3}}(2p)$ are the $m = n = 2p$ contributions to (7.73) and (7.71a) respectively. It is seen from the table that for increasing l the imaginary part of (7.74) dies away and the real part approaches (7.75). Thus at least the effective behaviour of $V_{1s, 1s}^{\text{OPT3}}(2p)$ at long range is given by $V_{1s, 1s}^{\text{AD3}}(2p)$, which varies as r_0^{-7} .

The second point. In section 7.2.2.3 we saw that the local second-order approximation* $V^{(2)}$ of (7.69) had a spurious r_0^{-3} long-range tail, the correct large distance variation of $V_{1s, 1s}^{\text{OPT2}}$ being r_0^{-4} . It would not be surprising if this spurious behaviour were carried into $V^{(3)}$ giving it a slower fall-off than the correct third-order result.

Clearly the long-range behaviour of $V^{(3)}$ and $V_{1s, 1s}^{\text{OPT3}}$ is an area requiring further investigation.

7.4. Calculations

Alton et al. [64] have made an *exact* evaluation of $V_{1s, 1s}^{\text{OPT2}}$ for electron-H (1s) elastic scattering at impact energies up to about 90 eV (taking $P = |\psi_{1s}\rangle\langle\psi_{1s}|$). By solving (see (7.9))

$$(\nabla_0^2 - 2V_{1s, 1s} - 2V_{1s, 1s}^{\text{OPT2}} + k_0^2)F_{1s}(\mathbf{r}_0) = 0 \quad (7.76)$$

they calculate cross sections which do not include electron exchange. Unfortunately electron exchange is important in this energy range. Coulter and Garrett [123] have tried to remedy this defect by incorporating exchange in a static exchange approximation, i.e., by solving

$$(\nabla_0^2 - 2V_{1s, 1s}^{\text{SE}} - 2V_{1s, 1s}^{\text{OPT2}} + k_0^2)F_{1s}(\mathbf{r}_0) = 0, \quad (7.77)$$

where $V_{1s, 1s}^{\text{SE}}$ is the (non-local) static exchange potential. However, Coulter and Garrett concentrate upon extracting total inelastic cross sections from their results [124] rather than on giving a complete picture of elastic scattering over the energy range.

Scott and Bransden [125] have solved (7.77) using a pseudostate approximation to $V_{1s, 1s}^{\text{OPT2}}$. Where comparison is possible their results are in quite good agreement with those of Coulter and Garrett. While this agreement is not perfect, it is reasonable to conclude that the pseudostate approximation gives a realistic representation of the exact $V_{1s, 1s}^{\text{OPT2}}$. Scott and Bransden's elastic differential cross sections are shown in fig. 24 for the energy range 1.22 eV to 50 eV. At 50 eV there is good agreement with experiment. With decreasing energy this agreement is lost at the important forward angles, until, at the lowest energy, 1.22 eV, theory once more gives an acceptable cross section.

It is not surprising that (7.77) works at high energies but not at lower energies; after all

$$V_{1s, 1s} + V_{1s, 1s}^{\text{OPT2}} \quad (7.78)$$

* In section 7.2.2.3 $V^{(2)}$ is called iV_{abs}^G .

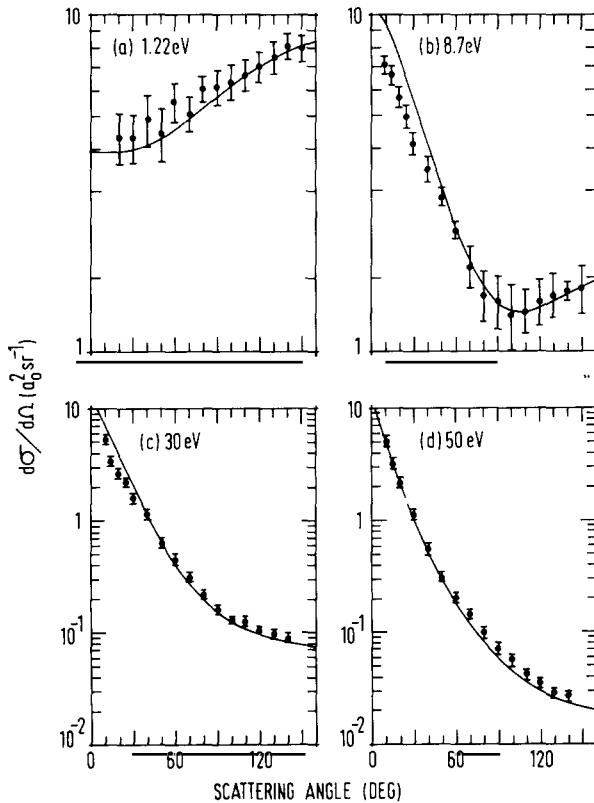


Fig. 24. Differential cross section for elastic scattering of electrons by H(1s) at (a) 1.22 eV, (b) 8.7 eV, (c) 30 eV and (d) 50 eV: (—) theoretical cross section of Scott and Bransden (SOPM) [125]; (●) experimental data of Williams [161, 164]. (Taken from Scott and Bransden [125], figs. 1 and 2.)

is really a high energy (perturbative) approximation to the full optical potential. At lower energies it is to be expected that one may have to go further than second order and/or include exchange properly in the optical potential formalism [8, 43, 54, 126, 127].

Historically, simple approximations based upon static exchange plus polarization potential/polarized orbitals have been regarded as respectable methods for dealing with low energy elastic scattering [128, 129, and references therein]. Often such methods are in essence just approximations to (7.77) (and usually adiabatic approximations), for example [129]. The results of fig. 24 put such methods under suspicion – they work perhaps because, in approximating (7.77), they make allowance in some mysterious way for effects, such as those mentioned in the previous paragraph, which are missing from (7.77) (the calculations and discussion in [129] are enlightening).

The second-order potential method (SOPM) of Bransden and Coleman [46] is an approximation to the coupled equations (7.9) in which the optical potential is treated only as far as second order. Early applications of this approximation to electron scattering adopted a semi-classical solution to (7.9) and usually neglected electron exchange [130–136]. These last two simplifications are rather gross and for a while concealed the strength of the SOPM. The first proper, i.e., partial wave, solutions of (7.9) including exchange, in the static-exchange approximation, were reported in [137, 138]. Until fairly recently the second-order optical potential terms were always evaluated in the closure approximation;

this has now given way to pseudostate methods [53, 125, 136, 139]. SOPM wavefunctions have been used in distorted-wave calculations of excitation and ionization [73, 74, 78, 140, 141]; the method has also been applied to proton impact where a semi-classical solution of (7.9) is valid [130, 131, 133, 136, 142]. In all of the references quoted above, except [134], the target has been either atomic hydrogen or helium; in [134] hydrogenic ions were considered.

Second-order potentials localized according to (7.36) have been used in calculations on elastic electron/positron-H (1s) [32, 51], electron-H (2s) [118] and electron-He (1^1S) [32, 78] scattering, and on the transitions H (1s) \rightarrow H (2s) [32, 69] and Li (2s) \rightarrow Li (3s) [76]. In addition (7.36) has been generalized to S \rightarrow P excitations and applied to the $1^1S \rightarrow 2^1P$ transition in He [23, 70].

McCarthy and co-workers have studied approximations to the optical potential for electron-hydrogen scattering which go beyond the second-order approximation although they are of the same kind of style [111–113, 143]; in particular they attempt to make full allowance for exchange. This should be contrasted with the work of Coulter and Garrett [123] and Scott and Bransden [125], where exchange is inserted in a cavalier way through the static-exchange approximation. Unfortunately McCarthy et al. use the localization approximation (7.33) which came in for some criticism in section 7.2.2.2, especially concerning long-range polarization behaviour.

McCarthy and co-workers have applied their methods to electron-H scattering in one-state ($P = 1s$) [144, 145], three-state ($P = 1s, 2s, 2p$) [143, 146] and six-state ($P = 1s, 2s, 2p, 3s, 3p, 3d$) [147] approximations. It should be noted that in the three- and six-state calculations the optical potential is treated only to first order in the non-diagonal couplings, i.e., from (7.7) and (7.9) (and neglecting exchange for simplicity),

$$(\nabla_0^2 + k_n^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^M \{\langle \psi_n | V | \psi_m \rangle + \delta_{m,n} \langle \psi_n | VQ[Q(E + i\eta - H_0 - V)Q]^{-1} QV | \psi_m \rangle\} F_m^+(\mathbf{r}_0). \quad (7.79)$$

In fact in the six-state calculation only the term $\langle \psi_n | V | \psi_m \rangle$ is kept in the curly bracket of (7.79) when $n = 3s, 3p, 3d$. As a result of these simplifications the calculated $1s \rightarrow 2s, 2p$ and $1s \rightarrow 3s, 3p, 3d$ amplitudes contain only the $n = 0$ to M contributions to the second Born term, i.e.,

$$\sum_{n=0}^M f_{f0}^{B2;n}. \quad (7.80)$$

The contributions from $n > M$ require the non-diagonal coupling $\langle \psi_f | VQ[Q(E + i\eta - H_0 - V)Q]^{-1} QV | \psi_0 \rangle$ which has been omitted from (7.79). For the three-state calculation ($1s, 2s, 2p$) (7.80) is exactly what is obtained in second order from an ordinary three-state $1s-2s-2p$ close-coupling calculation. It comes as no surprise to find that McCarthy and Stelbovics' three-state $1s \rightarrow 2s, 2p$ results are not greatly different from those of three-state close-coupling. The same is found for the six-state ($1s, 2s, 2p, 3s, 3p, 3d$) calculation, adding the $3s, 3p$ and $3d$ contributions to (7.80) does not make a great deal of difference. However, including all the intermediate states in the second Born term does lead to $n = 2$ excitation cross sections significantly different from three-state close-coupling, at least for $1s \rightarrow 2s$, as the DWSBA calculations of Kingston and Walters (section 5.3.2) show [9, 32]; or, in other words, the terms $\langle \psi_f | VQ[Q(E + i\eta - H_0 - V)Q]^{-1} QV | \psi_0 \rangle$ omitted by McCarthy et al. are very important for the excitation $\psi_0 \rightarrow \psi_f$.

Other related papers will be found in [77, 148–150]. The optical potential approximations of McCarthy et al. will be given fuller consideration in section 8.3.

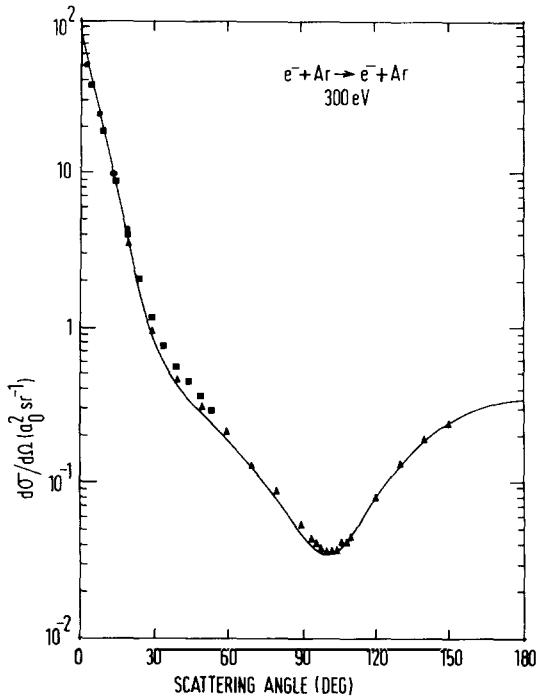


Fig. 25. Differential cross section for elastic scattering of electrons by Ar at 300 eV. Curve: calculation using (7.44) and (7.55). Experimental data: (●) Bromberg [15]; (▲) Williams and Willis [79]; (■) Jansen et al. [166]. (Taken from Joachain et al. [38], fig. 2c.)

Approximate local second-order potentials (section 7.2.2.3) have been used in calculations of e^\pm elastic scattering by He and Ne [115, 116, 122] and by Ar [38, 121] (fig. 25) and of electron elastic scattering by H [122], Li [88], Na [89] and K [92]. In all cases of electron scattering exchange has been included using a local exchange potential [122, 151]. Such potentials are essentially just approximations to the exchange part of static exchange.

8. Exchange

In fig. 26 the DWSBA of Dewangan and Walters [37], the EBS approximation of Byron and Joachain [50] and the SOPM of Winters et al. [138] are compared with experimental data on electron-He (1^1S) elastic scattering at 100 eV. There are two striking things about this figure. The first is the measure of agreement between the three calculations. The second is the manner in which the theoretical cross sections diverge from experiment at the smaller angles—the theoretical numbers become too large. This breakdown pattern is also observed in electron-H (1s) (fig. 24 and [32]) and electron-Ne [37] elastic scattering with decreasing impact energy.

It is thought that the breakdown illustrated in fig. 26 arises primarily from an inadequate treatment of exchange effects [43, 54, 62]. In the DWSBA and SOPM calculations of fig. 26 exchange is included only in the static-exchange approximation. In the EBS cross section the Ochkur approximation for exchange has been used, this can be considered as an approximation to static-exchange. A notable feature of nearly all of the approximations so far studied in this article has been the casual way in which exchange has been handled. This attitude is all right when the approximation is to be used at high energies where exchange is not very important; however, it is to be expected that such cavalier

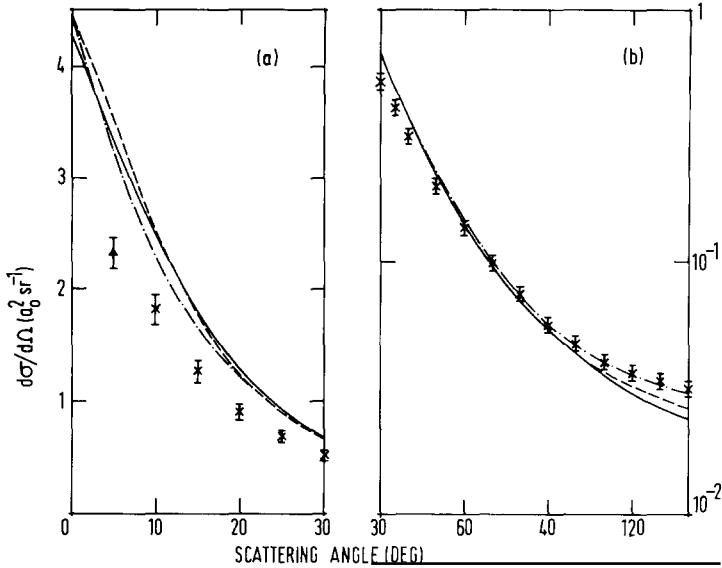


Fig. 26. Differential cross section for elastic scattering of electrons by He (1^1S) at 100 eV: (a) 0° to 30° ; (b) 30° to 140° . Curves: (—) DWSBA of [37]; (---) SOPM of [138]; (-·-·-) EBS approximation of [50]. Experimental data: (x) Register et al. [165]; (Δ) Jansen et al. [166]. (Only the measurement at 5° is shown, at other angles the results of Jansen et al. are in agreement with those of Register et al.)

treatment of exchange will eventually rebound on the approximation as it is pushed down to lower energies.

In this section I shall consider exchange in the context of perturbative methods. The situation at present is not really very satisfactory. I shall therefore content myself with a statement of what is known rather than with the presentation of a well-formed theory. Further, in order to make a simple illustration of principles, I shall assume everywhere in this section that the target atom is atomic hydrogen.

8.1. Notation

The Hamiltonian for electron scattering by atomic hydrogen is

$$H \equiv -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - 1/r_0 - 1/r_1 + 1/r_{01}. \quad (8.1)$$

The direct scattering amplitude for the transition $\psi_0 \rightarrow \psi_f$ is given by (2.7))

$$f_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle \mathbf{k}_f(\mathbf{r}_0)\psi_f(\mathbf{r}_1)| V(\mathbf{r}_0, \mathbf{r}_1)| \Psi^+(\mathbf{r}_0, \mathbf{r}_1) \rangle, \quad (8.2a)$$

$$= -(1/2\pi)\langle \Psi^-(\mathbf{r}_0, \mathbf{r}_1)| V(\mathbf{r}_0, \mathbf{r}_1)| \mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1) \rangle, \quad (8.2b)$$

while the exchange amplitude is

$$g_{f0}(\mathbf{k}_f, \mathbf{k}_0) = -(1/2\pi)\langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)| V(\mathbf{r}_1, \mathbf{r}_0)| \Psi^+(\mathbf{r}_0, \mathbf{r}_1) \rangle \quad (8.3a)$$

$$= -(1/2\pi)\langle \Psi^-(\mathbf{r}_1, \mathbf{r}_0)| V(\mathbf{r}_0, \mathbf{r}_1)| \mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1) \rangle. \quad (8.3b)$$

In (8.2) and (8.3)

$$V(\mathbf{r}_0, \mathbf{r}_1) \equiv -1/r_0 + 1/r_{01} . \quad (8.4)$$

The Ψ^\pm are solutions of

$$H\Psi^\pm = (\frac{1}{2}k_0^2 + \varepsilon_0)\Psi^\pm , \quad (8.5)$$

satisfying the boundary conditions

$$\Psi^+(\mathbf{r}_0, \mathbf{r}_1) \xrightarrow[r_1 \text{ finite}]{r_0 \rightarrow \infty} \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)\psi_0(\mathbf{r}_1) + \text{outgoing scattered waves} , \quad (8.6a)$$

$$\xrightarrow[r_0 \text{ finite}]{r_1 \rightarrow \infty} \text{only outgoing scattered waves} , \quad (8.6b)$$

and

$$\Psi^-(\mathbf{r}_0, \mathbf{r}_1) \xrightarrow[r_1 \text{ finite}]{r_0 \rightarrow \infty} \exp(i\mathbf{k}_f \cdot \mathbf{r}_0)\psi_f(\mathbf{r}_1) + \text{ingoing scattered waves} , \quad (8.7a)$$

$$\xrightarrow[r_0 \text{ finite}]{r_1 \rightarrow \infty} \text{only ingoing scattered waves} , \quad (8.7b)$$

Ψ^\pm satisfy the Lippmann–Schwinger equations ((3.1)):

$$\Psi^+(\mathbf{r}_0, \mathbf{r}_1) = \exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)\psi_0(\mathbf{r}_1) + G_0^+(0, 1)V(\mathbf{r}_0, \mathbf{r}_1)\Psi^+(\mathbf{r}_0, \mathbf{r}_1) , \quad (8.8a)$$

$$\Psi^-(\mathbf{r}_0, \mathbf{r}_1) = \exp(i\mathbf{k}_f \cdot \mathbf{r}_0)\psi_f(\mathbf{r}_1) + G_0^-(0, 1)V(\mathbf{r}_0, \mathbf{r}_1)\Psi^-(\mathbf{r}_0, \mathbf{r}_1) , \quad (8.8b)$$

$$G_0^\pm(0, 1) \equiv \lim_{\eta \rightarrow 0^+} (E - K_0 - H_1 \pm i\eta)^{-1} , \quad (8.8c)$$

$$E = \frac{1}{2}k_0^2 + \varepsilon_0 = \frac{1}{2}k_f^2 + \varepsilon_f , \quad (8.8d)$$

$$K_i \equiv -\frac{1}{2}\nabla_i^2 , \quad i = 0, 1 , \quad (8.8e)$$

$$H_i \equiv -\frac{1}{2}\nabla_i^2 - 1/r_i , \quad i = 0, 1 , \quad (8.8f)$$

8.2. The Born series for the exchange amplitude

Starting from (8.3a) and using (8.8a) we may generate the Born series

$$g_{f0}(\mathbf{k}_f, \mathbf{k}_0) = \sum_{n=1}^{\infty} g_{f0}^{Bn+}(\mathbf{k}_f, \mathbf{k}_0) , \quad (8.9a)$$

$$g_{f0}^{Bn+}(\mathbf{k}_f, \mathbf{k}_0) \equiv -(1/2\pi)\langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)|V(\mathbf{r}_1, \mathbf{r}_0)(G_0^+(0, 1)V(\mathbf{r}_0, \mathbf{r}_1))^{n-1}|\mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle. \quad (8.9b)$$

Alternatively, starting from (8.3b) and employing (8.8b) we get

$$g_{f0}(\mathbf{k}_f, \mathbf{k}_0) = \sum_{n=1}^{\infty} g_{f0}^{Bn-}(\mathbf{k}_f, \mathbf{k}_0), \quad (8.10a)$$

$$g_{f0}^{Bn-}(\mathbf{k}_f, \mathbf{k}_0) \equiv -(1/2\pi)\langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)|(V(\mathbf{r}_1, \mathbf{r}_0)G_0^+(1, 0))^{n-1}V(\mathbf{r}_0, \mathbf{r}_1)|\mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle. \quad (8.10b)$$

The expansion (8.9) is called the “post” form of the Born series, (8.10) is the “prior” form.

It is a trivial matter to show that

$$g_{f0}^{B1+} = g_{f0}^{B1-}. \quad (8.11)$$

However, in general,

$$g_{f0}^{Bn+} \neq g_{f0}^{Bn-}, \quad n \geq 2. \quad (8.12)$$

One exception to (8.12) is the case of elastic scattering off an S-state. Despite the inequality (8.12) the sum of the series (8.9a) and (8.10a) must be the same, i.e., g_{f0} . In the rest of this section I shall confine myself to the post form (8.9), unless otherwise indicated. An important point to note is that there is an infinite number of possible Born expansions of g_{f0} , depending upon the choice of expanding potential – (8.9) and (8.10) are just the two most obvious possibilities and perhaps not the best.

If the electron-electron interaction, $1/r_{01}$, is “switched off” then, from (8.1), (8.5) and (8.6), Ψ^+ becomes

$$\Psi^+(\mathbf{r}_0, \mathbf{r}_1) = (2\pi)^{3/2}\psi_{\mathbf{k}_0}^+(\mathbf{r}_0)\psi_0(\mathbf{r}_1), \quad (8.13)$$

where $\psi_{\mathbf{k}_0}^+(\mathbf{r}_0)$ is the Coulomb scattering wavefunction for an electron incident with momentum \mathbf{k}_0 upon the nuclear potential $-1/r_0$, the + once more indicates outgoing scattered waves. It is assumed that the normalization of $\psi_{\mathbf{k}}^+$ is such that

$$\langle \psi_{\kappa}^+ | \psi_{\kappa'}^+ \rangle = \delta(\kappa - \kappa'). \quad (8.14)$$

Putting (8.13) in (8.3a) (with $1/r_{01}$ off) gives

$$\begin{aligned} g_{f0}(\mathbf{k}_f, \mathbf{k}_0) &= -(1/2\pi)\langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)| -1/r_1 |\psi_{\mathbf{k}_0}^+(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle \\ &= 0, \end{aligned} \quad (8.15)$$

due to orthogonality of ψ_f and $\psi_{\mathbf{k}_0}^+$ (ψ_0 and ψ_f are bound states). This result is physically obvious: if $1/r_{01}$ is switched off then the two electrons do not interact and so cannot be exchanged. The result (8.15) has important implications for the Born series (8.9) and (8.10).

It is a simple matter to show that when $1/r_{01}$ is set to zero the Born terms $g_{f0}^{Bn\pm}$ do not vanish. For

example, g_{f0}^{B1+} then becomes

$$g_{f0}^{B1+} = -(1/2\pi) \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -\frac{1}{r_1} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle \neq 0. \quad (8.16)$$

However, since the full amplitude g_{f0} is zero there must be cancellations between the individual Born terms to produce this result. In other words, from (8.4) and (8.9),*

$$\sum_{n=1}^{\infty} -\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -\frac{1}{r_1} \left(G_0^+(0, 1) \left(-\frac{1}{r_0} \right) \right)^{n-1} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle = 0. \quad (8.17)$$

In a Born approximation only a finite number of terms from the Born series (8.9) and (8.10) are used; then the cancellation (8.17) cannot take place. It has therefore become customary to alter the Born approximation so that the terms which contribute to (8.17), and would therefore be cancelled by higher orders, are eliminated from the finite approximation. For example, the first Born approximation is

$$g_{f0}^{\text{Born } 1} = g_{f0}^{B1+} = g_{f0}^{B1-} = -\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -\frac{1}{r_1} + \frac{1}{r_{01}} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle. \quad (8.18)$$

This is altered to

$$\tilde{g}_{f0}^{\text{Born } 1} \equiv \tilde{g}_{f0}^{B1} \equiv -\frac{1}{2\pi} \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | \frac{1}{r_{01}} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle \quad (8.19)$$

by dropping the $-1/r_1$ contribution which according to (8.17) will be cancelled by higher-order Born terms.

The alteration of higher-order Born approximations is somewhat more problematical. Consider the second Born approximation

$$g_{f0}^{\text{Born } 2} = g_{f0}^{B1+} + g_{f0}^{B2+}. \quad (8.20)$$

Using the spectral representation (4.1) of the Green's function $G_0^+(0, 1)$ the second Born term may be written

$$g_{f0}^{B2+} = \sum_n g_{f0}^{B2+; n}, \quad (8.21a)$$

$$g_{f0}^{B2+; n} \equiv -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int d\mathbf{k} \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -1/r_1 + 1/r_{01} | \mathbf{k}(\mathbf{r}_0) \psi_n(\mathbf{r}_1) \rangle \\ \times \frac{\langle \mathbf{k}(\mathbf{r}_0) \psi_n(\mathbf{r}_1) | -1/r_0 + 1/r_{01} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle}{k_n^2 - k^2 + i\eta}. \quad (8.21b)$$

* Because of the long-range nature of the Coulomb potential (8.17) is not mathematically sound. As far as this kind of argument is concerned the Coulomb potential is to be considered to be of the form $-1/r$ with a cutoff to zero at arbitrarily large distance.

Since the nuclear potential $-1/r_0$ does not contribute to (8.21b) when $n \neq 0$, because of the orthogonality of ψ_0 and ψ_n , there is no need to alter $g_{f0}^{B2+;n}$ for $n \neq 0$ – it will automatically go to zero when $1/r_{01}$ is switched off. The only term we need to adjust is $g_{f0}^{B2+;0}$. This term may be separated into two pieces:

$$\begin{aligned} g_{f0}^{B2+;0} = & -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int dk \langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)|-1/r_1|\mathbf{k}(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle \\ & \times \frac{\langle \mathbf{k}(\mathbf{r}_0)\psi_0(\mathbf{r}_1)|-1/r_0|\mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle}{k_0^2 - k^2 + i\eta} + g_{f0}^{B2+;0}(\text{rest}). \end{aligned} \quad (8.22)$$

It is the first part of (8.22) which is cancelled by the other terms in the Born series. If the Coulombic interaction were of short range rather than long range the correct thing to do would be to remove the first term in (8.22) and therefore replace $g_{f0}^{B2+;0}$ by $g_{f0}^{B2+;0}(\text{rest})$. However, because of the long-range nature of the nuclear potentials the first term in (8.22) is infinite; since $g_{f0}^{B2+;0}$ is finite this means that $g_{f0}^{B2+;0}(\text{rest})$ is infinite; replacement of $g_{f0}^{B2+;0}$ by $g_{f0}^{B2+;0}(\text{rest})$ is therefore not acceptable.

In the papers of Byron, Joachain and Potvliege [28, 98] $g_{f0}^{B2+;0}$ is altered by following the example of g_{f0}^{B1+} in (8.18) and (8.19), i.e., by simply dropping the nuclear term $-1/r_1$. Thus

$$\begin{aligned} g_{f0}^{B2+;0} \rightarrow \tilde{g}_{f0}^{B2+;0} \equiv & -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int dk \langle \mathbf{k}_f(\mathbf{r}_1)\psi_f(\mathbf{r}_0)|1/r_{01}|\mathbf{k}(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle \\ & \times \frac{\langle \mathbf{k}(\mathbf{r}_0)\psi_0(\mathbf{r}_1)|-1/r_0+1/r_{01}|\mathbf{k}_0(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle}{k_0^2 - k^2 + i\eta}. \end{aligned} \quad (8.23)$$

While this prescription cannot be rigorously derived from theory it is simple and sensible. A reasonable form for the second Born approximation to exchange therefore is

$$\tilde{g}_{f0}^{\text{Born } 2+} = \tilde{g}_{f0}^{B1} + \tilde{g}_{f0}^{B2+;0} + \sum_{n \neq 0} g_{f0}^{B2+;n}. \quad (8.24)$$

The amplitude (8.24) satisfies the requirement of going to zero when $1/r_{01}$ is switched off.

It might be thought that a sensible two-state (ψ_0 and ψ_f)^{*} approximation to (8.24) would be

$$\tilde{g}_{f0}^{\text{Born } 2+} = \tilde{g}_{f0}^{B1} + \tilde{g}_{f0}^{B2+;0} + \tilde{g}_{f0}^{B2+;f}. \quad (8.25)$$

However, let us examine (8.25). In (8.19), (8.21b) and (8.23) matrix elements of the form $\langle \mathbf{k}_1(\mathbf{r}_1)\psi_1(\mathbf{r}_0)|\dots|\mathbf{k}_2(\mathbf{r}_0), \psi_2(\mathbf{r}_1)\rangle$ may be interpreted as representing exchange transitions while those of the form $\langle \mathbf{k}_1(\mathbf{r}_0)\psi_1(\mathbf{r}_1)|\dots|\mathbf{k}_2(\mathbf{r}_0)\psi_2(\mathbf{r}_1)\rangle$ correspond to direct transitions. With this in mind \tilde{g}_{f0}^{B1} is interpreted as a single exchange transition in which the atom goes from ψ_0 to ψ_f . In $\tilde{g}_{f0}^{B2+;0}$ and $\tilde{g}_{f0}^{B2+;f}$ on the other hand the incident electron first undergoes direct scattering which is then followed by exchange scattering to the final state. But what about transitions in which the incident electron is first exchange scattered and then directly scattered? These would be represented by terms of the form

^{*} The remarks which follow are easily modified for the case of elastic scattering, $\psi_0 = \psi_f$.

$$\begin{aligned} & -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int dk \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -1/r_1 + 1/r_{01} | \mathbf{k}(\mathbf{r}_1) \psi_0(\mathbf{r}_0) \rangle \frac{\langle \mathbf{k}(\mathbf{r}_1) \psi_0(\mathbf{r}_0) | -1/r_0 + 1/r_{01} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle}{k_0^2 - k^2 + i\eta} \\ & = g_{f0}^{B2-;0} \end{aligned} \quad (8.26a)$$

(see (8.10b)) and

$$\begin{aligned} & -\frac{1}{8\pi^4} \lim_{\eta \rightarrow 0+} \int dk \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | -1/r_1 + 1/r_{01} | \mathbf{k}(\mathbf{r}_1) \psi_f(\mathbf{r}_0) \rangle \frac{\langle \mathbf{k}(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | 1/r_{01} | \mathbf{k}_0(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle}{k_f^2 - k^2 + i\eta} \\ & = \tilde{g}_{f0}^{B2-;f} \end{aligned} \quad (8.26b)$$

where \sim in (8.26b) means that a correction analogous to (8.23) has been applied.

The term (8.26a) results from (8.21b) on making the replacements

$$(2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}_0) \rightarrow \psi_0(\mathbf{r}_0), \quad (8.27a)$$

$$k^2 \rightarrow 2\varepsilon_0 \quad \text{in the denominator}, \quad (8.27b)$$

$$\psi_n(\mathbf{r}_1) \rightarrow (2\pi)^{-3/2} \exp(i\mathbf{k} \cdot \mathbf{r}_1), \quad (8.27c)$$

$$k_m^2 = k_0^2 + 2(\varepsilon_0 - \varepsilon_n) \rightarrow k_0^2 + 2(\varepsilon_0 - \frac{1}{2}k^2) \quad \text{in the denominator}. \quad (8.27d)$$

This suggests that (8.26a) is contained, in some sense, in the continuum part, see (8.27c) and (8.27d), of the sum

$$\sum_{n \neq 0, f} g_{f0}^{B2+;n} \quad (8.28)$$

omitted in going from (8.24) to (8.25). A similar argument applies to (8.26b).

The above result implies, in agreement with intuition and with the kind of structure also observed in the two-state close-coupling approximation, that a consistent two-state approximation to (8.24) is not (8.25) but rather (8.25) plus (8.26), i.e.,

$$\tilde{g}_{f0}^{\text{Born } 2+} = \tilde{g}_{f0}^{B1} + \tilde{g}_{f0}^{B2+;0} + g_{f0}^{B2-;0} + g_{f0}^{B2+;f} + \tilde{g}_{f0}^{B2-;f}. \quad (8.29)$$

Further, it seems reasonable that all second Born terms in (8.29) should be treated on the same basis, i.e. $g_{f0}^{B2-;0}$ and $g_{f0}^{B2+;f}$ should be replaced by their \sim counterparts. This finally gives the two-state approximation of Byron et al. [28]:

$$\tilde{g}_{f0}^{\text{Born } 2, \text{ BJP}} = \tilde{g}_{f0}^{B1} + \tilde{g}_{f0}^{B2+;0} + \tilde{g}_{f0}^{B2-;0} + \tilde{g}_{f0}^{B2+;f} + \tilde{g}_{f0}^{B2-;f}. \quad (8.30)$$

Substituting (8.8a) in (8.3a) and using (4.1) and (8.9b) gives for the exchange amplitude

$$\begin{aligned} g_{f0}(\mathbf{k}_f, \mathbf{k}_0) &= g_{f0}^{B1+}(\mathbf{k}_f, \mathbf{k}_0) \\ & - \frac{1}{8\pi^4} \sum_n \lim_{\eta \rightarrow 0+} \int \frac{dk \langle \mathbf{k}_f(\mathbf{r}_1) \psi_f(\mathbf{r}_0) | V(\mathbf{r}_1, \mathbf{r}_0) | \mathbf{k}(\mathbf{r}_0) \psi_n(\mathbf{r}_1) \rangle \langle \mathbf{k}(\mathbf{r}_0) \psi_n(\mathbf{r}_1) | V(\mathbf{r}_0, \mathbf{r}_1) | \Psi^+(\mathbf{r}_0, \mathbf{r}_1) \rangle}{k_n^2 - k^2 + i\eta}. \end{aligned} \quad (8.31)$$

The first matrix element in (8.31) is the half-off-energy-shell* first Born exchange amplitude (see (8.9b))

$$-2\pi g_{fn}^{B1+}(\mathbf{k}_f, \mathbf{k}), \quad (8.32)$$

while the second matrix element is the half-off-energy-shell* direct amplitude (see (8.2a))

$$-2\pi f_{n0}(\mathbf{k}, \mathbf{k}_0). \quad (8.33)$$

Using (8.32) and (8.33), (8.31) may be rewritten

$$g_{f0}(\mathbf{k}_f, \mathbf{k}_0) = g_{f0}^{B1+}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi^2} \sum_n \lim_{\eta \rightarrow 0^+} \int \frac{d\mathbf{k} g_{fn}^{B1+}(\mathbf{k}_f, \mathbf{k}) f_{n0}(\mathbf{k}, \mathbf{k}_0)}{k_n^2 - k^2 + i\eta}. \quad (8.34)$$

Making a two-state approximation to (8.34) in the spirit of (8.30) yields the *non-perturbative* result

$$\begin{aligned} g_{f0}^{TS}(\mathbf{k}_f, \mathbf{k}_0) &= \tilde{g}_{f0}^{B1}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi^2} \int \frac{d\mathbf{k} \tilde{g}_{f0}^{B1}(\mathbf{k}_f, \mathbf{k}_0) f_{00}(\mathbf{k}, \mathbf{k}_0)}{k_0^2 - k^2 + i\eta} \\ &\quad - \frac{1}{2\pi^2} \int \frac{d\mathbf{k} f_{f0}(\mathbf{k}_f, \mathbf{k}) \tilde{g}_{00}^{B1}(\mathbf{k}, \mathbf{k}_0)}{k_0^2 - k^2 + i\eta} - \frac{1}{2\pi^2} \int \frac{d\mathbf{k} \tilde{g}_{ff}^{B1}(\mathbf{k}_f, \mathbf{k}) f_{f0}(\mathbf{k}, \mathbf{k}_0)}{k_f^2 - k^2 + i\eta} \\ &\quad - \frac{1}{2\pi^2} \int \frac{d\mathbf{k} f_{ff}(\mathbf{k}_f, \mathbf{k}) \tilde{g}_{f0}^{B1}(\mathbf{k}, \mathbf{k}_0)}{k_f^2 - k^2 + i\eta}. \end{aligned} \quad (8.35)$$

The UEBS exchange amplitude, g_{f0}^{UEBS} , of Byron et al. [28], which was mentioned in section 6.5, is obtained from (8.35) on replacing f by its UEBS approximation (6.24). In practice these authors have only used g_{f0}^{UEBS} in elastic scattering. The amplitude g_{00}^{UEBS} is derived from a one-state approximation to (8.34); the static-exchange approximation (section 8.3) is also a one-state approximation. As far as exchange is concerned, therefore, g_{00}^{UEBS} does not go very much further than the static-exchange approximation, in particular, like static-exchange, it does not take account of those exchange couplings which are presumed necessary to correct the erroneous behaviour of the theoretical cross sections of fig. 26.

Byron et al. [98] have employed the approximation (8.30) in a calculation of elastic scattering by H (1s) at 100 eV. This calculation differs from that reported in [28] only in the use of (8.30) rather than g_{00}^{UEBS} for the exchange amplitude. Comparing the 100 eV figures in these two references it is clear that there is a noticeable difference between the approximation (8.30) and g_{00}^{UEBS} . Thus, at 140° the cross section of [98] is about 25% larger than that of [28]. Of the two approximations, (8.30) and g_{00}^{UEBS} , the non-perturbative g_{00}^{UEBS} is preferable. Byron et al. [98] have also used a reduced form of (8.30) for the 1s → 2s excitation of H, namely,

$$\tilde{g}_{f0}^{B1} + \tilde{g}_{f0}^{B2+;0} + \tilde{g}_{f0}^{B2-;f}. \quad (8.36)$$

There is good reason to believe that the leading contribution to high energy large momentum transfer exchange scattering is contained in the second Born terms

* "Half-off" since k_0 and k_f are fixed by energy conservation, i.e., $k_0^2 + 2\varepsilon_0 = E = k_f^2 + 2\varepsilon_f$, but the magnitude of \mathbf{k} is not, see (8.31).

$$\tilde{g}_{f0}^{B2+;0} + \tilde{g}_{f0}^{B2-;f} \quad (8.37)$$

for inelastic scattering and in

$$\tilde{g}_{00}^{B2+;0} + \tilde{g}_{00}^{B2-;0} \quad (8.38)$$

for elastic scattering [5, 28, 98]. The situation is completely analogous to direct inelastic scattering at large momentum transfers (section 4.1.2). Thus the first Born term \tilde{g}_{f0}^{B1} does not have the electron-nucleus interaction which is responsible for large momentum transfer scattering. This interaction first becomes operative at the second Born level through the terms (8.37) and (8.38).

For small ($q \leq k_0^{-1}$) and intermediate momentum transfers q the first Born amplitude \tilde{g}^{B1} gives the leading (in k_0) behaviour for elastic scattering. However, for inelastic scattering at small q the second Born term dominates \tilde{g}^{B1} in the limit $k_0 \rightarrow \infty$ – this result has important implication for pure inelastic exchange collisions [5, 152]. At intermediate q for inelastic scattering \tilde{g}^{B1} gives the leading behaviour. In connection with the EBS approximation of section 6.2.3 it should be noted that \tilde{g}_{f0}^{B1} gives the exchange amplitude correct through order k_0^{-2} for both elastic and inelastic scattering [5].

Walters [54] has made an exact calculation of the second Born term $g_{1s,1s}^{B2+}$ ($= g_{1s,1s}^{B2-}$) for elastic scattering of electrons by H (1s) at 30 eV. A sample of his results is given in table 6. In this table the term $g_{1s,1s}^{B2+}$ is broken down into two components, $g_{1s,1s}^{B2+;1s}$ (see (8.21)) and

$$g_{1s,1s}^{B2+;n \neq 1s} \equiv \sum_{n \neq 1s} g_{1s,1s}^{B2+;n} \quad (8.39)$$

which are separately listed. Also shown in the table is the first Born term $g_{1s,1s}^{B1+}$ and a closure approximation to $g_{1s,1s}^{B2+;n \neq 1s}$ in which k_n^2 of (8.21b) has been replaced by an average value $\bar{k}^2 = k_0^2 + 2(\varepsilon_0 - \bar{\varepsilon})$ with $\bar{\varepsilon} = -1/18$ a.u.

From the table it is seen that $g_{1s,1s}^{B2+;n \neq 1s}$ is comparable with $g_{1s,1s}^{B1+} + g_{1s,1s}^{B2+;1s}$. This emphasises the importance of exchange couplings to states other than 1s at this energy. However, care must be exercised on this point since, in the sense of the argument leading to (8.29), part of the second-order exchange coupling to 1s is contained in $g_{1s,1s}^{B2+;n \neq 1s}$.

A second point to note is the generally poor performance of the closure approximation. This casts considerable doubt upon the use of the Glauber approximation for the exchange amplitude [153]. It will be remembered (section 6.1) that the Glauber approximation involves closure with the choice $\bar{\varepsilon} = \varepsilon_0$ ($= -1/2$ in this case); it is thought that a lower value of $\bar{\varepsilon}$ than that of table 6 will lead to worse closure results [54]. In view of the remarks preceding (8.28) one should probably not be surprised by the failure of the Glauber approximation – since the exchange amplitude receives very significant contributions from continuum intermediate states (8.27c) it is not a good idea to fix ε_n at the value ε_0 (see (8.27d)).

Studies of the high energy behaviour of the second Born exchange term have been made by Shakeshaft [152] and by Gavrila and Mandal [154]. These authors have not used the Green's function (8.8c) but have adopted the plane wave Green's function

$$(E - K_0 - K_1 + i\eta)^{-1}. \quad (8.40)$$

Byron and Joachain [155] have also studied the second Born exchange term in the context of forward dispersion relations.

Table 6
Exchange amplitudes for elastic electron-H (1s) scattering at 30 eV (as calculated by Walters [54])

(a) Real part

θ (degrees)*	Exact $g_{1s, 1s}^{B2+; n \neq 1s}$	Closure approximation** to $g_{1s, 1s}^{B2+; n \neq 1s}$	Exact $g_{1s, 1s}^{B2+, 1s}$	$g_{1s, 1s}^{B1+, 1s}$
0	0.510	0.539	-0.1707	-0.559
10	0.478	0.535	-0.1702	-0.533
20	0.396	0.521	-0.1687	-0.461
30	0.297	0.490	-0.1664	-0.361
40	0.209	0.441	-0.1635	-0.253
50	0.147	0.375	-0.1604	-0.151
60	0.108	0.303	-0.1571	-0.609×10^{-1}
90	0.797×10^{-1}	0.125	-0.1488	0.122
120	0.864×10^{-1}	0.388×10^{-1}	-0.1436	0.212
160	0.922×10^{-1}	0.170×10^{-2}	-0.1407	0.260
180	0.925×10^{-1}	-0.196×10^{-2}	-0.1404	0.265

(b) Imaginary part

0	0.182	0.581	-0.318×10^{-1}	0
10	0.149	0.532	-0.306×10^{-1}	0
20	0.669×10^{-1}	0.401	-0.269×10^{-1}	0
30	-0.334×10^{-1}	0.228	-0.211×10^{-1}	0
40	-0.121	0.569×10^{-1}	-0.136×10^{-1}	0
50	-0.179	-0.799×10^{-1}	-0.478×10^{-2}	0
60	-0.206	-0.169	0.478×10^{-2}	0
90	-0.164	-0.206	0.338×10^{-1}	0
120	-0.739×10^{-1}	-0.117	0.572×10^{-1}	0
160	0.924×10^{-3}	-0.304×10^{-1}	0.744×10^{-1}	0
180	0.104×10^{-1}	-0.189×10^{-1}	0.765×10^{-1}	0

* Scattering angle.

** All intermediate states approximated by closure with $\varepsilon = -1/18$ a.u.

Finally, I would mention the Ochkur (or Bonham-Ochkur) approximation [97, 156] to the first Born term \tilde{g}_{f0}^{B1} . The electron-electron potential $1/r_{01}$ may be alternatively written

$$\frac{1}{r_{01}} = \frac{1}{2\pi^2} \int \frac{\exp[i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_0)]}{k^2} d\mathbf{k}. \quad (8.41)$$

Using (8.41) in (8.19) gives

$$\tilde{g}_{f0}^{B1} = -\frac{1}{4\pi^3} \int \frac{d\mathbf{k}}{k^2} \left\{ \int \exp[i(\mathbf{k} - \mathbf{k}_f) \cdot \mathbf{r}_1] \exp[i(\mathbf{k}_0 - \mathbf{k}) \cdot \mathbf{r}_0] \psi_f^*(\mathbf{r}_0) \psi_0(\mathbf{r}_1) d\mathbf{r}_0 d\mathbf{r}_1 \right\}. \quad (8.42)$$

At high energies it is to be expected that the main contribution to the integral over \mathbf{k} in (8.42) will occur for $k \approx k_0 \approx k_f$. Setting* $k = k_0$ in the denominator of (8.42) enables the integral over \mathbf{k} to be trivially performed, giving $(2\pi)^3 \delta(\mathbf{r}_1 - \mathbf{r}_0)$, and leading to the Ochkur approximation

* A choice of average k more symmetric between k_0 and k_f may be desirable. However, the principle is the same.

$$\begin{aligned} g_{f0}^{\text{Och}} &= -\frac{2}{k_0^2} \int \psi_f^*(\mathbf{r}_0) \exp(i\mathbf{q} \cdot \mathbf{r}_0) \psi_0(\mathbf{r}_0) d\mathbf{r}_0 \\ &= \frac{1}{k_0^2} (q^2 f_{f0}^{\text{B1}} - 2\delta_{f0}), \end{aligned} \quad (8.43)$$

where f_{f0}^{B1} is the *direct* first Born amplitude of (3.5). The important thing about the Ockhur approximation (8.43), as far as the EBS approximation of section 6.2.3 is concerned, is that it gives $\tilde{g}_{f0}^{\text{B1}}$ correct through order k_0^{-2} .

8.3. Optical potentials

The approach to exchange outlined in section 8.2 might be described as the “asymmetric attitude” in that the calculation of the exchange amplitude proceeds independently from the calculation of the direct amplitude. This makes sense at high energies where exchange scattering dies rapidly away with respect to direct scattering – the situation here is asymmetric. At lower energies where direct and exchange scattering are more comparable it is better to treat both on the same footing (the “symmetric attitude”) by working with a wavefunction which has the correct symmetry from the beginning. The optical potential formalism provides a good starting point.

In section 7 the optical potential formalism was set up with the treatment of direct scattering only in mind. Here I shall extend the idea to symmetrized wavefunctions. For the electron–H system the correctly symmetrized (spatial) wavefunctions are

$$\Psi^+ = \sum_n (F_n^+(\mathbf{r}_0)\psi_n(\mathbf{r}_1) + \alpha F_n^+(\mathbf{r}_1)\psi_n(\mathbf{r}_0)) \quad (8.44)$$

where $\alpha = +1$ for the singlet case and $\alpha = -1$ for the triplet wave-function. The plan is to break the wavefunction space up into two parts, Ψ^{P+} and Ψ^{Q+} , where

$$\Psi^{P+} \equiv \sum_{n=0}^M (F_n^+(\mathbf{r}_0)\psi_n(\mathbf{r}_1) + \alpha F_n^+(\mathbf{r}_1)\psi_n(\mathbf{r}_0)), \quad (8.45)$$

and Ψ^{Q+} , the remaining terms in (8.44), is *orthogonal* to Ψ^{P+} . This can be achieved by defining the symmetrized projection operators [10, 157]

$$Q = Q_0 Q_1, \quad (8.46a)$$

$$P = 1 - Q, \quad (8.46b)$$

where

$$Q_i = 1 - P_i, \quad (8.46c)$$

$$P_i = \sum_{n=0}^M |\psi_n(\mathbf{r}_i)\rangle\langle\psi_n(\mathbf{r}_i)|. \quad (8.46d)$$

It is easily verified that (8.46a) and (8.46b) are projection operators, i.e.,

$$P^2 = P, \quad Q^2 = Q, \quad (8.47a)$$

$$PQ = QP = 0. \quad (8.47b)$$

The setting up of projection operators P and Q for targets other than H needs more careful consideration; Feshbach [157] has indicated how to do it.

It is not difficult to show that Ψ^{P+} must satisfy [10]

$$(PHP + PHQ[Q(E + i\eta - H)Q]^{-1}QHP - E)\Psi^{P+} = 0. \quad (8.48)$$

This can be reduced to a set of coupled equations for the F_n^+ ($n = 0$ to M) of the form (7.9), i.e.,

$$(\nabla_0^2 + k_0^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^M \langle \psi_n(\mathbf{r}_1) | V^{\text{OPT}} | \psi_m(\mathbf{r}_1) \rangle F_m^+(\mathbf{r}_0), \quad (8.49)$$

where the non-local operator V^{OPT} is the optical potential. Note that (8.49) does not explicitly display any exchange symmetry between electrons 0 and 1; this symmetry is absorbed into the definition of V^{OPT} so that the equations for the F_n^+ read like equations for a distinguishable incident electron labelled 0.

Since my aim here is to illustrate principles rather than give general formalisms, I shall now specialize (8.48) to the case of elastic scattering off the state ψ_0 and where P_i is chosen to be

$$P_i = |\psi_0(\mathbf{r}_i)\rangle\langle\psi_0(\mathbf{r}_i)|. \quad (8.50)$$

Taking the scalar product of (8.48) with $\langle\psi_0(\mathbf{r}_1)|$ on the left leads, after a little work, to the equation

$$\begin{aligned} (\nabla_0^2 + k_0^2)F_0^+(\mathbf{r}_0) &= 2V_{00}(\mathbf{r}_0)F_0^+(\mathbf{r}_0) + 2\alpha\langle\psi_0(\mathbf{r}_1)|\left(2\varepsilon_0 + \frac{1}{r_{01}}\right)|F_0^+(\mathbf{r}_1)\rangle\psi_0(\mathbf{r}_0) \\ &\quad + 2\langle\psi_0(\mathbf{r}_1)|\frac{1}{r_{01}}Q\frac{1}{Q(E + i\eta - H)Q}Q\frac{1}{r_{01}}|F_0^+(\mathbf{r}_0)\psi_0(\mathbf{r}_1) + \alpha F_0^+(\mathbf{r}_1)\psi_0(\mathbf{r}_0)\rangle, \end{aligned} \quad (8.51)$$

where V_{00} is the static potential (3.7b) of the state ψ_0 . The first two terms on the right-hand side of (8.51) arise exclusively from P-space, i.e., PHP ; the third term gives the effect of Q-space couplings upon P-space.

Let the eigenstates (both bound and continuum) of the two-electron Q-space operator QHQ be denoted by ϕ_q :

$$QHQ\phi_q(\mathbf{r}_0, \mathbf{r}_1) = E_q\phi_q(\mathbf{r}_0, \mathbf{r}_1). \quad (8.52)$$

These states are either singlets (S) or triplets (T). Their normalization is chosen so that

$$\sum_{\text{all } q} |\phi_q^S\rangle\langle\phi_q^S| + \sum_{\text{all } q} |\phi_q^T\rangle\langle\phi_q^T| = Q, \quad (8.53)$$

the Q-space unit operator. We may then write

$$\begin{aligned} \frac{1}{r_{01}} Q \frac{1}{Q(E + i\eta - H)Q} Q \frac{1}{r_{01}} &= \sum_q \frac{1}{r_{01}} \frac{|\phi_q^S\rangle\langle\phi_q^S|}{(E + i\eta - E_q^S)} \frac{1}{r_{01}} \\ &+ \sum_q \frac{1}{r_{01}} \frac{|\phi_q^T\rangle\langle\phi_q^T|}{(E + i\eta - E_q^T)} \frac{1}{r_{01}}. \end{aligned} \quad (8.54)$$

Using (8.54), eq. (8.51) may be cast in the form

$$(\nabla_0^2 + k_0^2)F_0^+(\mathbf{r}_0) = 2\langle\psi_0(\mathbf{r}_1)|V^{\text{OPT}}|\psi_0(\mathbf{r}_1)\rangle F_0^+(\mathbf{r}_0), \quad (8.55)$$

where the optical potential for singlet scattering is given by

$$V^{\text{OPT}, S} = V_P^{\text{OPT}, S} + V_Q^{\text{OPT}, S}, \quad (8.56)$$

with the P- and Q-space components being defined by

$$\langle\psi_0(\mathbf{r}_1)|V_P^{\text{OPT}, S}|\psi_0(\mathbf{r}_1)\rangle F_0^+(\mathbf{r}_0) \equiv V_{00}(\mathbf{r}_0)F_0^+(\mathbf{r}_0) + \langle\psi_0(\mathbf{r}_1)|(2\varepsilon_0 + 1/r_{01})|F_0^+(\mathbf{r}_1)\rangle\psi_0(\mathbf{r}_0), \quad (8.57a)$$

$$\begin{aligned} \langle\psi_0(\mathbf{r}_1)|V_Q^{\text{OPT}, S}|\psi_0(\mathbf{r}_1)\rangle F_0^+(\mathbf{r}_0) \\ = 2 \sum_q \frac{\langle\psi_0(\mathbf{r}_1)|\frac{1}{r_{01}}|\phi_q^S(\mathbf{r}_0, \mathbf{r}_1)\rangle\langle\phi_q^S(\mathbf{r}_0, \mathbf{r}_1)|\frac{1}{r_{01}}|F_0^+(\mathbf{r}_0)\psi_0(\mathbf{r}_1)\rangle}{(E + i\eta - E_q^S)}. \end{aligned} \quad (8.57b)$$

The potential for triplet scattering, $V^{\text{OPT}, T}$, is obtained from (8.56) and (8.57) on replacing S by T and changing the sign of the second term on the right-hand side of (8.57a).

The P-space part of (8.56), i.e., (8.57a), is just the (non-local) static-exchange potential. Solving (8.55) with the coupling to Q-space switched off, i.e., $V_Q^{\text{OPT}, S/T} = 0$, gives the static-exchange approximation which has been referred to in previous sections. Note that the static-exchange approximation is just a one-state approximation to (8.44) in which Ψ^+ is taken to be

$$\Psi^+ = F_0^+(\mathbf{r}_0)\psi_0(\mathbf{r}_1) + \alpha F_0^+(\mathbf{r}_1)\psi_0(\mathbf{r}_0), \quad (8.58)$$

The problem of interest here is how to build upon the static exchange approximation by using perturbative-style methods to evaluate $V_Q^{\text{OPT}, S/T}$.

Proceeding in a simple-minded fashion, and with the spectral decomposition (4.1) as an intuitive guide, it seems reasonable to suggest the approximation [111, 113, 143, 144]

$$\phi_q^{S/T}(\mathbf{r}_0, \mathbf{r}_1) \triangleq \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} (\exp(i\mathbf{k} \cdot \mathbf{r}_0)\psi_n(\mathbf{r}_1) \pm \exp(i\mathbf{k} \cdot \mathbf{r}_1)\psi_n(\mathbf{r}_0)), \quad (8.59a)$$

$$E_q^{S/T} \triangleq \frac{1}{2}\mathbf{k}^2 + \varepsilon_n, \quad n \neq 0, \quad (8.59b)$$

where ψ_n is, as usual, a hydrogen eigenstate and the minus sign is to be associated with the triplet case. The label q is to be understood as specifying \mathbf{k} and n .

When ψ_n is a bound state (8.59) requires no further comment. However, consider the case where ψ_n is a continuum state, ψ_κ^+ say*:

$$\phi_q^{S/T}(\mathbf{r}_0, \mathbf{r}_1) \triangleq \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} (\exp(i\mathbf{k} \cdot \mathbf{r}_0) \psi_\kappa^+(\mathbf{r}_1) \pm \exp(i\mathbf{k} \cdot \mathbf{r}_1) \psi_\kappa^+(\mathbf{r}_0)) , \quad (8.60a)$$

$$E_q^{S/T} \triangleq \frac{1}{2} k^2 + \frac{1}{2} \kappa^2 , \quad (8.60b)$$

where q is the label (\mathbf{k}, κ) . The state (8.60) is supposed to represent two electrons in the continuum with momenta \mathbf{k} and κ . Since the two electrons are indistinguishable the labels $q = (\mathbf{k}, \kappa)$ and $q = (\kappa, \mathbf{k})$ should represent the same state. However, this is not true of the right-hand side of (8.60a) and must therefore be imposed. Physically it makes sense that the slower of the two electrons should be under the influence of the nuclear Coulomb field while the faster electron should be the plane wave. We are therefore led to the approximation

$$\phi_q^{S/T}(\mathbf{r}_0, \mathbf{r}_1) \triangleq \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} [\exp(i\mathbf{k}_> \cdot \mathbf{r}_0) \psi_{\mathbf{k}<}^+(\mathbf{r}_1) \pm \exp(i\mathbf{k}_> \cdot \mathbf{r}_1) \psi_{\mathbf{k}<}^+(\mathbf{r}_0)] , \quad (8.61a)$$

where $q = (\mathbf{k}, \kappa) = (\kappa, \mathbf{k})$ and

$$\begin{aligned} \mathbf{k}_> &= \mathbf{k} & \text{if } k > \kappa & \quad \mathbf{k}_< = \mathbf{k} & \text{if } k < \kappa \\ &= \kappa & \text{if } \kappa > k , & & = \kappa & \text{if } \kappa < k . \end{aligned} \quad (8.61b)$$

In summing over the states (8.61) care must be taken to avoid double counting by taking the sum as

$$\int_0^\infty k_>^2 dk_> \int_0^{k_>} k_<^2 dk_< \int d\hat{\mathbf{k}}_> \int d\hat{\mathbf{k}}_< . \quad (8.62)$$

Good support for the approximation (8.61) is provided by some recent calculations of electron impact ionization [158].

Employing (8.59) and (8.61) in (8.57b) leads to what is perhaps the simplest generalization of (7.16) to include exchange. Of course, there are many unsatisfactory features about the approximations (8.59) and (8.61). For example, the state normalizations are not quite correct. Thus $\langle \phi_q^{S/T} | \phi_{q'}^{S/T} \rangle$ is not quite $\delta(\mathbf{k} - \mathbf{k}')\delta_{nn'}$ in the bound state case (8.59) or $\delta(\mathbf{k} - \mathbf{k}')\delta(\kappa - \kappa')$ in the continuum case (8.61), as is required by (8.53). Also (8.59) and (8.61) have components in P-space. This defect can be removed by orthogonalizing the plane waves in (8.59) and (8.61) to ψ_0 . McCarthy et al. [144] say that this orthogonalization is not important for electron-H (1s) scattering at 100 eV and above. The approximations (8.59) and (8.61) could obviously be simply extended by, for example, replacing the plane waves by more sophisticated functions (distorted waves), perhaps also altering ψ_n and ψ_κ^+ away from atomic eigenstates at the same time [144].

* Either ψ_κ^+ or ψ_κ^- form a complete set of continuum states, here I choose the set ψ_κ^+ . The ψ_κ^+ are normalized according to (8.14).

The above ideas have been implemented by McCarthy and co-workers [111, 113, 143–147] for electron–H scattering, although often further approximations have been made – the reader needs to study these papers carefully to see exactly what has been done. It is difficult to assess this work since McCarthy et al. use a localization prescription for V^{OPT} which came in for some criticism in section 7.2.2.2; also, most of the work has been carried out at energies ≥ 50 eV where the approximations of sections 5, 6 and 7 would suggest that exchange can be treated in a simple way, e.g., through static-exchange for elastic scattering.

Finally, one may contemplate making distorted-wave approximations to the optical potential equations (8.49) along the lines described in section 7.1. Thus using the decomposition (8.56) the eqs. (8.49) become

$$(\nabla_0^2 + k_n^2)F_n^+(\mathbf{r}_0) = 2 \sum_{m=0}^M \{\langle \psi_n(\mathbf{r}_1) | V_P^{\text{OPT}} | \psi_m(\mathbf{r}_1) \rangle + \langle \psi_n(\mathbf{r}_1) | V_Q^{\text{OPT}} | \psi_m(\mathbf{r}_1) \rangle\} F_m^+(\mathbf{r}_0). \quad (8.63)$$

If these equations are solved treating the terms in V_Q^{OPT} perturbatively the result is a distorted-wave approximation. For example, in the simple case (8.55), solving only to first order in V_Q^{OPT} gives the distorted wave amplitude (for elastic scattering)

$$f_{\text{se}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \langle F_0^-(\mathbf{r}_0) \psi_0(\mathbf{r}_1) | V_Q^{\text{OPT}} | F_0^+(\mathbf{r}_0) \psi_0(\mathbf{r}_1) \rangle. \quad (8.64)$$

In (8.64) f_{se} is the static-exchange amplitude obtained by solving

$$(\nabla_0^2 + k_0^2)F_0^+(\mathbf{r}_0) = 2\langle \psi_0(\mathbf{r}_1) | V_P^{\text{OPT}} | \psi_0(\mathbf{r}_1) \rangle F_0^+(\mathbf{r}_0), \quad (8.65)$$

F_0^+ and F_0^- are the solutions of (8.65) with outgoing and ingoing scattered waves respectively. Formula (8.64) should be compared with the non-exchange result (5.21); note, however, that unlike (5.21) I do not necessarily imply any perturbative evaluation of V_Q^{OPT} itself in (8.64). One may, of course, generate higher-order distorted-wave approximations than (8.64) by solving (8.55) to higher order in V_Q^{OPT} .

The advantage of a distorted-wave approximation is that one is required only to evaluate certain matrix elements of V_Q^{OPT} . Solving coupled equations which involve non-local potentials is a somewhat more difficult task, unless, of course, good local approximations to the potentials can be found (section 7.2.2.2). A disadvantage of the distorted-wave approach is that a unitary amplitude is not guaranteed [110]; solving coupled equations ensures unitarity. However, the success of distorted-wave methods (section 5) suggests that this is not, in general, an important point; further there is a flexibility in the distorted-wave approach in that one may be able to remove, in a simple way, any large effects in V_Q^{OPT} , lump them with V_P^{OPT} for the calculation of distorted waves, and then treat only the residue of V_Q^{OPT} perturbatively.

9. Positron–Atom scattering

In section 3.3 the approximate equality of total cross sections for electron and positron scattering, at high enough energy, was commented upon. Calculations using the (better) methods of sections 5 to 7 have established the inequality

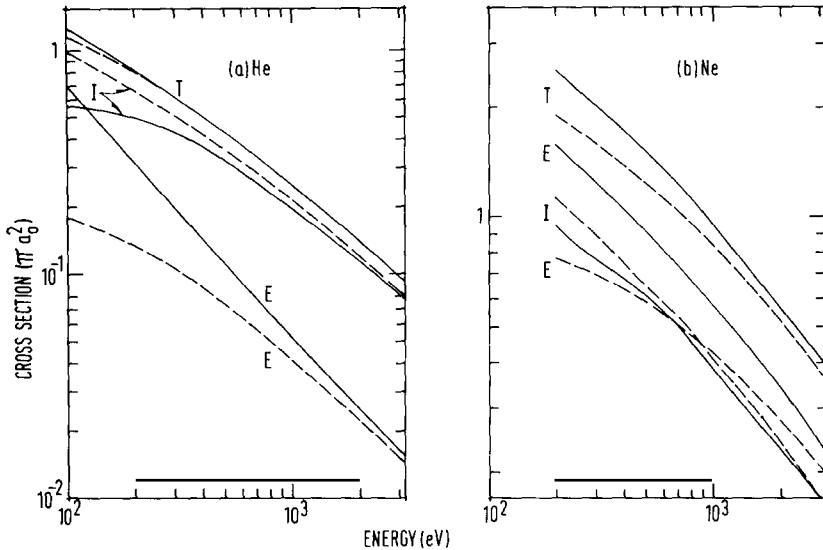


Fig. 27. Cross sections for e^\pm scattering by (a) He, (b) Ne. Notation: $T = \sigma_{\text{total}}$; $E = \sigma_{\text{elastic}}$; $I = \sigma_{\text{inelastic}}$. Curves: (—) electrons; (---) positrons. (The cross sections shown are based upon the experimental measurement of [29], the semi-empirical estimates of [167] and the DWSBA calculations of [37].)

$$\sigma_{\text{elastic}}(\text{positrons}) \leq \sigma_{\text{elastic}}(\text{electrons}) \quad (9.1)$$

for the integrated elastic cross section, where the equality sign holds only in the limit of asymptotically high energies. It is understood in (9.1) that the impact energy is not too low, since the methods of sections 5 to 7 do not apply to low energies. The inequality (9.1) is illustrated in fig. 27 for He and Ne targets, it is seen to be quite substantial at the lower energy end.

The corresponding differential cross sections are also very interesting, they are shown in fig. 28 for an impact energy of 400 eV. The most notable feature of the positron cross sections in this figure is the absence of the pronounced forward peak which is seen in electron scattering. This is explained by the fact that polarization effects add to shorter range effects in the case of electron scattering but subtract for positron collisions. For example, in the second Born approximation (3.9) f_{00}^{B1} and f_{00}^{B2} , which contains the polarization effect, have the same sign for electron scattering; changing from electrons to positrons reverses the sign of f_{00}^{B1} but leaves that of f_{00}^{B2} unchanged, with resulting cancellation of the forward polarization peak.

From the approximate equality*

$$\sigma_{\text{total}}(\text{positrons}) \approx \sigma_{\text{total}}(\text{electrons}) \quad (9.2)$$

and the inequality (9.1) it is tempting to deduce the approximate inequality*

$$\sigma_{\text{inelastic}}(\text{positrons}) \geq \sigma_{\text{inelastic}}(\text{electrons}), \quad (9.3)$$

where $\sigma_{\text{inelastic}}$ is the total inelastic cross section ($\sigma_{\text{total}} = \sigma_{\text{inelastic}} + \sigma_{\text{elastic}}$). However, the correctness of

* This is, of course, an exact equality at asymptotically high energies where the first Born approximation is valid.

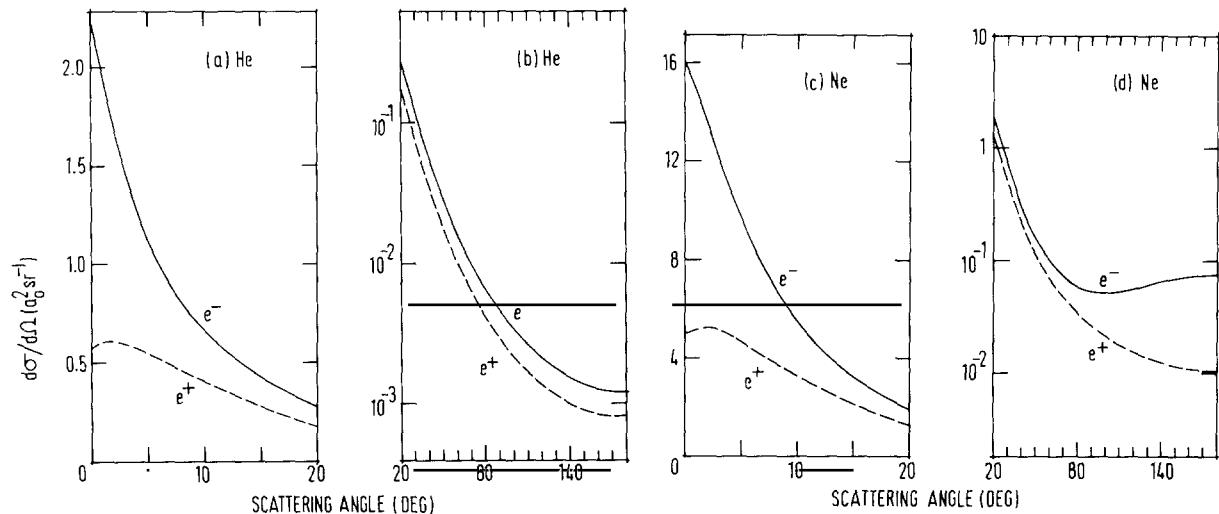


Fig. 28. DWSBA differential cross sections for elastic scattering of electrons by He and Ne at 400 eV [37]: (a) He, 0° to 20°; (b) He, 20° to 180°; (c) Ne, 0° to 20°; (d) Ne, 20° to 180°. Curves: (—) electrons; (---) positrons.

such a deduction depends upon: (i) what fraction of σ_{total} comes from $\sigma_{\text{inelastic}}$; (ii) how big the inequality (9.1) is; (iii) how good the equality (9.2) is. Under adverse conditions (9.3) could be totally erroneous.

Figure 27 shows $\sigma_{\text{inelastic}}$ for e^{\pm} scattering by He and Ne. It is seen that (9.3) holds in these two cases. Also shown, for completeness, is σ_{total} .

10. Addendum

In a very recent publication Byron et al. [159] have reported EBS (see (6.15)) calculations of the triple differential cross section, $d^3\sigma/d\Omega_A d\Omega_B dE_B$ (section 3.2), for electron impact ionization of H (1s) at 250 eV; electron exchange has also been taken into account. The collision geometry corresponds to the asymmetric case (i) of section 3.2. The results obtained are in good agreement with measurements of Lohmann and Weigold [160], although these data have quite large error bars. The calculation also confirms the viability of the second Born approximation (3.21).

11. Concluding remarks

Two main themes emerge from the preceding sections. The first is the undesirability of treating the singular e^{\pm} -nucleus interaction perturbatively (sections 3.2, 6.2.2 and 6.2.3). This leads to the idea of using distorted-wave Born series (section 5) rather than the ordinary plane-wave series. The second theme is the importance of the second Born term which contains in a dynamical way physical effects such as target polarization and flux loss. Indeed, as was recommended in section 5.2 and applied in sections 5.2, 6.1 and 7.4, Born series analysis of an approximation, at least up to second order, is a very useful way of assessing the quality of the approximation.

In section 6 methods based upon the Glauber and Wallace approximations were shown to be very successful. However, these methods have only been applied to light atoms such as H and He. In view of the practical difficulties in calculating the Glauber and Wallace approximations for more complicated atoms it is legitimate to ask whether these techniques can be viably extended to general atoms. It is not clear that the answer to this question is in the affirmative, except, of course, in cases where simplifying frozen core approximations can reasonably be used to reduce the labour [13].

The optical potential formalism (sections 7 and 8.3) provides a nice way of viewing e^\pm -atom collisions, particularly when exchange is to be consistently treated (section 8.3). One understandable weakness here is the desire to use local potential approximations. However, there is little point in making a sophisticated optical potential calculation only to mar the overall result by a poor, or unviable, local potential approximation.

As far as future developments are concerned it is to be anticipated that the use of the closure approximation to calculate the second Born term will fade away and be replaced by pseudostate methods, which may perhaps use the closure approximation as a standard for judging the effective completeness of the pseudostate set (section 4.2.2). Applications to e^\pm impact ionization will probably be a growth area (sections 3.2 and 10); indeed, inelastic scattering generally has not been satisfactorily analyzed. It is also likely that more effort will be devoted to the consistent treatment of electron exchange (section 8).

Even though present perturbative methods may not ultimately turn out to be the best way of handling the intermediate to high energy regime, it is likely that the perturbative view will long continue to provide valuable insight into e^\pm -atom collisions.

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