J. Phys. B: At. Mol. Phys. **15** (1982) 3915–3943. Printed in Great Britain

Unitarisation of the eikonal-Born series method for electron–atom and positron–atom collisions

F W Byron Jr†, C J Joachain‡§ and R M Potvliege‡

† Department of Physics and Astronomy, University of Massachusetts, Amherst, Massachusetts 01003, USA
‡ Physique Théorique, Faculté des Sciences, Université Libre de Bruxelles, Brussels, Belgium
§ Institut de Physique Corpusculaire, Université de Louvain, Louvain-la-Neuve, Belgium

Received 30 June 1982

Abstract. A systematic study is made of the unitarisation method which we recently proposed for the eikonal-Born series approximation, in the case of fast electron–atom and positron–atom collisions. Our unitarisation procedure is based on a generalisation of the potential scattering eikonal expansion of Wallace to the multiparticle case, suitably modified to take the long-range polarisation effects and absorption effects at small angles into account correctly. We also develop a new non-perturbative approximation for the exchange scattering amplitude, which is appropriate to use with our unitarised EBS direct scattering amplitude for electron–atom collisions. We then apply our unitarised EBS method to the elastic scattering of electrons and positrons by atomic hydrogen in the energy range 100–400 eV. A detailed comparison is made with other related theoretical methods and with recent absolute measurements of (e^-–H) elastic differential cross sections. Total (integrated) elastic and total (complete) cross sections for both electron and positron impact are also discussed.

1. Introduction

Following the introduction of the eikonal approximation in potential scattering theory (Molière 1947), it was natural that physicists should attempt to extend the basic eikonal concept to multiparticle scattering processes. This was accomplished by Glauber (1959) who essentially used a frozen-target approximation to convert the many-body scattering problem into a potential scattering problem in which the potential depends on the coordinates of the target. However, the original eikonal approximation is not free from serious drawbacks (Byron and Joachain 1973a, Byron *et al* 1973). A detailed comparison between the terms of the Born and eikonal series (in potential scattering) or the Born and Glauber series (for multiparticle collisions) led us to formulate the eikonal-Born series (EBS) method (Byron and Joachain 1973b, for a recent review see Byron and Joachain 1977a). In this approach the deficiencies of the eikonal approximation and the Glauber many-body generalisation of it are cured, within the framework of perturbation theory, by constructing scattering amplitudes which are consistent through order k_i^{-2}, where k_i is the incident wavenumber.

Another way of obtaining improvements over the eikonal approximation has been proposed recently by Wallace (1971, 1973). For the case of potential scattering,

0022-3700/82/213915+29$02.00

Wallace was able to write down in a systematic way the corrections to the eikonal phase, and detailed studies of the relationships between the terms of the Born, eikonal and Wallace series have been carried out by Byron *et al* (1975, 1979). In the light of these developments, we recently proposed (Byron *et al* 1981) a generalisation of the potential scattering Wallace amplitude to the multiparticle case, in the same spirit as that of Glauber's original extension of the potential scattering eikonal amplitude. This generalisation was also obtained subsequently by Franco and Iwinski (1982) and by Unnikrishnan and Prasad (1982). However, we also remarked (Byron *et al* 1981) that the resulting many-body Wallace amplitude does not eliminate all the difficulties inherent in the Glauber amplitude. In particular, the Wallace extension of the Glauber approximation is still a zero-excitation-energy approximation and therefore does not account for long-range polarisation effects at small angles and represents inadequately absorption effects in the same region. Fortunately, these difficulties can be eliminated by removing the term of the many-body Wallace amplitude which is of second order in the projectile–target interaction and replacing it by the second Born term (Byron *et al* 1981). The direct amplitude thus obtained, which we shall call the *unitarised eikonal-Born series* (UEBS) direct amplitude, has all the strengths of the EBS method at small and intermediate angles, where perturbation theory is rapidly convergent, but in addition it contains the *two* leading terms (in powers of k_i^{-1}) of each order of perturbation theory summed to *all* orders. Hence, at large angles, where the small-distance singularity of the central Coulomb potential is all-important, we are able to deal in a very satisfactory manner with the main feature of the scattering amplitude, which is similar to what is found in pure Coulomb scattering.

In this paper we present a detailed study of the unitarisation of the EBS method for electron–atom and positron–atom collisions, based on the considerations mentioned above. We begin in § 2 by reviewing some basic eikonal results from potential scattering in a form suitable for generalisation to the multiparticle case. Particular emphasis is given to the method of Wallace (1973) and the relationships between the Born, eikonal and Wallace series (Byron *et al* 1975, 1979). In § 3 we obtain the many-body Wallace amplitude by generalising the (non-central) potential scattering results of Wallace (1973). We also show in that section how several difficulties associated with long-range potentials can be overcome, discuss the relationships between the terms of the multiparticle Born, Glauber and Wallace series and develop a new non-perturbative approximation for the exchange scattering amplitude, which is appropriate to use with our unitarised EBS direct scattering amplitude for electron–atom collisions. In § 4 we evaluate the multiparticle Wallace phase in closed form for electron (positron)–atomic-hydrogen scattering and analyse the large momentum transfer properties of the direct amplitude for elastic scattering from the hydrogen ground state, as obtained from this phase. We then study in detail the elastic exchange amplitude. We conclude § 4 by presenting our results for electron and positron elastic scattering from the ground state of atomic hydrogen, in the energy range from 100 to 400 eV, using the unitarised EBS method for the direct scattering amplitude and our non-perturbative approximation for the exchange scattering amplitude. Values of the differential cross sections, integrated cross sections and total cross sections are given and compared with other recent calculations and with the experimental data. Finally, some interesting properties of the forward (zero-angle) elastic scattering amplitude are discussed in the context of our analysis of the electron and positron total cross sections results.

2. Potential scattering

In this section we briefly recall several important results from potential scattering theory, which are at the root of the many-body generalisations discussed in the next section.

Let us assume that an electron or a positron is scattered by a static potential $V(\boldsymbol{r})$. Using atomic units, we write the eikonal (Glauber) scattering amplitude as

$$f_{\mathrm{E}} = \frac{k}{2\pi \mathrm{i}} \int \exp(\mathrm{i}\boldsymbol{\Delta} \cdot \boldsymbol{b})[\exp(\mathrm{i}k^{-1}\chi_0(\boldsymbol{b})) - 1]\, \mathrm{d}^2\boldsymbol{b} \tag{2.1}$$

where $\boldsymbol{\Delta} = \boldsymbol{k}_{\mathrm{i}} - \boldsymbol{k}_{\mathrm{f}}$ is the momentum transfer ($\boldsymbol{k}_{\mathrm{i}}$ and $\boldsymbol{k}_{\mathrm{f}}$ being the initial and final momenta of the particle, respectively) and $k = |\boldsymbol{k}_{\mathrm{i}}| = |\boldsymbol{k}_{\mathrm{f}}|$ for the elastic scattering process considered here. The eikonal phase $\chi_0(\boldsymbol{b})$ which appears in equation (2.1) is given by

$$\chi_0(\boldsymbol{b}) = -\int_{-\infty}^{+\infty} V(\boldsymbol{b}, z)\, \mathrm{d}z = -\tfrac{1}{2}\int_{-\infty}^{+\infty} U(\boldsymbol{b}, z)\, \mathrm{d}z \tag{2.2}$$

where $U(\boldsymbol{r}) = 2V(\boldsymbol{r})$ is the reduced potential in the present case. We recall that we are working in a cylindrical coordinate system, with $\boldsymbol{r} = \boldsymbol{b} + z\hat{\boldsymbol{n}}$, $\hat{\boldsymbol{n}}$ being the direction perpendicular to $\boldsymbol{\Delta}$ (in the scattering plane). The eikonal series is obtained by expanding the amplitude f_{E} in powers of the potential, namely (Byron and Joachain 1977a)

$$f_{\mathrm{E}} = \sum_{n=1}^{\infty} \bar{f}_{\mathrm{E}n} \tag{2.3}$$

where

$$\bar{f}_{\mathrm{E}n} = \frac{1}{2\pi}\left(\frac{\mathrm{i}}{k}\right)^{n-1} \frac{1}{n!} \int \exp(\mathrm{i}\boldsymbol{\Delta} \cdot \boldsymbol{b})\, (\chi_0(\boldsymbol{b}))^n\, \mathrm{d}^2\boldsymbol{b}. \tag{2.4}$$

Detailed studies of the properties of the eikonal amplitude (2.1) and of the terms $\bar{f}_{\mathrm{E}n}$ of the eikonal series have been made for various central potentials (both real and complex) by Byron *et al* (1973, 1975, 1979). In particular, a comparison of the terms $\bar{f}_{\mathrm{E}n}$ with the corresponding terms $\bar{f}_{\mathrm{B}n}$ of the Born series leads to the eikonal-Born series amplitudes

$$f_{\mathrm{EBS}} = \bar{f}_{\mathrm{B}1} + \bar{f}_{\mathrm{B}2} + \bar{f}_{\mathrm{E}3} \tag{2.5}$$

and

$$\begin{aligned} f'_{\mathrm{EBS}} &= f_{\mathrm{E}} - \bar{f}_{\mathrm{E}2} + \bar{f}_{\mathrm{B}2} \\ &= \bar{f}_{\mathrm{B}1} + \bar{f}_{\mathrm{B}2} + \sum_{n=3}^{\infty} \bar{f}_{\mathrm{E}n} \end{aligned} \tag{2.6}$$

which provide a consistent picture of the scattering amplitude through order k^{-2}.

Another method of obtaining improvements over the eikonal scattering amplitude (2.1) has been proposed by Wallace (1971, 1973), who has obtained the leading corrections to the eikonal phase, within the impact parameter formalism. In what follows we shall be interested in the Wallace improved scattering amplitude containing

the leading correction to the eikonal phase, namely (Wallace 1973)

$$f_{\mathrm{W}} = \frac{k}{2\pi \mathrm{i}} \int \exp(\mathrm{i}\boldsymbol{\Delta} \cdot \boldsymbol{b}) \{\exp[\mathrm{i}(k^{-1}\chi_0(\boldsymbol{b}) + k^{-3}\chi_1(\boldsymbol{b}))] - 1\} \, \mathrm{d}^2\boldsymbol{b} \tag{2.7}$$

where the Wallace correction χ_1 is given by

$$\chi_1(\boldsymbol{b}) = \tfrac{1}{2} \int_{-\infty}^{+\infty} (\boldsymbol{\nabla} \chi_+) \cdot (\boldsymbol{\nabla} \chi_-) \, \mathrm{d}z \tag{2.8}$$

with

$$\chi_+(\boldsymbol{b}, z) = -\int_{-\infty}^{z} V(\boldsymbol{b}, z') \, \mathrm{d}z' \tag{2.9}$$

and

$$\chi_-(\boldsymbol{b}, z) = -\int_{z}^{\infty} V(\boldsymbol{b}, z') \, \mathrm{d}z'. \tag{2.10}$$

We remark that χ_1 is of *second order* in the interaction potential.

By analogy with the eikonal series (2.3), we define a Wallace series by expanding the amplitude f_{W} in powers of the potential. Calling $\bar{f}_{\mathrm{W}n}$ the term of order n in the potential strength, we therefore write

$$f_{\mathrm{W}} = \sum_{n=1}^{\infty} \bar{f}_{\mathrm{W}n} \tag{2.11}$$

and we note that

$$\bar{f}_{\mathrm{W}1} = \bar{f}_{\mathrm{E}1} = \bar{f}_{\mathrm{B}1} \tag{2.12}$$

for all interaction potentials, all energies and all momentum transfers.

It should be emphasised that the above formulae have been written down for the general case of a potential $V(\boldsymbol{r})$ which is *not* necessarily central. Indeed, it is this general case which will provide the starting point of our many-body generalisation of the Wallace amplitude, discussed in the next section. However, since at intermediate and high energies the large momentum transfer behaviour of the elastic electron (or positron)–atom scattering amplitude is governed by the *static* potential (which is *central* for target atoms such as atomic hydrogen, helium and the noble gases), it is also useful to summarise the most important results concerning the Wallace amplitude for central potentials,. In that case the Wallace correction to the phase, equation (2.8), can be written in the simpler form

$$\chi_1(b) = -\int_{-\infty}^{+\infty} V(r) \left(V(r) + r \frac{\mathrm{d}}{\mathrm{d}r} V(r) \right) \mathrm{d}z \tag{2.13}$$

with $r = (b^2 + z^2)^{1/2}$. A detailed study of the amplitude (2.7) and of the terms $\bar{f}_{\mathrm{W}n}$ has been made by Byron *et al* (1975, 1979) for various central potentials, and in particular for Yukawa-type potentials of the form

$$V(r) = V_0 \int_{\alpha_0 > 0}^{\infty} \rho(\alpha) r^{-1} \exp(-\alpha r) \, \mathrm{d}\alpha \tag{2.14}$$

where U_0 is a strength parameter (which may be complex). In equation (2.14) $\rho(\alpha)$ is a real weight function which may contain δ functions or derivatives of δ functions,

so that exponential potentials and/or potentials of the form $r^N \exp(-\mu r)$ can be represented by equation (2.14) as well as linear combinations of Yukawa potentials. For Yukawa-type potentials of the form (2.14) one may expand the Born term $\bar{f}_{Bn}(n \geq 2)$ for all momentum transfers as

$$\bar{f}_{Bn}(k, \Delta) = i^{n-1} U_0^n \left(\frac{A_{Bn}(\Delta)}{k^{n-1}} + i \frac{B_{Bn}(\Delta)}{k^n} + O(k^{-n-1}) \right) \tag{2.15}$$

where $A_{Bn}(\Delta)$ and $B_{Bn}(\Delta)$ are real functions of Δ. The work of Wallace (1973) and of Byron *et al* (1975, 1979) strongly suggests that for Yukawa-type potentials of the form (2.14) one has for *all* Δ

$$\bar{f}_{En}(k, \Delta) = i^{n-1} U_0^n \frac{A_{Bn}(\Delta)}{k^{n-1}} \qquad n \geq 1 \tag{2.16}$$

and

$$\bar{f}_{Wn}(k, \Delta) = i^{n-1} U_0^n \left(\frac{A_{Bn}(\Delta)}{k^{n-1}} + i \frac{B_{Bn}(\Delta)}{k^n} \right) \qquad n \geq 2. \tag{2.17}$$

Thus, for large k, each term $\bar{f}_{En}$ of the eikonal series gives the *leading contribution* to the corresponding Born term $\bar{f}_{Bn}$ for all momentum transfers, while the Wallace amplitude (2.7) also provides in each order of perturbation theory the *next term* to relative order k^{-1} beyond the eikonal contribution, at all momentum transfers.

3. The unitarised eikonal-Born series method for electron–atom or positron–atom collisions

Let us now turn to the realistic case of the scattering of an electron or a positron by a neutral target atom containing Z electrons. We shall establish our basic equations for both elastic and inelastic (excitation) processes. We begin by considering direct collisions; exchange effects will be discussed at the end of this section.

3.1. The unitarised EBS direct amplitude

We choose the nucleus of the target atom as the origin of our coordinate system, and denote the coordinates of the incident particle (electron or positron) and of the atomic electrons by $\boldsymbol{r}_0$ and $\boldsymbol{r}_j$ respectively ($j = 1, 2, \ldots Z$). We shall also use the symbol X to represent all the target coordinates. All quantities will be expressed in atomic units.

In the initial, direct channel the total Hamiltonian H of the system may be decomposed as

$$H = H_d + V_d \tag{3.1}$$

where the direct arrangement channel Hamiltonian H_d describes the two colliding particles (projectile and target atom) before the collision. It is such that $H_d = K + h$, where K is the kinetic energy operator of the incident particle and h the internal Hamiltonian describing the target atom before the collision. The momenta of the projectile before and after the collision are $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$, respectively, and $\boldsymbol{\Delta} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the momentum transfer. We shall denote by w_n the eigenenergies and by $|n\rangle$ the eigenvectors of the internal Hamiltonian h, so that

$$h|n\rangle = w_n|n\rangle. \tag{3.2}$$

The wavefunctions corresponding to the eigenvectors $|n\rangle$ will be written in the coordinate representation as $\psi_n(X)$. We shall assume that before the collision the target atom is in the eigenstate $|0\rangle$, with eigenenergy w_0. We shall also write

$$H_d\Phi_a = E_a\Phi_a \tag{3.3}$$

where $E_a = \frac{1}{2}k_i^2 + w_0 = E + w_0$ ($E = \frac{1}{2}k_i^2$ being the incident particle energy) and Φ_a is the 'free' state vector in the initial channel. We shall also need the Green's operator in the direct arrangement channel, which we write as

$$G_d^{(+)} = (E - H_d + i\varepsilon)^{-1} \qquad \varepsilon \to 0^+. \tag{3.4}$$

Neglecting all but the Coulomb interactions, the interaction potential between the projectile and the target in the direct arrangement channel is

$$V_d(\boldsymbol{r}_0, X) = \frac{ZQ}{r_0} - Q\sum_{j=1}^{Z} r_{0j}^{-1} \tag{3.5}$$

where $Q = -1$ for incident electrons, $Q = +1$ for incident positrons and $r_{0j} = |\boldsymbol{r}_0 - \boldsymbol{r}_j|$. Finally, we shall denote by $\Psi_a^{(+)}$ the exact scattering state vector, satisfying the Lippmann–Schwinger equation

$$\Psi_a^{(+)} = \Phi_a + G_d^{(+)}V_d\Psi_a^{(+)}. \tag{3.6}$$

Let us now assume that we are working within the framework of a 'frozen-target' approximation similar to that used by Glauber (1959) to obtain the many-body Glauber eikonal amplitude. We may then construct for a direct transition $|\boldsymbol{k}_i, 0\rangle \to |\boldsymbol{k}_f, m\rangle$ the many-body Wallace amplitude

$$f_W = \frac{k_i}{2\pi i}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(X)|\{\exp[i(k_i^{-1}\chi_0(\boldsymbol{b}, X) + k_i^{-3}\chi_1(\boldsymbol{b}, X))] - 1\}|\psi_0(X)\rangle\, d^2\boldsymbol{b} \tag{3.7}$$

where we have written $\boldsymbol{r}_0 = \boldsymbol{b} + z\hat{\boldsymbol{n}}$, $\hat{\boldsymbol{n}}$ being perpendicular to $\boldsymbol{\Delta}$, as in § 2. The quantity χ_0 is the familiar Glauber phase

$$\chi_0(\boldsymbol{b}, X) = -\int_{-\infty}^{+\infty} V_d(\boldsymbol{b}, z, X)\, dz \tag{3.8}$$

while the Wallace correction χ_1, which is of second order in the interaction potential V_d, is the generalisation of equation (2.8), namely

$$\chi_1(\boldsymbol{b}, X) = \tfrac{1}{2}\int_{-\infty}^{+\infty} (\boldsymbol{\nabla}\chi_+)\cdot(\boldsymbol{\nabla}\chi_-)\, dz \tag{3.9}$$

with

$$\chi_+(\boldsymbol{b}, z, X) = -\int_{-\infty}^{z} V_d(\boldsymbol{b}, z', X)\, dz' \tag{3.10}$$

and

$$\chi_-(\boldsymbol{b}, z, X) = -\int_{z}^{\infty} V_d(\boldsymbol{b}, z', X)\, dz'. \tag{3.11}$$

It should be stressed that because of the complexity of χ_1, the many-body Wallace

amplitude (3.7) is vastly more difficult to evaluate than the potential scattering Wallace amplitude (2.7) or the many-body Glauber amplitude

$$f_G = \frac{k_i}{2\pi i}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(X)|[\exp(ik_i^{-1}\chi_0(\boldsymbol{b},X))-1]|\psi_0(X)\rangle\,d^2\boldsymbol{b}. \tag{3.12}$$

An important property of the many-body Wallace amplitude (3.7) is that it is *unitary* (as is the Glauber amplitude f_G). Both f_G and f_W treat the interaction potential V_d to all orders in the coupling constant Q, and since f_W contains the phase correction χ_1, it appears to be a good candidate for the direct scattering amplitude. We shall examine this point below by using perturbation theory.

We shall assume that *LS* coupling holds for the target atom and that both ψ_0 and ψ_m correspond to definite values of the total orbital angular momentum and magnetic quantum number of the target, and are expressed as antisymmetrised products of one-electron orbitals. The integration on the azimuthal angle ϕ of $\boldsymbol{b}$ can then be performed in equations (3.7) and (3.12). For example, if both ψ_0 and ψ_m correspond to S states, then the many-body Wallace amplitude (3.7) becomes

$$f_W(S\to S) = -ik_i\int_0^\infty J_0(\Delta b)\langle\psi_m(X)|\{\exp[i(k_i^{-1}\chi_0(b,X)+k_i^{-3}\chi_1(b,X))]-1\}|\psi_0(X)\rangle b\,db \tag{3.13}$$

where $\chi_0(b,X)$ and $\chi_1(b,X)$ are obtained by setting $\phi=0$ in $\chi_0(\boldsymbol{b},X)$ and $\chi_1(\boldsymbol{b},X)$, respectively. The Glauber amplitude for S–S transitions, $f_G(S\to S)$ is obtained by setting $\chi_1=0$ in equation (3.13), so that

$$f_G(S\to S) = -ik_i\int_0^\infty J_0(\Delta b)\langle\psi_m(X)|[\exp(ik_i^{-1}\chi_0(b,X))-1]|\psi_0(X)\rangle b\,db. \tag{3.14}$$

Expressions which are similar to equation (3.13) can readily be written down for the many-body Wallace and Glauber amplitudes corresponding to non-S→S transitions; the main difference from equations (3.13) and (3.14) is the replacement of $J_0(\Delta b)$ by $i^{|\delta M|}J_{|\delta M|}(\Delta b)$, where δM is the difference between the initial and final magnetic quantum numbers.

Let us expand the many-body Wallace amplitude f_W and the Glauber amplitude f_G in powers of the interaction potential V_d. In this way we generate the many-body Wallace series and the Glauber series, the general terms of which will be denoted by $\bar{f}_{Wn}$ and $\bar{f}_{Gn}$, respectively. Both $\bar{f}_{Wn}$ and $\bar{f}_{Gn}$ provide approximations to the general term $\bar{f}_{Bn}$ of the (many-body) Born series for the direct scattering amplitude. The relationships between the terms $\bar{f}_{Gn}$ and $\bar{f}_{Bn}$ have been discussed elsewhere (see, for example, Byron and Joachain, 1977a). We shall now investigate the properties of the Wallace terms $\bar{f}_{Wn}$.

First of all, it is clear that we have in first order

$$\bar{f}_{W1} = \bar{f}_{G1} = \bar{f}_{B1} = (2\pi)^{-1}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(X)|\chi_0(\boldsymbol{b},X)|\psi_0(X)\rangle\,d^2\boldsymbol{b}. \tag{3.15}$$

Remembering that χ_1 is of second order in V_d, we see from equation (3.7) that for $n>1$

$$\bar{f}_{Wn} = (2\pi)^{-1}\left(\frac{i}{k_i}\right)^{n-1}\frac{1}{n!}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(X)|\chi_0^n(\boldsymbol{b},X)$$
$$-n(n-1)ik_i^{-1}\chi_0^{n-2}(\boldsymbol{b},X)\chi_1(\boldsymbol{b},X)+\ldots|\psi_0(X)\rangle\,d^2\boldsymbol{b} \tag{3.16}$$

where we have only written explicitly the two leading contributions to $\bar{f}_{Wn}$ in inverse powers of k_i. For $n \geqslant 4$, terms involving higher powers of χ_1 (such as $\chi_0^{n-4}\chi_1^2$) occur in equation (3.16). We shall see in § 4 (for the case of $e^{\pm}$–H collisions) that these terms are sufficiently singular that the integral implied by equation (3.16) diverges. This, of course, does not imply that the full many-body Wallace amplitude f_W diverges, since in this case the quantity χ_1 occurs in the phase. We also see that the first term on the right-hand side of equation (3.16), involving χ_0^n, is just the nth term of the Glauber series,

$$\bar{f}_{Gn} = (2\pi)^{-1}\left(\frac{i}{k_i}\right)^{n-1}\frac{1}{n!}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(\boldsymbol{X})|\chi_0^n(\boldsymbol{b},\boldsymbol{X})|\psi_0(\boldsymbol{X})\rangle\, d^2\boldsymbol{b} \tag{3.17}$$

which provides the leading contribution to $\bar{f}_{Wn}$ in inverse powers of k_i; the second term on the right-hand side of equation (3.16) yields a correction of order k_i^{-1} relative to the first term.

The second-order Wallace term, $\bar{f}_{W2}$, is of particular interest. It is given by

$$\bar{f}_{W2} = (2\pi)^{-1}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b})\langle\psi_m(\boldsymbol{X})|\tfrac{1}{2}ik_i^{-1}\chi_0^2(\boldsymbol{b},\boldsymbol{X}) + k_i^{-2}\chi_1(\boldsymbol{b},\boldsymbol{X})|\psi_0(\boldsymbol{X})\rangle\, d^2\boldsymbol{b}. \tag{3.18}$$

If we are dealing with an S→S transition we may write the real and imaginary parts of $\bar{f}_{W2}$ as

$$\mathrm{Re}\,\bar{f}_{W2}(S\to S) = k_i^{-2}\int_0^\infty J_0(\Delta b)\langle\psi_m(\boldsymbol{X})|\chi_1(b,\boldsymbol{X})|\psi_0(\boldsymbol{X})\rangle b\, db \tag{3.19}$$

and

$$\mathrm{Im}\,\bar{f}_{W2}(S\to S) = \tfrac{1}{2}k_i^{-1}\int_0^\infty J_0(\Delta b)\langle\psi_m(\boldsymbol{X})|\chi_0^2(b,\boldsymbol{X})|\psi_0(\boldsymbol{X})\rangle b\, db \tag{3.20}$$

and we recall that $\mathrm{Re}\,\bar{f}_{G2} = 0$ in that case.

At this point, we remark that since the 'frozen target' model is derived from a many-body Green's function in which closure has been applied and the average excitation energies in both the initial and final channels have been set equal to zero, the long-range dynamic polarisation effects will be missing from the many-body Wallace amplitude f_W. In particular, the term $\mathrm{Re}\,\bar{f}_{W2}$ given by (3.19) is just the k_i^{-2} part of $\mathrm{Re}\,\bar{f}_{SB2}$ (where SB2 denotes the simplified second Born term, obtained in the closure approximation) with an average excitation energy $\bar{w} = 0$, and thus lacks the all-important contribution of order k_i^{-1} which is characteristic of dipole polarisation effects. Also, the term $\mathrm{Im}\,\bar{f}_{W2}$ (which is identical to $\mathrm{Im}\,\bar{f}_{G2}$) and hence $\mathrm{Im}\,\bar{f}_W$ diverge at $\Delta = 0$.

In order to avoid the above deficiencies due to the term $\bar{f}_{W2}$, while keeping the advantages of f_W, and remembering that the second Born term can be evaluated with good accuracy in many cases of interest, we construct a new amplitude with $\bar{f}_{B2}$ inserted in the place of $\bar{f}_{W2}$, namely

$$f_{UEBS} = f_W - \bar{f}_{W2} + \bar{f}_{B2}. \tag{3.21}$$

At small momentum transfers, where higher-order terms of perturbation theory are rather unimportant, we see that if we keep the terms through order k_i^{-2} in (3.21), we retrieve the eikonal-Born series (EBS) amplitude (Byron and Joachain 1973b, 1977c)

$$f_{EBS} = \bar{f}_{B1} + \bar{f}_{B2} + \bar{f}_{G3}. \tag{3.22}$$

On the other hand, the terms $\bar{f}_{B2}$ and $\bar{f}_{W2}$ will differ negligibly at large momentum transfers because when Δ is large, off-shell elastic scattering (for which the correct excitation energy is zero) dominates. Thus, at large Δ, f_{UEBS} will differ negligibly from f_W, and will provide a more accurate value of the direct scattering amplitude than the EBS′ amplitude (Byron and Joachain 1975)

$$f_{EBS'} = f_G - \bar{f}_{G2} + \bar{f}_{B2}. \tag{3.23}$$

Moreover, the amplitude f_{UEBS} will be nearly unitary at all angles. In what follows we shall call f_{UEBS} the 'unitarised EBS direct amplitude'. It is this amplitude which is used in § 4 as our approximation to the direct scattering amplitude for elastic collisions of electrons and positrons with atomic hydrogen.

3.2. The unitarised EBS exchange amplitude

Given the very careful, non-perturbative treatment which we have developed for the direct scattering amplitude, it is natural to look beyond first order (Born or Ochkur) approximations for the exchange amplitude. We begin by splitting the total Hamiltonian in the exchange arrangement channel as

$$H = H_P + V_P \tag{3.24}$$

where V_P, the interaction between the outgoing electron (coordinate $\boldsymbol{r}_1$) and the target, is obtained by permutating in V_d the coordinates of the electrons (0) and (1). Let $a \equiv (\boldsymbol{k}_i, 0)$ be the initial state of the system, with the incident electron having momentum $\boldsymbol{k}_i$ and the target in the state $|0\rangle$, and $b \equiv (\boldsymbol{k}_f, m)$ the final state in the exchange arrangement channel, with the outgoing (initially bound) electron having momentum $\boldsymbol{k}_f$ and the target in the state $|m\rangle$. The exchange amplitude corresponding to the transition $a \to b$ is given by (see, for example, Joachain, 1975)

$$g_{ba} = -(2\pi)^2 \langle \Phi_{Pb} | V_P | \Psi_a^{(+)} \rangle \tag{3.25}$$

where $\Psi_a^{(+)} \equiv \Psi_{\boldsymbol{k}_i,0}^{(+)}$ is the exact scattering state vector, satisfying equation (3.6), and $\Phi_{Pb} \equiv \Phi_{m,\boldsymbol{k}_f}$ is the final asymptotic state in the exchange arrangement channel, such that

$$H_P \Phi_{Pb} = E_b \Phi_{Pb} \tag{3.26}$$

with $E_b = \frac{1}{2}k_f^2 + w_m$. Using equation (3.6), we may also write

$$g_{ba} = -(2\pi)^2 (\langle \Phi_{Pb} | V_P | \Phi_a \rangle + \langle \Phi_{Pb} | V_P G_d^{(+)} V_d | \Psi_a^{(+)} \rangle). \tag{3.27}$$

Let us use in equation (3.27) the spectral representation of the Green's operator $G_d^{(+)}$, namely

$$G_d^{(+)} = \sum_n \int d\boldsymbol{q} \frac{|\Phi_{\boldsymbol{q},n}\rangle\langle\Phi_{\boldsymbol{q},n}|}{\frac{1}{2}k_i^2 + w_0 - \frac{1}{2}q^2 - w_n + i\varepsilon} \qquad \varepsilon \to 0^+ \tag{3.28}$$

(where the sum over n implies an integration on the continuum part of the spectrum) and introduce a more explicit notation, with $g_{ba} \equiv g(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0)$. In this way we obtain

$$g(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0) = g_{B1}(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0) + (2\pi^2)^{-1} \sum_n \int d\boldsymbol{q} \frac{1}{q^2 - k_n^2 - i\varepsilon}$$
$$\times g_{B1}(\boldsymbol{k}_f, m; \boldsymbol{q}, n) f(\boldsymbol{q}, n; \boldsymbol{k}_i, 0) \qquad \varepsilon \to 0^+ \tag{3.29}$$

with $k_n^2 = k_i^2 - 2(w_n - w_0)$. In the above equation

$$g_{B1}(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0) = -(2\pi)^2 \langle \Phi_{m,\boldsymbol{k}_f} | V_P \text{ (or } V_d) | \Phi_{\boldsymbol{k}_i,0} \rangle \tag{3.30}$$

is the first Born (or Born–Oppenheimer) approximation to the exchange amplitude (on shell), while

$$g_{B1}(\boldsymbol{k}_f, m; \boldsymbol{q}, n) = -(2\pi)^2 \langle \Phi_{m,\boldsymbol{k}_f} | V_P | \Phi_{\boldsymbol{q},n} \rangle \tag{3.31}$$

is the *half-off-shell* first Born exchange amplitude for the transition $(\boldsymbol{q}, n) \to (\boldsymbol{k}_f, m)$ from a virtual initial state $(\boldsymbol{q}, n)$ to the final state $(\boldsymbol{k}_f, m)$, and

$$f(\boldsymbol{q}, n; \boldsymbol{k}_i, 0) = -(2\pi)^2 \langle \Phi_{\boldsymbol{q},n} | V_d | \Psi^{(+)}_{\boldsymbol{k}_i,0} \rangle \tag{3.32}$$

is the *half-off-shell* direct scattering amplitude for the transition $(\boldsymbol{k}_i, 0) \to (\boldsymbol{q}, n)$ from the initial state $(\boldsymbol{k}_i, 0)$ to a virtual state $(\boldsymbol{q}, n)$.

Equation (3.29) is an interesting one, since it tells us that if we know all the half-off-shell *direct* amplitudes, then the *exchange* amplitude may be obtained by quadratures. More importantly, equation (3.29) is completely *non-perturbative* in nature although, if one wishes, one can of course expand $f(\boldsymbol{q}, n; \boldsymbol{k}_i, 0)$ in a Born series and generate in this way a Born series for $g(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0)$.

We remark that an equation which is formally equivalent to equation (3.29) may be derived by starting from the expression (Joachain 1975)

$$g_{ba} = -(2\pi)^2 \langle \Psi^{(-)}_{Pb} | V_d | \Phi_a \rangle \tag{3.33}$$

where the exact state vector $\Psi^{(-)}_{Pb} \equiv \Psi^{(-)}_{m,\boldsymbol{k}_f}$ satisfies the Lippmann–Schwinger equation

$$\Psi^{(-)}_{Pb} = \Phi_{Pb} + G_P^{(-)} V_P \Psi^{(-)}_{Pb} \tag{3.34}$$

and

$$G_P^{(-)} = (E - H_P - i\varepsilon)^{-1} \qquad \varepsilon \to 0^+. \tag{3.35}$$

By using the spectral representation of the Green's operator $G_P^{(-)}$ in the exchange arrangement channel, we then obtain

$$g(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0) = g_{B1}(\boldsymbol{k}_f, m; \boldsymbol{k}_i, 0) + (2\pi^2)^{-1} \sum_n \int d\boldsymbol{q} \frac{1}{q^2 - k_n^2 - i\varepsilon}$$
$$\times f(\boldsymbol{k}_f, m; \boldsymbol{q}, n) g_{B1}(\boldsymbol{q}, n; \boldsymbol{k}_i, 0) \tag{3.36}$$

which is the desired result. In the above equation $g_{B1}(\boldsymbol{q}, n; \boldsymbol{k}_i, 0)$ is the (prior) half-off-shell first Born exchange amplitude, namely

$$g_{B1}(\boldsymbol{q}, n; \boldsymbol{k}_i, 0) = -(2\pi)^2 \langle \Phi_{n,\boldsymbol{q}} | V_d | \Phi_{\boldsymbol{k}_i,0} \rangle. \tag{3.37}$$

In attempting to make approximations in equations (3.29) or (3.36) one must be very careful. In the spirit of few-state approximations, it is tempting to consider the possibility of including only the initial and final target states in the sum over the index n which appears in these equations. For example, in equation (3.29) and for the case of *elastic* scattering, this approach would yield an approximation in which there is initial channel elastic scattering. On the other hand, in an optical model approach with a 'direct' optical potential V^d_{opt} and an exchange pseudopotential V^{ex}_{opt} (see Byron and Joachain 1977b, 1981), one obtains higher-order corrections to g_{B1} which account for both initial and final channel elastic scattering. Similar conclusions can be inferred from the distorted wave approximation. What happens in equation (3.29) is that terms in the high continuum of the *initial* (direct) arrangement channel target state

summation (with corresponding values of q of order unity) give rise to *final* (exchange) arrangement channel elastic scattering. Thus, it is reasonable to conjecture that a consistent 'elastic' approximation to the elastic exchange amplitude is given by

$$\begin{aligned} g_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) &= \tilde{g}_{\mathrm{B1}}(\boldsymbol{k}_{\mathrm{f}}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{i}}^2 - \mathrm{i}\varepsilon} \tilde{g}_{\mathrm{B1}}(\boldsymbol{k}_{\mathrm{f}}, 0; \boldsymbol{q}, 0) f_{\mathrm{UEBS}}(\boldsymbol{q}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{i}}^2 - \mathrm{i}\varepsilon} f_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, 0; \boldsymbol{q}, 0) \tilde{g}_{\mathrm{B1}}(\boldsymbol{q}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) \qquad \varepsilon \to 0^+. \end{aligned} \tag{3.38}$$

In writing equation (3.38) we have used our unitarised EBS amplitude f_{UEBS} defined by equation (3.21) to approximate the exact half-off-shell direct elastic amplitude f. Moreover, we have replaced g_{B1} by $\tilde{g}_{\mathrm{B1}}$, which is the first Born exchange amplitude from which the contribution due to the electron–nucleus interaction has been removed. This reflects the well known property that if the electron–electron interactions are set equal to zero in the interaction potentials V_{P} or V_{d} then the exchange amplitude g_{ba}, as given by equation (3.25) or (3.33), vanishes (see Goldberger and Watson 1964, Joachain 1975). In other words the sum of all the terms of the Born series for the exchange amplitude which do not involve the electron–electron interactions must add up to zero (Shakeshaft 1978). By setting the electron–nucleus term equal to zero in the expression of $\tilde{g}_{\mathrm{B1}}$ we guarantee that this property is obeyed.

The elastic exchange amplitude $g_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, 0; \boldsymbol{k}_{\mathrm{i}}, 0)$ given by equation (3.38) will be denoted in what follows as the unitarised EBS elastic exchange amplitude. It is this amplitude which, together with the direct amplitude f_{UEBS}, will be used in § 4 to analyse the elastic scattering of fast electrons by atomic hydrogen in the ground state. We remark that the last two terms in equation (3.38) are particularly important at large angles where scattering through elastic intermediate states is expected to dominate at sufficiently high impact energies.

The generalisation of equation (3.38) to the case of *inelastic* exchange amplitudes is straightforward. For example, in the case of an inelastic transition $(\boldsymbol{k}_{\mathrm{i}}, 0) \to (\boldsymbol{k}_{\mathrm{f}}, m)$, with $m \neq 0$, the unitarised EBS exchange amplitude, obtained by including the initial and final target states in both the initial (direct) and final (exchange) arrangement channels is given by

$$\begin{aligned} g_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{k}_{\mathrm{i}}, 0) &= \tilde{g}_{\mathrm{B1}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{i}}^2 - \mathrm{i}\varepsilon} \tilde{g}_{\mathrm{B1}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{q}, 0) f_{\mathrm{UEBS}}(\boldsymbol{q}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{f}}^2 - \mathrm{i}\varepsilon} \tilde{g}_{\mathrm{B1}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{q}, m) f_{\mathrm{UEBS}}(\boldsymbol{q}, m; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{i}}^2 - \mathrm{i}\varepsilon} f_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{q}, 0) \tilde{g}_{\mathrm{B1}}(\boldsymbol{q}, 0; \boldsymbol{k}_{\mathrm{i}}, 0) \\ &\quad + (2\pi^2)^{-1} \int \mathrm{d}\boldsymbol{q} \frac{1}{q^2 - k_{\mathrm{f}}^2 - \mathrm{i}\varepsilon} f_{\mathrm{UEBS}}(\boldsymbol{k}_{\mathrm{f}}, m; \boldsymbol{q}, m) \tilde{g}_{\mathrm{B1}}(\boldsymbol{q}, m; \boldsymbol{k}_{\mathrm{i}}, 0) \qquad \varepsilon \to 0^+ \end{aligned} \tag{3.39}$$

4. Elastic electron and positron scattering by atomic hydrogen

In order to illustrate the discussion of § 3, we shall consider here the simple case of elastic collisions of electrons or positrons by the ground state of atomic hydrogen.

4.1. Calculation of the unitarised EBS direct amplitude

Let $\boldsymbol{r}_0$ be the coordinate of the incident electron and $\boldsymbol{r}_1$ that of the target electron. Then

$$V_d(\boldsymbol{r}_0, \boldsymbol{r}_1) = Q\left(\frac{1}{r_0} - \frac{1}{r_{01}}\right) \tag{4.1}$$

with $r_{01} = |\boldsymbol{r}_0 - \boldsymbol{r}_1|$. Using equation (3.8) we obtain for the Glauber phase the well known expression

$$\chi_0(\boldsymbol{b}, \boldsymbol{b}_1) = -Q \ln(\beta^2/b^2) \tag{4.2}$$

where we have written $\boldsymbol{r}_0 = \boldsymbol{b} + z\hat{\boldsymbol{n}}$, $\boldsymbol{r}_1 = \boldsymbol{b}_1 + z_1\hat{\boldsymbol{n}}$ and $\boldsymbol{\beta} = \boldsymbol{b} - \boldsymbol{b}_1$.

Our next task is to calculate the Wallace correction χ_1. From equations (3.10) and (4.1) we have

$$\begin{aligned}\chi_+(\boldsymbol{b}, z, \boldsymbol{r}_1) &= -Q\int_{-\infty}^{z} \{(b^2+z'^2)^{-2} - [\beta^2 + (z'-z_1)^2]^{-1/2}\}\,dz' \\ &= Q \ln \frac{r_0 - z}{|\boldsymbol{r}_0 - \boldsymbol{r}_1| - (z - z_1)}\end{aligned} \tag{4.3}$$

while equation (3.11) yields in a similar way

$$\chi_-(\boldsymbol{b}, z, \boldsymbol{r}_1) = Q \ln \frac{r_0 + z}{|\boldsymbol{r}_0 - \boldsymbol{r}_1| + (z - z_1)}. \tag{4.4}$$

From equations (3.9), (4.3) and (4.4) we then obtain, after a straightforward calculation,

$$\chi_1(\boldsymbol{b}, \boldsymbol{r}_1) = Q^2\left(I_1(b, \beta, z_1) - \frac{\boldsymbol{b}\cdot\boldsymbol{\beta}}{b^2\beta^2} I_2(b, \beta, z_1)\right) \tag{4.5}$$

where

$$I_1(b, \beta, z_1) = \int_{-\infty}^{+\infty} (b^2+z^2)^{-1/2}[\beta^2 + (z-z_1)^2]^{-1/2}\,dz \tag{4.6}$$

and

$$I_2(b, \beta, z_1) = \int_{-\infty}^{+\infty} \{1 - z(z-z_1)(b^2+z^2)^{-1/2}[\beta^2 + (z-z_1)^2]^{-1/2}\}\,dz. \tag{4.7}$$

In equation (4.5) we have written explicitly the quantity $Q^2(=1)$ to emphasise that the correction χ_1 is of second order in the direct interaction potential V_d.

The integrals I_1 and I_2 are evaluated in appendix 1, where it is shown that

$$\begin{aligned}I_1(b, \beta, z_1) &= \frac{\pi}{(b\beta)^{1/2}} P_{-1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right) \\ &= \frac{\pi}{(b\beta)^{1/2}} {}_2F_1\left(\tfrac{1}{2}, \tfrac{1}{2}; 1; -\frac{(\beta-b)^2+z_1^2}{4b\beta}\right)\end{aligned} \tag{4.8}$$

and

$$I_2(b,\beta,z_1)=\pi(b\beta)^{1/2}P_{1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right)$$
$$=\pi(b\beta)^{1/2}{}_2F_1\left(-\tfrac{1}{2},\tfrac{3}{2};1;-\frac{(\beta-b)^2+z_1^2}{4b\beta}\right). \tag{4.9}$$

In the above equations $P_{1/2}$ and $P_{-1/2}$ are Legendre functions.

Using equation (4.5) and the results (4.8) and (4.9), we may now write the Wallace correction in closed form as

$$\chi_1(\boldsymbol{b},\boldsymbol{r}_1)=\frac{Q^2\pi}{(b\beta)^{1/2}}\left(P_{-1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right)-\hat{\boldsymbol{b}}\cdot\hat{\boldsymbol{\beta}}P_{1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right)\right)$$
$$=\frac{Q^2\pi}{(b\beta)^{1/2}}\left({}_2F_1\left(\tfrac{1}{2},\tfrac{1}{2};1;-\frac{(\beta-b)^2+z_1^2}{4b\beta}\right)\right.$$
$$\left.-\hat{\boldsymbol{b}}\cdot\hat{\boldsymbol{\beta}}{}_2F_1\left(-\tfrac{1}{2},\tfrac{3}{2};1;-\frac{(\beta-b)^2+z_1^2}{4b\beta}\right)\right). \tag{4.10}$$

This result is identical to that obtained by Byron *et al* (1981) (and subsequently by Unnikrishnan and Prasad (1982), and Franco and Iwinski (1982)). We remark that χ_1 is an even function of z_1, a fact which allows only transitions such that $\Delta L+\Delta M$ is even.

With the Glauber phase given by equation (4.2) and the Wallace correction χ_1 obtained from equation (4.10), we must now perform the five-dimensional integrals implied by equations (3.7) and (3.18) to determine the quantities f_{W} and $\bar{f}_{\mathrm{W2}}$ which, together with the second Born term $\bar{f}_{\mathrm{B2}}$—obtained in the way described in the recent paper of Byron and Joachain (1981)—are required in order to obtain the unitarised EBS amplitude f_{UEBS}. In fact, as explained above, once the symmetries of ψ_0 and ψ_m are specified the integral on the azimuthal angle ϕ can be done analytically, and we are left with four-dimensional integrals. For example, in the case of S→S transitions, and in particular for the elastic scattering case considered here, the relevant four-dimensional integrals corresponding to f_{W} and $\bar{f}_{\mathrm{W2}}$ are given by equations (3.13), (3.19) and (3.20), respectively.

The four-dimensional integrals giving f_{W} and $\bar{f}_{\mathrm{W2}}$ for the case of elastic scattering by the ground state of atomic hydrogen (with $\psi_0\equiv\psi_m\equiv\psi_{1s}$) have been calculated by direct numerical integration. Excellent checks on the numerical procedures may be obtained by noting that

(i) the quantity $\mathrm{Re}\,\bar{f}_{\mathrm{W2}}$, as given by equation (3.19) is the k_i^{-2} part of $\mathrm{Re}\,\bar{f}_{\mathrm{SB2}}$, calculated with an average excitation energy $\bar{w}=0$. This property, which was pointed out in § 3 on general grounds, is proved explicitly in appendix 2 for the case of elastic $e^{\pm}$–H scattering considered here.

(ii) The quantity $\mathrm{Im}\,\bar{f}_{\mathrm{W2}}$, as given by equation (3.20) is equal to $\mathrm{Im}\,\bar{f}_{\mathrm{G2}}$, which can be obtained in closed form for the case of elastic $e^{\pm}$–H scattering (Yates 1974).

4.2. The large momentum transfer limit of the direct amplitude

Since at large momentum transfers the influence of higher-order terms in perturbation theory is enhanced, it is of particular interest to examine the behaviour of the terms

$\bar{f}_{\mathrm{W}n}$ in the limit of large Δ. We shall do this by following a method similar to that used in appendix B of Byron and Joachain (1977a) to obtain the asymptotic form of the Glauber series for large Δ.

First of all, we remark that the large-Δ behaviour of the Wallace amplitude is controlled by the small-b behaviour of the phases $\chi_0(b, \boldsymbol{b}_1)$ and $\chi_1(b, \boldsymbol{b}_1)$. From equation (4.2) we see immediately that for small b

$$\chi_0 \simeq Q \ln b^2 - Q \ln b_1^2. \tag{4.11}$$

The small-b behaviour of the Wallace correction is readily obtained from equation (4.10). We find that

$$\chi_1(b, r_1) \simeq Q^2 \left(-\frac{2r_1 \cos\phi_1}{b_1} \frac{1}{b} - \frac{1}{r_1} \ln b^2 + \frac{2}{r_1} \ln \frac{4r_1^2}{b_1} \right). \tag{4.12}$$

Substituting equations (4.11) and (4.12) into equation (3.13), and setting $\psi_0 = \psi_m = \psi_{1\mathrm{s}}$, we obtain in the limit of large Δ, for the elastic scattering case,

$$f_{\mathrm{W}} \simeq -\mathrm{i}k_{\mathrm{i}} \int_0^\infty J_0(\Delta b) \left\langle \psi_{1\mathrm{s}} \right| \left\{ \exp\left[\mathrm{i} \left(\frac{Q}{k_{\mathrm{i}}} \ln b^2 - \frac{Q}{k_{\mathrm{i}}} \ln b_1^2 \right.\right.\right.$$
$$\left.\left.\left. - \frac{Q^2}{k_{\mathrm{i}}^3 r_1} \ln b^2 + \frac{2Q^2}{k_{\mathrm{i}}^3 r_1} \ln \frac{4r_1^2}{b_1} - \frac{2Q^2 r_1 \cos\phi_1}{k_{\mathrm{i}}^3 b b_1} \right) \right] - 1 \right\} \left| \psi_{1\mathrm{s}} \right\rangle b \, \mathrm{d}b. \tag{4.13}$$

To extract the various terms in the Wallace series, one merely expands the exponential in powers of Q. However, we see that this procedure leads to a term in b^{-2}, proportional to Q^4, which will yield a divergent integral. Hence, in what follows, we shall consider only terms up to order Q^3, and therefore shall neglect the last term in the exponential bracket, since in lowest orders (Q^2 and Q^3) it gives zero because of the ϕ_1 integration.

Setting

$$\alpha = \frac{Q}{k_{\mathrm{i}}} - \frac{Q^2}{k_{\mathrm{i}}^3 r_1} \tag{4.14}$$

and neglecting the term in $\cos\phi_1$, we find that for large Δ

$$f_{\mathrm{W}} \simeq -\mathrm{i}k_{\mathrm{i}} \int_0^\infty J_0(\Delta b) \left\langle \psi_{1\mathrm{s}} \right| b^{1+2\mathrm{i}\alpha} \exp\left[\mathrm{i} \left(-\frac{Q}{k_{\mathrm{i}}} \ln b_1^2 + \frac{2Q^2}{k_{\mathrm{i}}^3 r_1} \ln \frac{4r_1^2}{b_1} \right) \right] \left| \psi_{1\mathrm{s}} \right\rangle \mathrm{d}b. \tag{4.15}$$

The integration over b can be done with the aid of a large-b cut-off, and we obtain in the limit of large Δ

$$f_{\mathrm{W}} \simeq -\frac{2}{\Delta^2} \left\langle \psi_{1\mathrm{s}} \right| \left(Q - \frac{Q^2}{k_{\mathrm{i}}^2 r_1} \right) \frac{\Gamma(1+\mathrm{i}\alpha)}{\Gamma(1-\mathrm{i}\alpha)} \exp(-2\mathrm{i}\alpha \ln \tfrac{1}{2}\Delta)$$
$$\times \exp\left[\mathrm{i} \left(-\frac{Q}{k_{\mathrm{i}}} \ln b_1^2 + \frac{2Q^2}{k_{\mathrm{i}}^3 r_1} \ln \frac{4r_1^2}{b_1} \right) \right] \left| \psi_{1\mathrm{s}} \right\rangle. \tag{4.16}$$

It is now a simple matter to expand equation (4.16) in powers of Q up to third order, and thereby obtain the first three terms of the Wallace series in the limit of large Δ.

That is,

$$\bar{f}_{W1} \simeq -2Q/\Delta^2 \tag{4.17a}$$

$$\mathrm{Re}\,\bar{f}_{W2} \simeq -(2Q^2/k_i^2\Delta^2)\langle\psi_{1s}|r_1^{-1}|\psi_{1s}\rangle = 2Q^2/k_i^2\Delta^2 \tag{4.17b}$$

$$\begin{aligned}\mathrm{Im}\,\bar{f}_{W2} &\simeq (4Q^2/k_i\Delta^2)\langle\psi_{1s}|\ln b_1 + \ln\tfrac{1}{2}\Delta + \gamma|\psi_{1s}\rangle \\ &= (4Q^2/k_i\Delta^2)(\ln\tfrac{1}{2}\Delta + \tfrac{1}{2})\end{aligned} \tag{4.17c}$$

$$\begin{aligned}\mathrm{Re}\,\bar{f}_{W3} &\simeq (4Q^3/k_i^2\Delta^2)\langle\psi_{1s}|(\ln b_1 + \ln\tfrac{1}{2}\Delta + \gamma)^2|\psi_{1s}\rangle \\ &= (4Q^3/k_i^2\Delta^2)(\ln^2\tfrac{1}{2}\Delta + \ln\tfrac{1}{2}\Delta + \tfrac{1}{12}\pi^2)\end{aligned} \tag{4.17d}$$

$$\begin{aligned}\mathrm{Im}\,\bar{f}_{W3} &\simeq -(8Q^3/k_i^3\Delta^2)\langle\psi_{1s}|(\ln r_1 + \ln\Delta + \gamma)r_1^{-1}|\psi_{1s}\rangle \\ &= -(8Q^3/k_i^3\Delta^2)(\ln\tfrac{1}{2}\Delta + 1).\end{aligned} \tag{4.17e}$$

In equations (4.17), $\gamma = 0.57721566\ldots$ is the Euler constant. Note that in using equation (4.13) to obtain equations (4.17) we assume that the region near $r_1 = 0$ is unimportant in evaluating the various matrix elements. This is clearly the case here.

The terms $\bar{f}_{W1}$, $\mathrm{Im}\,\bar{f}_{W2}$ and $\mathrm{Re}\,\bar{f}_{W3}$ of course duplicate the large-Δ behaviour of the corresponding terms in the Glauber series. From the point of view of the unitarised EBS approximation, the interesting new terms are $\mathrm{Re}\,\bar{f}_{W2}$, $\mathrm{Im}\,\bar{f}_{W3}, \ldots,$ namely those terms which are missing from the Glauber series. We remark that the large-Δ expression of $\mathrm{Re}\,\bar{f}_{W2}$ agrees precisely with the large-Δ expression for $\mathrm{Re}\,\bar{f}_{SB2}$ (see Byron and Joachain 1973b), evaluated with $\bar{w} = 0$, as we expect from our discussion of the term $\mathrm{Re}\,\bar{f}_{W2}$ in § 3 and appendix 2. In addition, the part of $\mathrm{Im}\,\bar{f}_{W3}$ proportional to $\ln\frac{1}{2}\Delta$ is just what one obtains in the large-Δ limit when one does an elastic unitarity calculation of $\mathrm{Im}\,\bar{f}_{B3}$ (Byron and Joachain 1973c). However, the part of $\mathrm{Im}\,\bar{f}_{W3}$ which contains no logarithms arises from the contributions of an infinite number of intermediate states in the unitarity relation. It is also interesting to note that, unlike the Glauber approximation, the Wallace approximation will yield a differential cross section containing terms in $\ln\Delta$. This is readily seen from equation (4.16) where α, as given by equation (4.14) is a function of r_1. For the simple Glauber approximation, α is independent of r_1, and hence the term in $\ln\Delta$ appears only as an overall phase factor in the scattering amplitude at large momentum transfers.

Finally, we return to the question of the singular term in b^{-1} which we have discarded. As pointed out above, the existence of this term implies that one cannot expand indefinitely in powers of the Wallace phase and hence in inverse powers of k_i. This strongly suggests that, in fact, one does not have a power series in k_i^{-1} for the scattering amplitude, even though such an expansion may occur for the first few orders. At first glance, this conclusion appears disturbing. However, one should remember that Byron and Latour (1976) have shown that for large k_i and large Δ the imaginary part of the second Born term for 1s–2p excitation in atomic hydrogen falls off very slowly, namely like $k_i^{-2}\Delta^{-1}$. Through the unitarity relation such a term will contribute to $\mathrm{Im}\,\bar{f}_{B4}$ via an expression of the form (see, for example, Joachain 1975)

$$\frac{k_i}{4\pi}\int (\mathrm{Im}\,\bar{f}_{B2}^{1s2p})(\mathrm{Im}\,\bar{f}_{B2}^{1s2p})\,d\Omega. \tag{4.18}$$

Because of the very slow fall-off of $\mathrm{Im}\,\bar{f}_{B2}^{1s2p}$ with increasing Δ, this expression yields terms in $\ln k_i$, in addition to terms of a more conventional type. This gives some

support for the idea that an expansion of the elastic amplitude in powers of k_i^{-1} may not exist beyond the first few orders of perturbation theory.

4.3. The exchange amplitude

Let us now consider the elastic exchange amplitude $g(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s)$ for electron scattering from the ground state of atomic hydrogen. The potential V_P is given by

$$V_P(\boldsymbol{r}_0, \boldsymbol{r}_1) = r_{01}^{-1} - r_1^{-1}. \tag{4.19}$$

Before applying our treatment of § 3.2 to the present case, we briefly discuss some properties of the first two terms of the Born series for the elastic exchange amplitude g.

The first Born approximation to the exchange amplitude, given by equation (3.30), reads in the present case

$$g_{B1}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) = g_{B1}^{(01)}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) + g_{B1}^{(1)}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) \tag{4.20}$$

where

$$g_{B1}^{(01)}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) = -(2\pi)^{-1}\langle \exp(i\boldsymbol{k}_f \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|r_{01}^{-1}|\exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle \tag{4.21}$$

and

$$g_{B1}^{(1)}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) = -(2\pi)^{-1}\langle \exp(i\boldsymbol{k}_f \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|-r_1^{-1}|\exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle. \tag{4.22}$$

The quantity $g_{B1}^{(01)}$ which is obtained from g_{B1} by omitting the contribution due to the electron–nucleus interaction $(-r_1^{-1})$ is what we called $\tilde{g}_{B1}$ in § 3.2. We use here the more explicit notation $g_{B1}^{(01)}$ since this term arises only from the electron–electron repulsion term r_{01}^{-1}. It is readily evaluated by using standard Dalitz integrals (see, for example, Joachain 1975). We recall that for large $k_i (= k_f)$ the term $g_{B1}^{(01)}$ reduces to the Ochkur amplitude

$$g_{Och} = -32/k_i^2(\Delta^2+4)^2. \tag{4.23}$$

The quantity $g_{B1}^{(1)}$, which is the contribution to g_{B1} arising from the electron–nucleus interaction $(-r_1^{-1})$ is straightforward to evaluate, giving the result $g_{B1}^{(1)} = 16(k_i^2+1)^{-3}$. As pointed out in § 3.2, the term $g_{B1}^{(1)}$ must be omitted, because if the electron–electron interaction r_{01}^{-1} were turned off, the exact amplitude would vanish. In fact, as Byron and Joachain (1973b) pointed out, one can show explicitly that for large k_i the dominant part of $g_{B1}^{(1)}$ (namely $16k_i^{-6}$) is exactly cancelled by part of the second Born term $\bar{g}_{B2}$. This part is the contribution to $\bar{g}_{B2}$ arising from the ground state (1s) acting as an intermediate state, and involving the electron–nucleus interaction $(-r_1^{-1})$ in the off-shell exchange matrix element, namely

$$\bar{g}_{B2}^{(1)}(1s) = (8\pi^4)^{-1}\int d\boldsymbol{q}\,\frac{1}{q^2 - k_i^2 - i\varepsilon}\langle \exp(i\boldsymbol{k}_f \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|-r_1^{-1}|\exp(i\boldsymbol{q} \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle$$

$$\times\langle \exp(i\boldsymbol{q} \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)|r_{01}^{-1} - r_0^{-1}|\exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle \qquad \varepsilon \to 0^+. \tag{4.24}$$

An exact calculation of the full second term of the Born series for the exchange amplitude, $\bar{g}_{B2}$ (including the electron–nucleus interaction term in the exchange matrix element) has been performed recently by Walters (1980) for elastic e^-–H scattering

at 30 eV. In adding the exact quantity $\bar{g}_{B2}$ so obtained to g_{B1}, the cancellation mentioned above between the terms $g_{B1}^{(1)}$ and $\bar{g}_{B2}^{(1)}(1s)$ is, of course, taken into account. However, other cancellations, involving the electron–nucleus interaction $(-r_1^{-1})$, and arising between $\bar{g}_{B2}$ and higher-order terms $\bar{g}_{Bn}$ of the Born series for the exchange amplitude, are then neglected. For this reason we are interested here only in $\bar{g}_{B2}^{(01)}$, the part of the second Born exchange amplitude containing only the term r_{01}^{-1} in the exchange matrix element. Moreover, in line with the 'elastic' approximation to the exchange amplitude discussed in § 3.2, we shall consider only the contributions to $\bar{g}_{B2}^{(01)}$ coming from the ground state acting as an intermediate state in both the initial and final arrangement channels. Denoting these contributions by $\bar{g}_{B2}^{(01)}(1s)$ and $\bar{g}_{B2}^{(01)}(1s')$, we have

$$\bar{g}_{B2}^{(01)}(1s) = (8\pi^4)^{-1} \int d\boldsymbol{q} \frac{1}{q^2 - k_i^2 - i\varepsilon} \langle \exp(i\boldsymbol{k}_f \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|r_{01}^{-1}|\exp(i\boldsymbol{q} \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle$$

$$\times \langle \exp(i\boldsymbol{q} \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)|r_{01}^{-1} - r_0^{-1}|\exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle \qquad \varepsilon \to 0^+ \quad (4.25a)$$

and

$$\bar{g}_{B2}^{(01)}(1s') = (8\pi^4)^{-1} \int d\boldsymbol{q} \frac{1}{q^2 - k_i^2 - i\varepsilon} \langle \exp(i\boldsymbol{k}_f \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|r_{01}^{-1} - r_1^{-1}|\exp(i\boldsymbol{q} \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)\rangle$$

$$\times \langle \exp(i\boldsymbol{q} \cdot \boldsymbol{r}_1)\psi_{1s}(r_0)|r_{01}^{-1}|\exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_0)\psi_{1s}(r_1)\rangle \qquad \varepsilon \to 0^+. \quad (4.25b)$$

The two terms $\bar{g}_{B2}^{(01)}(1s)$ and $\bar{g}_{B2}^{(01)}(1s')$ are of particular importance at large momentum transfers. Indeed, when k_i and Δ are large, the leading part of both terms, which is provided by their imaginary part, is given by

$$\text{Im}\, \bar{g}_{B2}^{(01)}(1s) = \text{Im}\, \bar{g}_{B2}^{(01)}(1s') \simeq -4/k_i^3 \Delta^2 \quad (4.26)$$

and therefore falls off like $k_i^{-3}\Delta^{-2}$ rather than like $k_i^{-2}\Delta^{-4}$ as is the case with $g_{B1}^{(01)}$ (see equation (4.23)). Since the term $g_{B1}^{(01)}$ contains the leading piece of the elastic exchange amplitude at small Δ, the approximate second-order amplitude

$$g \simeq g_{B1}^{(01)} + \bar{g}_{B2}^{(01)}(1s) + \bar{g}_{B2}^{(01)}(1s') \quad (4.27)$$

which was used by Byron *et al* (1981) contains the leading contribution to the elastic exchange amplitude at all angles. However, as explained in § 3.2 we can use equation (3.38) and our knowledge of the direct elastic, unitarised EBS amplitude f_{UEBS} to construct an improved elastic exchange amplitude

$$g_{UEBS}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s)$$

$$= g_{B1}^{(01)}(\boldsymbol{k}_f, 1s; \boldsymbol{k}_i, 1s) + (2\pi^2)^{-1} \int d\boldsymbol{q} \frac{1}{q^2 - k_i^2 - i\varepsilon}$$

$$\times g_{B1}^{(01)}(\boldsymbol{k}_f, 1s; \boldsymbol{q}, n) f_{UEBS}(\boldsymbol{q}, 1s; \boldsymbol{k}_i, 1s) + (2\pi^2)^{-1} \int d\boldsymbol{q} \frac{1}{q^2 - k_i^2 - i\varepsilon}$$

$$\times f_{UEBS}(\boldsymbol{k}_f, 1s; \boldsymbol{q}, 1s) g_{B1}^{(01)}(\boldsymbol{q}, 1s; \boldsymbol{k}_i, 1s) \qquad \varepsilon \to 0^+. \quad (4.28)$$

In addition to exhibiting the nice properties of the second-order amplitude (4.27), the amplitude (4.28) has the important advantage of being non-perturbative, as it contains the interaction potential to all orders via f_{UEBS}.

4.4. Results and discussion

Using the unitarised EBS direct amplitude f_{UEBS} given by equation (3.21) (with $Q=-1$ in V_{d}) as our approximation to the direct amplitude, f^{-}, and the amplitude g_{UEBS} given by equation (4.28) as our approximation to the exchange amplitude, g, we have obtained differential scattering cross sections for electron–atomic-hydrogen elastic scattering from the relation

$$\mathrm{d}\sigma^{-}/\mathrm{d}\Omega=\tfrac{1}{4}|f^{-}+g|^{2}+\tfrac{3}{4}|f^{-}-g|^{2}. \tag{4.29}$$

Similarly, for positron–atomic-hydrogen elastic scattering we have used equation (3.21) (with $Q=+1$ in V_{d}) to obtain the scattering amplitude f^{+} and hence the differential cross section

$$\mathrm{d}\sigma^{+}/\mathrm{d}\Omega=|f^{+}|^{2}. \tag{4.30}$$

Our UEBS results for electron and positron scattering are listed in tables 1 and 2, respectively, for incident energies of 100, 200, 300 and 400 eV. In tables 3 and 4 we present a detailed comparison, at an incident energy of 100 eV, of our present UEBS results with those obtained by using several related theoretical approximations, namely the eikonal-Born series (EBS) method (with f_{B2} obtained from Byron and Joachain (1981)), the third-order optical model (OM) calculations of Byron and Joachain (1981), and the many-body Wallace approximation, namely

$$\frac{\mathrm{d}\sigma_{\mathrm{W}}^{\pm}}{\mathrm{d}\Omega}=|f_{\mathrm{W}}^{\pm}|^{2} \tag{4.31}$$

where f_{W}^{-} is the many-body Wallace amplitude (3.7) for electrons and f_{W}^{+} that for positrons. In table 3 we have also added for comparison EBS and UEBS results in which exchange effects have been omitted.

Table 1. Differential cross sections (in $a_0^2\ \mathrm{sr}^{-1}$) for the elastic scattering of electrons by atomic hydrogen in the energy range 100–400 eV, as obtained from the present unitarised eikonal-Born series theory. The numbers in parentheses indicate powers of ten.

θ	Energy (eV)			
(deg)	100	200	300	400
0	8.22	5.59	4.50	3.88
5	4.46	2.19	1.51	1.21
10	2.40	1.12	7.84(−1)	6.27(−1)
15	1.39	6.41(−1)	4.32(−1)	3.23(−1)
20	8.46(−1)	3.80(−1)	2.39(−1)	1.67(−1)
25	5.35(−1)	2.30(−1)	1.35(−1)	8.92(−2)
30	3.50(−1)	1.43(−1)	7.96(−2)	5.03(−2)
35	2.35(−1)	9.21(−2)	4.88(−2)	3.00(−2)
40	1.63(−1)	6.10(−2)	3.13(−2)	1.88(−2)
50	8.43(−2)	2.95(−2)	1.44(−2)	8.45(−3)
60	4.80(−2)	1.59(−2)	7.57(−3)	4.39(−3)
70	2.96(−2)	9.43(−3)	4.42(−3)	2.55(−3)
80	1.96(−2)	6.04(−3)	2.81(−3)	1.62(−3)
90	1.38(−2)	4.14(−3)	1.92(−3)	1.11(−3)
100	1.02(−2)	3.01(−3)	1.39(−3)	8.04(−4)
120	6.43(−3)	1.84(−3)	8.49(−4)	4.90(−4)
140	4.72(−3)	1.33(−3)	6.10(−4)	3.52(−4)
160	3.96(−3)	1.10(−3)	5.04(−4)	2.91(−4)
180	3.73(−3)	1.03(−3)	4.73(−4)	2.74(−4)

Table 2. Differential cross sections (in a_0^2 sr^{-1}) for the elastic scattering of positrons by atomic hydrogen in the energy range 100–400 eV, as obtained from the present unitarised eikonal-Born series theory. The numbers in parentheses indicate powers of ten.

θ (deg)	Energy (eV)			
	100	200	300	400
0	2.37	1.67	1.39	1.25
5	1.67	1.17	9.95(−1)	9.04(−1)
10	1.05	7.18(−1)	5.98(−1)	5.18(−1)
15	6.68(−1)	4.51(−1)	3.46(−1)	2.75(−1)
20	4.44(−1)	2.79(−1)	1.94(−1)	1.42(−1)
25	3.01(−1)	1.72(−1)	1.10(−1)	7.57(−2)
30	2.06(−1)	1.07(−1)	6.42(−2)	4.25(−2)
35	1.42(−1)	6.78(−2)	3.92(−2)	2.52(−2)
40	9.90(−2)	4.46(−2)	2.50(−2)	1.58(−2)
50	5.05(−2)	2.12(−2)	1.15(−2)	7.14(−3)
60	2.79(−2)	1.14(−2)	6.06(−3)	3.73(−3)
70	1.68(−2)	6.75(−3)	3.56(−3)	2.17(−3)
80	1.09(−2)	4.34(−3)	2.27(−3)	1.39(−3)
90	7.56(−3)	2.99(−3)	1.56(−3)	9.50(−4)
100	5.57(−3)	2.18(−3)	1.13(−3)	6.92(−4)
120	3.48(−3)	1.34(−3)	6.97(−4)	4.23(−4)
140	2.56(−3)	9.68(−4)	5.03(−4)	3.05(−4)
160	2.14(−3)	8.03(−4)	4.16(−4)	2.53(−4)
180	2.02(−3)	7.55(−4)	3.91(−4)	2.38(−4)

Table 3. Comparison of various differential cross sections (in a_0^2 sr^{-1}) for elastic electron–atomic-hydrogen scattering at 100 eV, as obtained from several approximations, namely: eikonal-Born series (EBS), Wallace (W), unitarised EBS (UEBS) and third-order optical model (OM) of Byron and Joachain (1981). The numbers in parentheses indicate powers of ten.

θ (deg)	No exchange			With exchange		
	EBS	W	UEBS	EBS	OM	UEBS
0	8.01	∞	7.56	8.73	8.54	8.22
5	4.31	2.94	4.00	4.81	4.73	4.46
10	2.27	1.66	2.08	2.63	2.57	2.40
15	1.28	1.07	1.17	1.53	1.48	1.39
20	7.69(−1)	7.14(−1)	7.03(−1)	9.41(−1)	9.02(−1)	8.46(−1)
25	4.85(−1)	4.84(−1)	4.44(−1)	6.01(−1)	5.71(−1)	5.35(−1)
30	3.20(−1)	3.32(−1)	2.92(−1)	3.96(−1)	3.75(−1)	3.50(−1)
35	2.19(−1)	2.31(−1)	1.99(−1)	2.69(−1)	2.53(−1)	2.35(−1)
40	1.55(−1)	1.63(−1)	1.39(−1)	1.88(−1)	1.77(−1)	1.63(−1)
50	8.43(−2)	8.56(−2)	7.43(−2)	9.92(−2)	9.28(−2)	8.43(−2)
60	5.08(−2)	4.87(−2)	4.34(−2)	5.79(−2)	5.37(−2)	4.80(−2)
70	3.32(−2)	2.98(−2)	2.73(−2)	3.68(−2)	3.36(−2)	2.96(−2)
80	2.32(−2)	1.95(−2)	1.82(−2)	2.52(−2)	2.25(−2)	1.96(−2)
90	1.72(−2)	1.36(−2)	1.29(−2)	1.83(−2)	1.60(−2)	1.38(−2)
100	1.33(−2)	9.94(−3)	9.53(−3)	1.40(−2)	1.19(−2)	1.02(−2)
120	9.06(−3)	6.12(−3)	5.94(−3)	9.37(−3)	7.51(−3)	6.43(−3)
140	7.02(−3)	4.41(−3)	4.31(−3)	7.20(−3)	5.50(−3)	4.72(−3)
160	6.07(−3)	3.66(−3)	3.57(−3)	6.20(−3)	4.59(−3)	3.96(−3)
180	5.79(−3)	3.44(−3)	3.36(−3)	5.91(−3)	4.33(−3)	3.73(−3)

Table 4. Comparison of various differential cross sections (in a_0^2 sr^{-1}) for elastic positron–atomic-hydrogen scattering at 100 eV, as obtained from several approximations, namely: eikonal-Born series (EBS), Wallace (W), third-order optical model (OM) and unitarised EBS (UEBS). The numbers in parentheses indicate powers of ten.

θ (deg)	EBS	W	OM	UEBS
0	2.63	∞	2.20	2.37
5	1.81	2.36	1.55	1.67
10	1.08	1.18	9.66(−1)	1.05
15	6.61(−1)	6.89(−1)	6.17(−1)	6.68(−1)
20	4.25(−1)	4.31(−1)	4.14(−1)	4.44(−1)
25	2.83(−1)	2.80(−1)	2.85(−1)	3.01(−1)
30	1.93(−1)	1.87(−1)	1.99(−1)	2.06(−1)
35	1.35(−1)	1.28(−1)	1.41(−1)	1.42(−1)
40	9.64(−2)	8.97(−2)	1.01(−1)	9.90(−2)
50	5.35(−2)	4.70(−2)	5.42(−2)	5.05(−2)
60	3.31(−2)	2.69(−2)	3.14(−2)	2.79(−2)
70	2.25(−2)	1.66(−2)	1.96(−2)	1.68(−2)
80	1.65(−2)	1.10(−2)	1.31(−2)	1.09(−2)
90	1.28(−2)	7.70(−3)	9.22(−3)	7.56(−3)
100	1.03(−2)	5.70(−3)	6.86(−3)	5.57(−3)
120	7.51(−3)	3.58(−3)	4.32(−3)	3.48(−3)
140	6.08(−3)	2.63(−3)	3.17(−3)	2.56(−3)
160	5.39(−3)	2.20(−3)	2.65(−3)	2.14(−3)
180	5.18(−3)	2.08(−3)	2.50(−3)	2.02(−3)

In figures 1–3 we show our present UEBS electron results along with those obtained from the EBS approximation and the third-order OM approach (Byron and Joachain 1981). The OM results are in close accord with the DWSBA calculations of Kingston and Walters (1980), particularly at large angles. The experimental values of Williams (1975) are also shown, together with some experimental values of Lloyd *et al* (1974)—as renormalised by van Wingerden *et al* (1977)—whenever these differ significantly from (or complete) the Williams data. Also shown in figures 1–3 are our UEBS positron scattering results. The difference between electron and positron scattering is striking throughout the entire angular range. We recall that the Glauber method gives electron and positron differential cross sections which are exactly equal. Clearly, the addition of the Wallace correction, χ_1, to the Glauber phase, χ_0, has a significant effect.

Looking at figures 1 and 2, we see that at small angles our present UEBS results agree very well with the EBS and third-order OM values, but at larger angles the three methods split, with the EBS method giving the largest results of the three and the present method giving the smallest. We remark that the difference between the present UEBS results and our previously published ones (Byron *et al* 1981) is due entirely to our treatment of exchange. In our previous work we used the approximate second-order elastic exchange amplitude (4.27), while here we use the elastic exchange amplitude given by equation (4.28), which leads to lower differential cross sections at large angles. We also note that at large angles the no-exchange UEBS (or Wallace) electron results are lower than the corresponding no-exchange electron third-order OM results, the difference being about 25% at $\theta = 180°$ for an incident energy of 100 eV, and becoming smaller as the energy increases. The experimental values of Williams (1975) and of Lloyd *et al* (1974)—as renormalised by van Wingerden *et al*

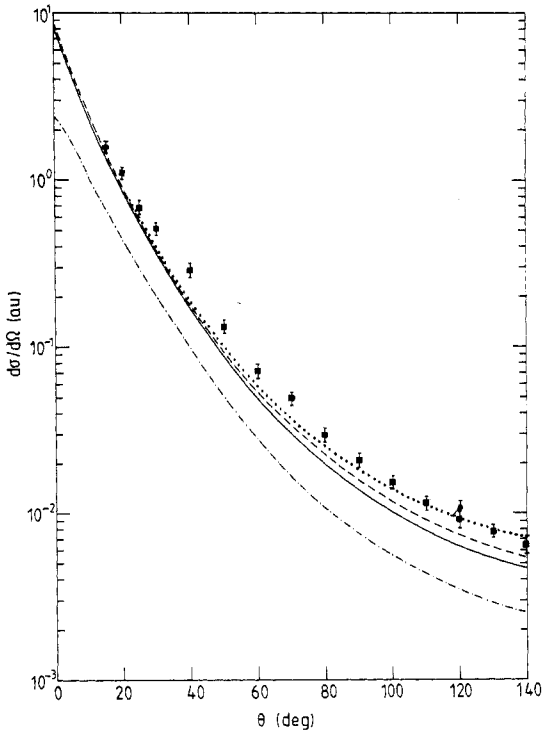

Figure 1. Differential cross sections for the elastic scattering of 100 eV electrons and positrons by atomic hydrogen. The full curve is the present unitarised EBS result for electrons, the broken curve is the third-order optical model of Byron and Joachain (1981) for electrons, the dotted curve is the EBS result for electrons and the chain curve is the present unitarised EBS result for positrons. The squares (■) represent the experimental data of Williams (1975) for incident electrons and the dots (●) those of Lloyd *et al* (1974), renormalised by van Wingerden *et al* (1977).

(1977)—lie consistently above our present UEBS results by roughly 25–30% at 100 eV and by 10–30% at 200 eV. In the light of the excellent agreement between the three theoretical results at small and intermediate angles, it is difficult to see what effects could be invoked on the theoretical side to explain the differences between theory and experiment.

In figure 3, at an energy of 400 eV, the optical model results and the present UEBS results are nearly indistinguishable from each other, while the EBS results are still on the high side at larger angles. The agreement between theory and experiment is better than at 100 and 200 eV, but it is still far from excellent, especially at larger angles.

In tables 5 and 6 we list the total (integrated) elastic cross sections for electron and positron scattering, respectively. As we would expect from figures 1–3, the present UEBS method gives values which are in good agreement with those obtained from the third-order OM potential. It is encouraging to see that these two distinctly different methods of unitarising the EBS method give such similar results. We also note the close agreement between the present results and the DWSBA values of Kingston and Walters (1980). All the theoretical results fall below the experimental results of Williams (1975) and of van Wingerden *et al* (1977), the discrepancy at 200 eV between the UEBS result and the value obtained by Williams being about 10%, while it is larger

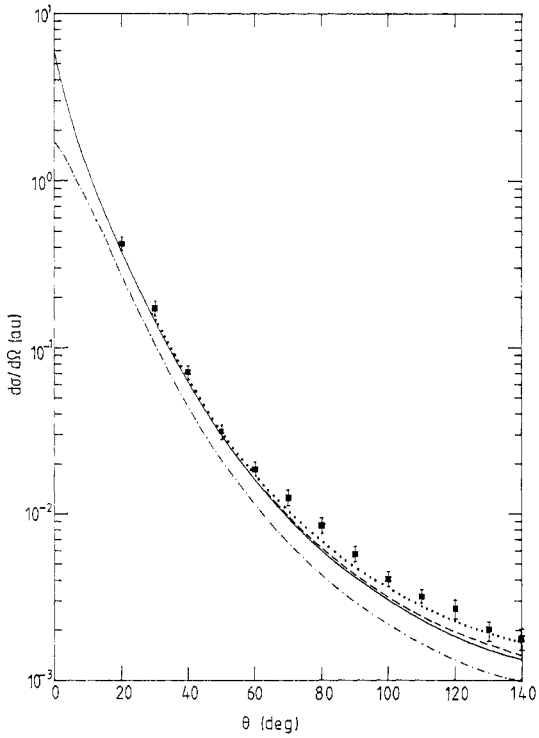

Figure 2. Same as figure 1, but at 200 eV.

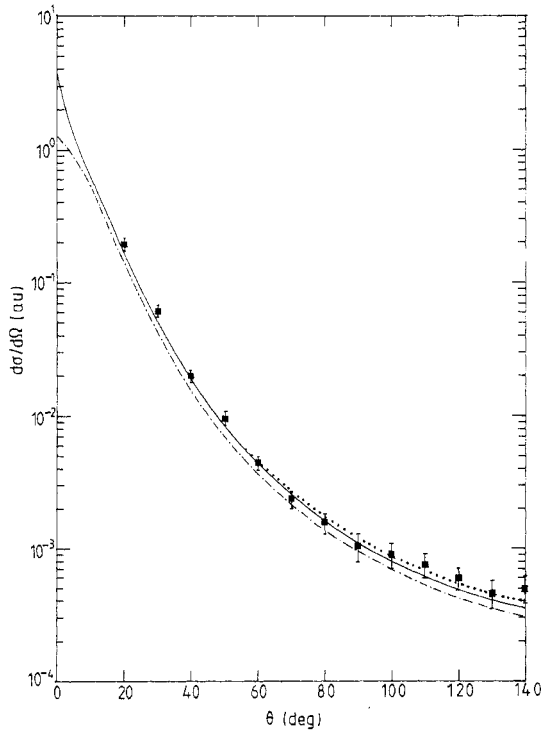

Figure 3. Same as figure 1, but at 400 eV. The full curve represents both the third-order optical model results of Byron and Joachain (1981) and the present UEBS results.

Table 5. Total elastic cross sections (in units of a_0^2) for electron scattering by atomic hydrogen. The numbers in parentheses indicate powers of ten.

Energy (eV)	First Born approximation	DWSBA†	EBS	Third-order optical model‡	Present UEBS	Williams (1975)	van Wingerden *et al* (1977)
100	9.39(−1)	1.45	1.61	1.54	1.43	1.75§	1.83
200	4.84(−1)	6.09(−1)	6.39(−1)	6.31(−1)	6.13(−1)	6.69(−1)§	7.89(−1)
300	3.26(−1)	3.80(−1)	3.90(−1)	3.91(−1)	3.82(−1)		
400	1.97(−1)	2.76(−1)	2.80(−1)	2.82(−1)	2.76(−1)		

† Kingston and Walters (1980).
‡ Byron and Joachain (1981).
§ Values quoted by van Wingerden *et al* (1977).

Table 6. Total elastic cross sections (in units of a_0^2) for positron scattering by atomic hydrogen. The numbers in parentheses indicate powers of ten.

Energy (eV)	First Born approximation	EBS	Third-order optical model†	Present UEBS
100	9.39(−1)	7.59(−1)	7.02(−1)	6.09(−1)
200	4.84(−1)	4.22(−1)	4.13(−1)	3.74(−1)
300	3.26(−1)	2.95(−1)	2.92(−1)	2.72(−1)
400	1.97(−1)	2.27(−1)	2.26(−1)	2.14(−1)

† Byron and Joachain (1981).

than 20% between the UEBS value and the result of van Wingerden *et al*. Regarding positron scattering, it is interesting to note that the differences between the present UEBS method and the third-order optical potential results are more important than in the electron scattering case.

By using the optical theorem applied separately to the singlet and triplet cross sections for electron–atomic-hydrogen elastic scattering, we obtain for the total (complete) electron scattering cross section

$$\sigma_{\mathrm{tot}}^{-} = (4\pi/k_{\mathrm{i}})\mathrm{Im}(f^{-}(\theta = 0) - \tfrac{1}{2}g(\theta = 0)) \tag{4.32}$$

while for the total positron scattering cross section we have simply

$$\sigma_{\mathrm{tot}}^{+} = (4\pi/k_{\mathrm{i}})\,\mathrm{Im}\,f^{+}(\theta = 0). \tag{4.33}$$

Results for $\sigma_{\mathrm{tot}}^{-}$ obtained from our present UEBS calculations are given in table 7, where they are compared with the first Born values, the DWSBA values of Kingston and Walters (1980), the EBS values, the results of the third-order OM calculation and the semi-empirical values obtained by de Heer *et al* (1977). The various theoretical results agree closely for incident energies $E \geqslant 200$ eV, but at 100 eV they split, with the present UEBS results being on the lower side, in better agreement with the semi-empirical values of de Heer *et al*.

In table 8 we show the results for $\sigma_{\mathrm{tot}}^{+}$, obtained from our present UEBS calculations, and compare them with the third-order OM values and the EBS results. The EBS values of $\sigma_{\mathrm{tot}}^{+}$ are the same as the EBS values of $\sigma_{\mathrm{tot}}^{-}$, and are just the sum of the first Born integrated cross sections, since in the EBS approximation the imaginary part of the scattering amplitude is given by $\mathrm{Im}\,\bar{f}_{\mathrm{B2}}$.

Table 7. Total cross sections (in units of a_0^2) for electron scattering by atomic hydrogen.

Energy (eV)	DWSBA†	EBS	Third-order optical model‡	Present UEBS	Semi-empirical§
100	7.40	7.49	7.68	7.19	6.85
200	4.34	4.39	4.38	4.27	4.18
300	3.11	3.17	3.14	3.10	3.06
400	2.46	2.50	2.48	2.45	2.43

† Kingston and Walters (1980).
‡ Byron and Joachain (1981).
§ de Heer *et al* (1977).

Table 8. Total cross sections (in units of a_0^2) for positron scattering by atomic hydrogen.

Energy (eV)	EBS	Third-order optical model†	Present UEBS
100	7.49	6.76	7.01
200	4.39	4.14	4.21
300	3.17	3.03	3.07
400	2.50	2.42	2.44

† Byron and Joachain (1981).

It is interesting to note from tables 7 and 8 that in the present UEBS method we find electron and positron total (complete) cross sections which are nearly equal. This near equality follows from the fact that in any method which employs a closure approximation for the Green's function all *odd* order terms of the Born series for the direct scattering amplitude (except the first, f_{B1}) vanish at $\theta = 0°$ for $e^{\pm}$–H elastic scattering (Dewangan 1980). Since the even orders of the Born series are the same at all angles for e^-–H and e^+–H scattering, we see that in any pure closure calculation

$$\operatorname{Im} f^-(\theta = 0) = \operatorname{Im} f^+(\theta = 0) \tag{4.34}$$

and that this equality will also hold for the unitarised EBS direct amplitudes given by equation (3.21). Thus, the difference between σ_{tot}^- and σ_{tot}^+ in the present calculations is due entirely to the presence of the exchange amplitude, g, in the electron scattering case. Since the imaginary part of our exchange amplitude, g_{UEBS}, is rather small, we find that σ_{tot}^- and σ_{tot}^+ are nearly equal.

Unfortunately, at small angles our evaluation of the exchange amplitude via the essentially 'elastic' approximation (4.28) is not likely to be very precise. We have estimated the effect of adding the 2s and 2p intermediate states contributions in equation (4.28). The result is that the value of $\operatorname{Im} g(\theta = 0)$ is reduced from the simple 'elastic' value obtained directly from equation (4.28). (We remark in this connection that intermediate p states do *not* dominate $\operatorname{Im} g(\theta = 0)$ as they do in the case of $\operatorname{Im} f(\theta = 0)$). Thus, the differences between σ_{tot}^- and σ_{tot}^+ may be even smaller than those inferred from tables 7 and 8.

Dewangan (1980) has suggested that the vanishing of the terms $\bar{f}_{Bn}$ (n odd $\geqslant 3$) of the Born series for direct scattering indicates a deficiency of the closure approximation. This conclusion is probably correct, but it is nevertheless possible that these terms $\bar{f}_{Bn}$ (n odd $\geqslant 3$) vanish at $\theta = 0°$ *to leading order* in k_i^{-1}. If this is the case, then $\bar{f}_{Bn}$

($\theta = 0$) will be small for n odd $\geqslant 3$ at the energies considered here, and the near equality of σ^{-}_{tot} and σ^{+}_{tot} will still exist. We remark in this connection that while the present method gives total (integrated) elastic cross sections for e^{-}–H scattering which are larger than those for e^{+}–H scattering (see tables 5 and 6) the same method applied to 1s–2s excitation of atomic hydrogen (Byron *et al* 1981) gives total (integrated) electron cross sections, $\sigma^{-}_{1s,2s}$, much smaller than those corresponding to positron impact, $\sigma^{+}_{1s,2s}$. In other words, in studying the differences between integrated electron and positron collision cross sections in atomic hydrogen one may find that there is a good deal of cancellation between different processes. On the experimental side, we note further that recent electron and positron total cross section measurements by Kauppila *et al* (1981), in which σ^{-}_{tot} and σ^{+}_{tot} are measured in the same apparatus on a *helium* target, give nearly equal total cross sections down to about 100 eV incident energy.

Acknowledgments

This work was supported in part by the NATO Scientific Affairs Division under Grant 1394. One of us (RMP) is supported by the IRSIA Institute.

Appendix 1

In this appendix we shall calculate the integrals $I_1(b, \beta, z_1)$ and $I_2(b, \beta, z_1)$ defined by equations (4.6) and (4.7), respectively.

The first integral, I_1, can readily be evaluated by using the Fourier convolution theorem. For this purpose, we write I_1 in the form

$$I_1 = \int_{-\infty}^{+\infty} f(z) g^*(z - z_1)\, \mathrm{d}z \tag{A.1}$$

where

$$f(z) = (b^2 + z^2)^{-1/2} \qquad g(z - z_1) = [\beta^2 + (z - z_1)^2]^{-1/2}. \tag{A.2}$$

Let us denote the Fourier transforms of the functions $f(z)$ and $g(z)$ by $F(p)$ and $G(p)$, respectively. We then have

$$I_1 = 2\pi \int_{-\infty}^{+\infty} \exp(\mathrm{i}pz_1) F(p) G^*(p)\, \mathrm{d}p. \tag{A.3}$$

In our case

$$F(p) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \exp(\mathrm{i}pz) f(z)\, \mathrm{d}z$$

$$= \pi^{-1} \int_0^{\infty} \frac{\cos(pz)}{(b^2 + z^2)^{1/2}}\, \mathrm{d}z = \pi^{-1} K_0(bp) \tag{A.4a}$$

and

$$G(p) = \pi^{-1} K_0(\beta p) \tag{A.4b}$$

where K_0 is the modified Bessel function of order zero. Hence, using equations (A.3) and (A.4), we find that

$$I_1(b,\beta,z_1)=\frac{4}{\pi}\int_0^\infty \cos(pz_1)K_0(bp)K_0(\beta p)\,\mathrm{d}p$$
$$=\frac{\pi}{(b\beta)^{1/2}}P_{-1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right)$$
$$=\frac{\pi}{(b\beta)^{1/2}}{}_2F_1\left(\tfrac{1}{2},\tfrac{1}{2};1;-\frac{(\beta-b)^2+z_1^2}{4b\beta}\right) \tag{A.5}$$

where $P_{-1/2}$ is a Legendre function, and we have used a known integral (Gradshteyn and Ryzhik 1965). This is the result quoted in equation (4.8).

The second integral, I_2, can be obtained in the following way. We first differentiate I_2 with respect to z_1:

$$\frac{\partial}{\partial z_1}I_2(b,\beta,z_1)=\beta^2\int_{-\infty}^{+\infty}(b^2+z^2)^{-1/2}[\beta^2+(z-z_1)^2]^{-3/2}z\,\mathrm{d}z \tag{A.6}$$

Using again the Fourier convolution theorem to evaluate the integral on the right-hand side of equation (A.6), we have (Gradshteyn and Ryzhik 1965)

$$\frac{\partial}{\partial z_1}I_2(b,\beta,z_1)=\frac{4}{\pi}b\beta\int_0^\infty p\,\sin(pz_1)K_1(bp)K_1(\beta p)\,\mathrm{d}p$$
$$=\frac{3\pi}{4(b\beta)^{1/2}}\frac{P_{1/2}^{-1}(u)}{(u^2-1)^{1/2}}z_1$$
$$=\frac{\pi}{(b\beta)^{1/2}}\frac{P_{1/2}^{1}(u)}{(u^2-1)^{1/2}}z_1 \tag{A.7}$$

where K_1 is the modified Bessel function of order one,

$$u=(b^2+\beta^2+z_1^2)/2b\beta \tag{A.8}$$

and we have used the fact that $P_{1/2}^{-1}(u)=\frac{4}{3}P_{1/2}^{1}(u)$. From equations (A.7) and (A.8) we see that

$$I_2(b,\beta,z_1)-I_2(b,\beta,0)=\pi(b\beta)^{1/2}\int_{u_1}^{u_2}\frac{P_{1/2}^{1}(u)}{(u^2-1)^{1/2}}\,\mathrm{d}u \tag{A.9}$$

with $u_1=(b^2+\beta^2+z_1^2)/2b\beta$ and $u_2=(b^2+\beta^2)/2b\beta$. Now, since (Abramowitz and Stegun 1964)

$$\frac{P_\nu^1(u)}{(u^2-1)^{1/2}}=\frac{\mathrm{d}}{\mathrm{d}u}P_\nu(u) \tag{A.10}$$

we have

$$I_2(b,\beta,z_1)-I_2(b,\beta,0)=\pi(b\beta)^{1/2}\left(P_{1/2}\left(\frac{b^2+\beta^2+z_1^2}{2b\beta}\right)-P_{1/2}\left(\frac{b^2+\beta^2}{2b\beta}\right)\right). \tag{A.11}$$

However,

$$I_2(b,\beta,0)=\pi b\,{}_2F_1(-\tfrac{1}{2},\tfrac{1}{2};1;(b^2-\beta^2)/b^2)$$
$$=\pi(b\beta)^{1/2}P_{1/2}((b^2+\beta^2)/2b\beta) \tag{A.12}$$

and therefore

$$I_2(b,\beta,z_1)=\pi(b\beta)^{1/2}P_{1/2}((b^2+\beta^2+z_1^2)/2b)$$
$$=\pi(b\beta)^{1/2}{}_2F_1(-\tfrac{1}{2},\tfrac{3}{2};1;-[(\beta-b)^2+z_1^2]/4b\beta) \tag{A.13}$$

which is the result quoted in equation (4.9).

Appendix 2

In this appendix we shall prove explicitly, for the case of electron (positron)–scattering by the ground state of atomic hydrogen, that the real part of the second-order Wallace term, $\mathrm{Re}\,\bar{f}_{W2}$, is identical to the k_i^{-2} part of $\mathrm{Re}\,\bar{f}_{SB2}$, evaluated with an average excitation energy $\bar{w}=0$. This constitutes an excellent check of the correctness of our result (4.10) for the Wallace phase correction χ_1. The integrals required in the following calculation are all given by Gradshteyn and Ryzhik (1965).

From (3.19), we have in the present case

$$\mathrm{Re}\,\bar{f}_{W2}=k_i^{-2}\int_0^{\infty}J_0(\Delta b)A(b)b\,\mathrm{d}b \tag{A.14}$$

where

$$A(b)=\int|\psi_{1s}(r_1)|^2\chi_1(b,\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1$$
$$=\pi^{-1}\int_0^{\infty}\mathrm{d}b_1\,b_1\int_{-\infty}^{+\infty}\mathrm{d}z_1\exp[-2(b_1^2+z_1^2)^{1/2}]\int_0^{2\pi}\mathrm{d}\omega\,\chi_1(b,\boldsymbol{r}_1). \tag{A.15}$$

Here ω is the angle between $\boldsymbol{b}$ and $\boldsymbol{b}_1$, and

$$\chi_1(b,\boldsymbol{r}_1)=\frac{\pi}{(b\beta)^{1/2}}(P_{-1/2}(u)-\hat{\boldsymbol{b}}\cdot\hat{\boldsymbol{\beta}}P_{1/2}(u)) \qquad u=(b^2+\beta^2+z_1^2)/2b\beta. \tag{A.16}$$

Since $\boldsymbol{\beta}=\boldsymbol{b}-\boldsymbol{b}_1$, we have

$$\hat{\boldsymbol{b}}\cdot\hat{\boldsymbol{\beta}}=(b^2-bb_1\cos\omega)/b\beta=\mathrm{d}\beta/\mathrm{d}b. \tag{A.17}$$

We begin by performing the integral over ω in (A.15). Using the results

$$\frac{\pi}{(b\beta)^{1/2}}P_{-1/2}(u)=\frac{4}{\pi}\int_0^{\infty}\cos(pz_1)K_0(bp)K_0(\beta p)\,\mathrm{d}p \tag{A.18a}$$

and

$$\frac{\pi}{(b\beta)^{1/2}}P_{1/2}(u)=\frac{8}{\pi}\frac{b\beta}{z_1}\int_0^{\infty}p\sin(pz_1)(uK_1(bp)K_1(\beta p)+K_0(bp)K_0(\beta p))\,\mathrm{d}p \tag{A.18b}$$

together with

$$\int_0^{2\pi}\mathrm{d}\omega\,K_0(p\beta)=\int_0^{2\pi}\mathrm{d}\omega\,K_0(p(b^2+b_1^2-2bb_1\cos\omega)^{1/2})$$

$$= \int_0^\infty \mathrm{d}x \frac{x}{x^2+p^2} \int_0^{2\pi} \mathrm{d}\omega\, J_0(x(b^2+b_1^2-2bb_1\cos\omega)^{1/2})$$

$$= 2\pi \int_0^\infty \mathrm{d}x \frac{x}{x^2+p^2} J_0(xb)J_0(xb_1) \tag{A.19}$$

we have

$$\int_0^{2\pi} \mathrm{d}\omega \frac{\pi}{(b\beta)^{1/2}} P_{-1/2}(u)$$

$$= 8 \int_0^\infty \mathrm{d}x\, xJ_0(xb)J_0(xb_1) \int_0^\infty \mathrm{d}p \cos(pz_1)K_0(bp)/(x^2+p^2). \tag{A.20}$$

Similarly, using the fact that

$$\frac{b-b_1\cos\omega}{\beta} K_1(\beta p) = -\frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}b} K_0(\beta p) \tag{A.21}$$

we find that

$$\int_0^{2\pi} \mathrm{d}\omega\, \boldsymbol{b}\cdot\boldsymbol{\beta} \frac{\pi}{(b\beta)^{1/2}} P_{1/2}(u) = \frac{16}{z_1} \int_0^\infty \mathrm{d}x\, x^2 J_1(xb)J_0(xb_1) \int_0^\infty \mathrm{d}p\, p \sin(pz_1)C_1$$

and

$$C_1 = \tfrac{1}{2}(b^2+z_1^2)\frac{1}{p}\frac{K_1(bp)}{x^2+p^2} + \frac{4p}{(x^2+p^2)^3} K_1(bp) + \frac{2b}{(x^2+p^2)^2} K_0(bp). \tag{A.22}$$

Integrating by parts over the variable p, we have

$$\int_0^{2\pi} \mathrm{d}\omega\, \boldsymbol{b}\cdot\boldsymbol{\beta} \frac{\pi}{(b\beta)^{1/2}} P_{1/2}(u) = 8 \int_0^\infty \mathrm{d}x\, x^2 \frac{J_1(xb)J_0(xb_1)}{x^2+p^2} C_2$$

and

$$C_2 = \int_0^\infty \mathrm{d}p \cos(pz_1)\left(bK_0(bp) + 2p\frac{K_1(bp)}{x^2+p^2}\right) + z_1 \int_0^\infty \mathrm{d}p \sin(pz_1)K_1(bp). \tag{A.23}$$

We may now perform the integrals over b_1 and z, which appear in (A.15), so that

$$A(b) = \frac{64}{\pi} \int_0^\infty \mathrm{d}p\, K_0(bp) \int_0^\infty \mathrm{d}x \frac{x}{x^2+p^2} \frac{1}{(x^2+p^2+4)^2} (J_0(xb) - bxJ_1(xb))$$

$$- \frac{128}{\pi} \int_0^\infty \mathrm{d}p\, pK_1(bp) \int_0^\infty \mathrm{d}x \frac{x^2}{x^2+p^2} \frac{J_1(xb)}{(x^2+p^2+4)^2}$$

$$\times \left(\frac{1}{x^2+p^2} + \frac{2}{(x^2+p^2+4)}\right) \tag{A.24}$$

which may also be written after some manipulation as

$$A(b) = -\frac{64}{\pi}\frac{1}{2\alpha}\frac{\partial}{\partial\alpha}\frac{\partial}{\partial b} b \int_0^\infty \mathrm{d}p\, K_0(bp) \int_0^\infty \mathrm{d}x \frac{x}{x^2+p^2} \frac{J_0(xb)}{x^2+p^2+\alpha^2}. \tag{A.25}$$

where α must be set equal to two after differentiation. The quantity $A(b)$ may be further reduced. Indeed, using in (A.25) the integral representation

$$\frac{1}{(x^2+p^2)^{1/2}}\frac{1}{x^2+p^2+\alpha^2}=\frac{1}{\alpha}\int_0^\infty \mathrm{d}t\, tJ_1(\alpha t)K_1(t(p^2+x^2)^{1/2}) \tag{A.26}$$

and performing successively the integrals on the variables x, p and t, we find that

$$A(b)=2(K_0(2b)+2bK_1(2b)). \tag{A.27}$$

Finally, upon inserting this result in (A.14) we obtain

$$\mathrm{Re}\,\bar{f}_{\mathrm{W2}}=\frac{2}{k_i^2(\Delta^2+4)}+\frac{16}{k_i^2(\Delta^2+4)^2}$$

which is precisely the k_i^{-2} part of $\mathrm{Re}\,\bar{f}_{\mathrm{SB2}}(\bar{w}=0)$ as obtained by Byron and Joachain (1973b).

References

Abramowitz M and Stegun I A 1964 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards)

Byron F W Jr and Joachain C J 1973a *Physica* **66** 33–42

—— 1973b *Phys. Rev.* A **8** 1267–82

—— 1973c *Phys. Rev.* A **8** 3266–9

—— 1975 *J. Phys. B: At. Mol. Phys.* **8** L284–8

—— 1977a *Phys. Rep.* **34** 233–324

—— 1977b *Phys. Rev.* A **15** 128–46

—— 1977c *J. Phys. B: At. Mol. Phys.* **10** 207–26

—— 1981 *J. Phys. B: At. Mol. Phys.* **14** 2429–48

Byron F W Jr, Joachain C J and Mund E H 1973 *Phys. Rev.* D **8** 2622–39

—— 1975 *Phys. Rev.* D **11** 1662–72

—— 1979 *Phys. Rev.* C **20** 2325–38

Byron F W Jr, Joachain C J and Potvliege R M 1981 *J. Phys. B: At. Mol. Phys.* **14** L609–15

Byron F W Jr and Latour L J Jr 1976 *Phys. Rev.* A **13** 649–64

Dewangan D P 1980 *J. Phys. B: At. Mol. Phys.* **13** L595–8

Franco V and Iwinski Z 1982 *Phys. Rev.* A **25** 1900–4

Glauber R J 1959 *Lectures in Theoretical Physics* vol 1, ed W F Brittin (New York: Interscience) pp 315–414

Goldberger M L and Watson K M 1964 *Collision Theory* (New York: Wiley)

Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series and Products* (New York: Academic)

de Heer F J, McDowell M R C and Wagenaar R W 1977 *J. Phys. B: At. Mol. Phys.* **10** 1945–53

Joachain C J 1975 *Quantum Collision Theory* (Amsterdam: North-Holland)

Kauppila W E, Stein T S, Smart J H, Dababneh M S, Ho Y K, Downing J P and Pol V 1981 *Phys. Rev.* A **24** 725–42

Kingston A E and Walters H R J 1980 *J. Phys. B: At. Mol. Phys.* **13** 4633–62

Lloyd C R, Teubner P J O, Weigold E and Lewis B R 1974 *Phys. Rev.* A **10** 175–81

Molière G 1947 *Z. Naturf.* **2A** 133–52

Shakeshaft R 1978 *Phys. Rev.* A **18** 2047–57

Unnikrishnan K and Prasad M A 1982 *J. Phys. B: At. Mol. Phys.* **15** 1549–57

Wallace S J 1971 *Phys. Rev. Lett.* **27** 622–5

—— 1973 *Ann. Phys., NY* **78** 190–257

Walters H R J 1980 *J. Phys. B: At. Mol. Phys.* **13** L749–55

Williams J F 1975 *J. Phys. B: At. Mol. Phys.* **8** 2191–9

van Wingerden B, Weigold E, de Heer F J and Nygaard K J 1977 *J. Phys. B: At. Mol. Phys.* **10** 1345–62

Yates A C 1974 *Chem. Phys. Lett.* **25** 480–6