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Computation of Scattering Functions in Second-Order Many-Body Theory

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A noniterative method is discussed for solving the electron–atom scattering equation derived in second-order many-body theory. The incident electron energy is taken to lie above the first inelastic threshold of the target atom. The method is applied to electron–helium collisions and elastic phase shifts for *s*-, *p*-, and *d*-wave scattering, computed in various models arising from the formalism, are tabulated.

1. INTRODUCTION

In the theoretical study of electron–atom collisions, one is frequently confronted with the problem of solving an equation of the type

$$[\nabla^2 + k^2] f_k(\mathbf{r}) = \int \Sigma(\mathbf{r}, \mathbf{r}'; k^2) f_k(\mathbf{r}')\, d\mathbf{r}' \tag{1}$$

for the scattering function $f_k(\mathbf{r})$. The expression on the left-hand side is the familiar free-particle operator describing the external electron in the absence of the target atom. The presence of the atom is recognized by the potential term $\Sigma(\mathbf{r}, \mathbf{r}'; k^2)$, appearing under the integral on the right-hand side, which will be referred to as the optical potential. This potential is in general dependent upon the incoming electron energy (k^2) and nonlocal. If k^2 is less than the energy of the first inelastic threshold, so that only the elastic channel is open, the potential is real, otherwise inelastic channels also become open and flux removed from the entrance channel, giving rise to absorptive effects, which will introduce an imaginary component to $\Sigma(\mathbf{r}, \mathbf{r}'; k^2)$. Because of the extremely complicated and complex nature of such a potential, one is forced to adopt some kind of approximation. It is the purpose of this paper to show how Eq. (1) may be solved in the case of elastic electron–atom scattering when the optical potential is approximated to second order according to the many-body theory scheme introduced by Schneider *et al.* [1]. To be specific, the target will be taken as a two-electron atomic system with nuclear charge Z.

The formulation of this many-body scheme for application to such a target has

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already been carried out by Scott and Taylor [2] so that here only their final result for $\Sigma(\mathbf{r}, \mathbf{r}'; k^2)$ need be given, viz.,

$$\Sigma(\mathbf{r}, \mathbf{r}'; k^2) = \Sigma^{\mathrm{HF}}(\mathbf{r}, \mathbf{r}') + \Sigma^{\mathrm{P}}(\mathbf{r}, \mathbf{r}'; k^2) - \Sigma^{\mathrm{EP}}(\mathbf{r}, \mathbf{r}'; k^2). \tag{2}$$

The first term on the right-hand side of Eq. (2) is the familiar first-order Hartree–Fock potential which will represent the static-exchange model introduced by Morse and Allis [3]. This is followed by the second-order polarization term Σ^{P} together with exchange counterpart Σ^{EP}. Denoting the atomic wavefunctions by $\psi_n(\mathbf{r}, \mathbf{r}')$, with $n = 0$ corresponding to the ground state of the target, let us put

$$V_{mn}(r) = \int \psi_m^*(\mathbf{x}, \mathbf{y})\, v(\mathbf{r} - \mathbf{x})\, \psi_n(\mathbf{x}, \mathbf{y})\, d\mathbf{x}\, d\mathbf{y}, \tag{3}$$

where

$$v(\mathbf{r} - \mathbf{r}') = 2/|\,\mathbf{r} - \mathbf{r}'\,|, \tag{4}$$

so that the components of the model optical potential in Eq. (2) can be expressed as

$$\begin{aligned} \Sigma^{\mathrm{HF}}(\mathbf{r}, \mathbf{r}') = {} & [-2Z/r + 2V_{00}(r)]\, \delta(\mathbf{r} - \mathbf{r}') \\ & - v(\mathbf{r} - \mathbf{r}') \int \psi_0^*(\mathbf{r}, \mathbf{x})\, \psi_0(\mathbf{r}', \mathbf{x})\, d\mathbf{x}, \end{aligned} \tag{5a}$$

$$\Sigma^{\mathrm{P}}(\mathbf{r}, \mathbf{r}'; k^2) = 2 \sum_{n \neq 0} V_{0n}(r)\, G(\mathbf{r}, \mathbf{r}'; k_n^2)\, V_{n0}(r'), \tag{5b}$$

$$\Sigma^{\mathrm{EP}}(\mathbf{r}, \mathbf{r}'; k^2) = \sum_{n \neq 0} V_{0n}(r) \int G(\mathbf{r}, \mathbf{x}; k_n^2)\, \psi_n^*(\mathbf{x}, \mathbf{y})\, v(\mathbf{r}' - \mathbf{x})\, \psi_0(\mathbf{r}', \mathbf{y})\, d\mathbf{x}\, d\mathbf{y}. \tag{5c}$$

Here, the summations over n include a discrete contribution from the bound states and an integral over the continuum states. Potential terms of similar structure arise also in the second-order optical potential approach of Bransden and Coleman [4]. The second-order terms defined by Eqs. (5b) and (5c) require knowledge of a suitable Green's function (propagator); below, the computation of such a function for scattering in the field of a local potential will be discussed. Energy dependence of the Green's function, which is the energy of the total system in channel n, is denoted by k_n^2.

Having defined the approximation of $\Sigma(\mathbf{r}, \mathbf{r}'; k^2)$ to be adopted, one proceeds to separate its radial and angular dependence, using the methods of partial wave analysis. Then, by introducing a partial wave decomposition of the function $f_k(\mathbf{r})$, Eq. (1) is reduced from a three-dimensional equation to a one-dimensional (radial) equation, thus making the problem more amenable to numerical solution. This analysis will form the material for Section 2. In Section 3 techniques to compute the radial Green's function will be discussed and then the radial optical potential reduced to a simpler mathematical expression. Section 4 will be concerned with the transformation of the simplified radial equation to an integral equation in preparation for application of a suitable numerical procedure to solve this particular type of equation. Finally, in

Section 5 the methods developed are specialized to the calculation of elastic scattering *s*-, *p*- and *d*-wave phase shifts for electron–helium collisions.

2. PARTIAL WAVE ANALYSIS

The summations over target states in Eqs. (5b) and (5c) present a special problem; for present purposes, it will be assumed adequate to retain a finite (discrete) number of terms, the specific nature of such terms to be otherwise determined by physical considerations as appropriate to a particular scattering system. The states so retained will be expressed as products of one-particle orbitals. Further, from the work of, for example, Yarlagadda [5], it can easily be shown that these states must possess a singlet spin configuration. Hence, let us write

$$\psi_0(\mathbf{r}, \mathbf{r}') = \phi_{1s}(\mathbf{r})\, \phi_{1s}(\mathbf{r}'), \tag{6}$$

$$\psi_n(\mathbf{r}, \mathbf{r}') = 2^{-1/2}[\phi_0(\mathbf{r})\, \phi_n(\mathbf{r}') + \phi_n(\mathbf{r})\, \phi_0(\mathbf{r}')], \tag{7}$$

where the one-particle orbitals will be written in terms of their radial (r) and angular ($\hat{r}$) components as

$$\phi_{1s}(\mathbf{r}) = R_{1s}(r)\, Y_{00}(\hat{r}), \tag{8}$$

$$\phi_0(\mathbf{r}) = w(r)\, Y_{00}(\hat{r}), \tag{9}$$

$$\phi_n(\mathbf{r}) = R_{nl}(r)\, Y_{lm}(\hat{r}). \tag{10}$$

The familiar multipole expansion of the electron–electron interaction term (Eq. (4)) is given by

$$v(\mathbf{r} - \mathbf{r}') = 2 \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1}\, \gamma_l(r, r')\, Y_{lm}(\hat{r})\, Y_{lm}^*(\hat{r}'), \tag{11}$$

where, employing the Heaviside function $\theta(x)$,

$$\gamma_l(r, r') = \theta(r' - r)\, r^l/r'^{l+1} + \theta(r - r')\, r'^l/r^{l+1}. \tag{12}$$

Expanding also the Green's function into its radial and angular parts, one has from Newton [6] that

$$G(\mathbf{r}, \mathbf{r}'; k_n^2) = 2 \sum_{l=0}^{\infty} \sum_{m=-l}^{l} G_l(r, r'; k_n^2)\, r^{-1} r'^{-1} Y_{lm}(\hat{r})\, Y_{lm}^*(\hat{r}'). \tag{13}$$

Hence, returning to Eq. (2) and substituting Eqs. (3)–(13), the following partial wave representation for the optical potential is derived:

$$\Sigma(\mathbf{r}, \mathbf{r}'; k^2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \Sigma_l(r, r'; k^2)\, r^{-1} r'^{-1} Y_{lm}(\hat{r})\, Y_{lm}^*(\hat{r}'), \tag{14}$$

where the radial component is given by

$$
\begin{aligned}
&\Sigma_l(r, r'; k^2) \\
&\quad = \left[-2Z/r + 4 \int_0^\infty \gamma_0(r, x) \mid x R_{1s}(x)|^2 \, dx\right] \delta(r - r') \\
&\quad - 2\gamma_l(r, r')\, r R_{1s}(r)\, r' R_{1s}(r')/(2l + 1) \\
&\quad + 4B^2 \sum_n \sum_{l'} \sum_\lambda f_{1s,nl'}(r) \Big[2(2\lambda + 1)(2l' + 1)^{-1} f_{1s,nl'}(r)\, G_\lambda(r, r'; k_n{}^2) \\
&\quad - (z\lambda + 1)(zl + 1)^{-1} r' R_{1s}(r') \int_0^\infty \gamma_l(x, r')\, R_{nl'}(x)\, G_\lambda(r, x; k_n{}^2)\, x \, dx\Big] \begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 .
\end{aligned}
\tag{15}
$$

In the above expression, the notation

$$B = \int_0^\infty w(x)\, R_{1s}(x)\, x^2 \, dx, \tag{16}$$

and

$$f_{1s,nl}(r) = \int_0^\infty \gamma_l(r, x)\, R_{1s}(x)\, R_{nl}(x)\, x^2 \, dx \tag{17}$$

has been introduced. The sum over n has already been discussed, while the sum over l' includes all principal angular-momentum states associated with a particular n ($l' < n$). Because of the presence of the Wigner 3-j symbols, the sum over λ is such that $\lambda = | l - l' |, | l - l' + 2 |, \ldots, | l + l' - 2 |, | l + l' |$.

Taking the z-axis parallel to the direction of the incoming electron, the scattering function is expanded into the partial wave series

$$f_k(\mathbf{r}) = k^{-1/2} \sum_{l=0}^{\infty} a_l r^{-1} f_l(k, r)\, Y_{l0}(\hat{r}), \tag{18}$$

where the lth partial wave satisfies regular boundary conditions at the origin and at large radial distances has the usual asymptotic behavior

$$\lim_{r\to\infty} f_l(k, r) = k^{-1/2} \sin(\phi(r) + \delta_l) \tag{19}$$

with $\phi(r)$ and δ_l defined, for example, by Mott and Massey [7].

Substituting Eqs. (14) and (18) into Eq. (1), one derives the integro-differential equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l + 1)}{r^2} + k^2\right] f_l(k, r) = \int_0^\infty \Sigma_l(r, r'; k^2)\, f_l(k, r')\, dr'. \tag{20}$$

This is the radial with which the remainder of this paper will be concerned.

3. REDUCTION OF $\sum_l(r, r'; k^2)$

This section will begin with the computation of the partial wave Green's function $G_l(r, r'; q^2)$ introduced in Eq. (13). For scattering by a local spherically symmetric potential $U(r)$, the Green's function can be expressed as (Newton [6])

$$G_l(r, r'; q^2) = a_l(r)\, b_l(r')\theta(r' - r) + a_l(r')\, b_l(r)\theta(r - r'), \tag{21}$$

where $a_l(r)$ and $b_l(r)$ are solutions of the differential equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + q^2 - U(r)\right] \psi_l(q, r) = 0 \tag{22}$$

constructed so that $G_l(r, r'; q^2)$ satisfies outgoing wave boundary conditions. The regular solution $a_l(r)$, which satisfies the same boundary conditions as given in Eq. (19) for $f_l(k, r)$, is readily obtained from Eq. (22) by a standard Numerov integration scheme provided initial power series solutions can be derived at small r. In order to compute $b_l(r)$, which depends upon the irregular solution, it is more convenient to use the integral version of Eq. (22), thus building in the appropriate boundary conditions:

$$\psi_l(q, r) = \hat{h}_l(qr) + q^{-1} \int_r^\infty U(x)[\hat{\jmath}_l(qr)\, \hat{n}_l(qx) - \hat{\jmath}_l(qx)\, \hat{n}_l(qr)]\, \psi_l(q, x)\, dx, \tag{23}$$

where

$$\hat{h}_l(qr) = -q^{-1/2}[\hat{n}_l(qr) - i\hat{\jmath}_l(qr)]. \tag{24}$$

For a neutral target, $U(r)$ will decay exponentially at large r and $\hat{\jmath}_l(x)$ and $\hat{n}_l(x)$ will denote the regular and irregular Riccati–Bessel functions, respectively, normalized such that as $x \to \infty$, $\hat{\jmath}_l(x) \to \sin(x - l\pi/2)$ and $\hat{n}_l(x) \to -\cos(x - l\pi/2)$.

Equation (23) is integrated inwards from the asymptotic region where it is assumed $U(r)$ is negligible. However, for an ionic target, which generates a long-range Coulomb potential of strength $-(Z - 2)/r$, this assumption will not be true. The problem is circumvented by using appropriate spherical Coulomb functions for $\hat{\jmath}_l(x)$ and $\hat{n}_l(x)$ and hence retaining only the exponentially decreasing part of the potential under the integral. Simpson's rule is used to perform the integration.

A mesh of points is set up from the origin which consists of several grids such that the step length of each grid is twice that of the previous grid. For notational purposes, let n denote evaluation at the point r_n and $n = N$ correspond to the end point farthest from the origin. It is convenient in Eq. (23) to drop the subscript l and to absorb the factor q^{-1} into $U(x)$. Then application of Simpson's rule yields

$$\begin{aligned}\psi(n) = \hat{h}(n) &+ \hat{\jmath}(n)\{I(n+2) + \tfrac{1}{3}h[U(n+2)\hat{n}(n+2)\psi(n+2) \\ &+ 4U(n+1)\hat{n}(n+1)\psi(n+1)]\} - \hat{n}(n)\{J(n+2) \\ &+ \tfrac{1}{3}h[U(n+2)\hat{\jmath}(n+2)\psi(n+2) + 4U(n+1)\hat{\jmath}(n+1)\psi(n+1)]\},\end{aligned} \tag{25}$$

where h denotes step length and

$$I(n) = \int_n^N U(x)\,\hat{n}(x)\,\psi(x)\,dx, \qquad J(n) = \int_n^N U(x)\,\hat{j}(x)\,\psi(x)\,dx. \tag{26}$$

These integrals may be evaluated by further use of Simpson's rule.

The formula given in Eq. (25) requires a constant step length so that in the present work a modification is needed to overcome the change in step length at the end of each grid. Letting h denote the new step length, use is made of the formal result

$$\begin{aligned}\int_r^{r+h} & f(x)\,g(x)\,dx \\ & = h[f(r)\,g(r) + 2f(r+h/2)\{g(r) + g(r+h)\} + f(r+h)\,g(r+h)]/6,\end{aligned} \tag{27}$$

where it is assumed that the function $f(x)$ may be evaluated at any value of x but that $g(x)$ is only known at the end points; hence, the mean value of g with respect to these end points has been used at the midpoint $r + h/2$. Associating ψ with g and since $U(x)$, $\hat{j}(x)$, and $\hat{n}(x)$ may be evaluated at any x, Eq. (27) is applied to Eq. (23) to compute ψ at the first point of the new grid. A similar method is used to evaluate also the integrals defined in Eq. (26) at this point. Thereafter, the formula of Eq. (25) is used to compute ψ at the second and subsequent points of the grid.

Having discussed the computation of $G_l(r, r'; q^2)$, let us now turn our attention to the integral term appearing in Eq. (15) which depends upon a knowledge of $G_\lambda(r, r'; q^2)$ and denote this exchange integral by $H^l_{\lambda l'}(r, r'; q^2)$:

$$H^l_{\lambda l'}(r, r'; q^2) = \int_0^\infty \gamma_l(x, r')\,R_{nl'}(x)\,G_\lambda(r, x; q^2)\,x\,dx. \tag{28}$$

Substituting for $\gamma_l(x, r')$ and $G_\lambda(r, x; q^2)$ according to Eqs. (12) and (21), respectively, it is convenient to define the resulting integrals by

$$f_\lambda{}^1(r) = \int_0^r R_{nl'}(x)\,a_\lambda(x)\,x^{l+1}\,dx, \tag{29a}$$

$$f_\lambda{}^2(r) = \int_0^r R_{nl'}(x)\,b_\lambda(x)\,x^{l+1}\,dx, \tag{29b}$$

$$f_\lambda{}^3(r) = \int_0^r R_{nl'}(x)\,a_\lambda(x)\,x^{-l}\,dx, \tag{29c}$$

$$f_\lambda{}^4(r) = \int_r^\infty R_{nl'}(x)\,b_\lambda(x)\,x^{-l}\,dx, \tag{29d}$$

so that putting

$$g_\lambda{}^1(r) = r^{-(l+1)} f_\lambda{}^2(r) + r^l f_\lambda{}^4(r), \tag{30a}$$

$$g_\lambda{}^2(r) = b_\lambda(r) f_\lambda{}^1(r) - a_\lambda(r) f_\lambda{}^2(r), \tag{30b}$$

$$h_\lambda{}^1(r) = r^{-(l+1)} f_\lambda{}^1(r) - r^l f_\lambda{}^3(r), \tag{30c}$$

$$h_\lambda{}^2(r) = b_\lambda(r) f_\lambda{}^3(r) + a_\lambda(r) f_\lambda{}^4(r), \tag{30d}$$

Eq. (28) becomes

$$\begin{aligned} H^l_{\lambda l'}(r, r'; q^2) &= [a_\lambda(r)\, g_\lambda{}^1(r') + g_\lambda{}^2(r)\, r'^{-(l+1)}]\theta(r' - r) \\ &\quad + [b_\lambda(r)\, h_\lambda{}^1(r') + h_\lambda{}^2(r)\, r'^l]\theta(r - r'). \end{aligned} \tag{31}$$

While the integrands of Eqs. (29a)–(29c) are regular at the origin and may hence be evaluated by outward integration (using, for example, Simpson's rule), that of Eq. (29d) is irregular. However, since the integrand of $f_\lambda{}^4(r)$ also contains the exponentially decaying bound state function $R_{nl'}(r)$, the integral is most conveniently obtained by inward integration from the asymptotic region (where the integrand is effectively zero) using Simpson's rule. The formula given in Eq. (27) is employed at the beginning of each new grid.

Finally, by adopting the notation

$$C_{ll'\lambda} = \frac{2(2l+1)}{2l'+1} D_{ll'\lambda}, \qquad D_{ll'\lambda} = 4B^2 \frac{(2\lambda+1)}{2l+1} \begin{pmatrix} l & l' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2,$$

the expression for the partial wave optical potential of Eq. (15) reduces to the form

$$\begin{aligned} \Sigma_l(r, r'; k^2) &= \left[-2Z/r + 4\int_0^\infty \gamma_0(r, x)\, |\, xR_{1s}(x)|^2\, dx\right] \delta(r - r') \\ &\quad - 2\gamma_l(r, r')\, rR_{1s}(r)\, r'R_{1s}(r')/(2l+1) + \sum_n \sum_{l'} \sum_\lambda f_{1s,nl'}(r) \\ &\quad \times [C_{ll'\lambda} f_{1s,nl'}(r)\, G_\lambda(r, r'; k_n{}^2) - D_{ll'\lambda} r'R_{1s}(r')\, H^l_{\lambda l'}(r, r'; k_n{}^2)]. \end{aligned} \tag{32}$$

For a suitable choice of atomic wavefunctions, the integrals defined in Eqs. (16) and (17) and that appearing in Eq. (32) may be evaluated analytically so that all the terms arising in Eq. (32) are now known at the mesh points.

4. Method of Solution

By introducing the Green's function operator $K_0(r, r'; k^2)$ associated with the left-hand side of Eq. (20), one transforms this equation to read

$$f_l(k, r) = R(r) + \int_0^\infty \int_0^\infty K_0(r, x; k^2)\, \Sigma_l(x, r'; k^2) f_l(k, r')\, dx\, dr', \tag{33}$$

where

$$K_0(r, r'; k^2) = R(r)I(r')\theta(r' - r) + I(r)R(r')\theta(r - r'). \tag{34}$$

The regular and irregular functions are given respectively by

$$R(r) = \hat{j}_l(kr) \qquad \text{and} \qquad I(r) = k^{-1}\hat{n}_l(kr)$$

with $\hat{\jmath}_l(x)$ and $\hat{n}_l(x)$ defined following Eq. (24). With this choice of Green's function operator, and introducing the phase shift δ_l, $f_l(k, r)$ has the asymptotic behavior

$$f_l(k, r) \underset{r\to\infty}{\sim} \hat{\jmath}_l(kr) - \tan \delta_l \hat{n}_l(kr) \tag{35}$$

which is equivalent to the boundary condition specified in Eq. (19).

It is convenient at this point to let $V(r)$ denote the first-order direct term (the nuclear plus static potential), viz,

$$\begin{aligned} V(r) &= -2Z/r + 4 \int_0^\infty \gamma_0(r, x) \mid xR_{1s}(x)|^2 \, dx \\ &\xrightarrow[r\to\infty]{} -2(Z-2)/r. \end{aligned} \tag{36}$$

In subsequent numerical work it is essential that $V(r)$ decrease rapidly at large r so that $V(r_{N-1})$ and $V(r_N)$ may be taken as effectively zero. For neutral helium this condition is satisfied, otherwise for ionic targets ($Z > 2$) one must adopt the procedure outlined in connection with computing the Green's function discussed in Section 3 for such a target. That is, the term $-2(Z-2)/r$ is transferred to the left-hand side of Eq. (20) leaving the remainder of the first-order direct term with the required decay behavior and using spherical Coulomb functions in the construction of $K_0(r, r'; k^2)$.

Defining a new integral function

$$K(r, r'; k^2) = \int_0^\infty K_0(r, x; k^2)\, \Sigma_l(x, r'; k^2)\, dx, \tag{37}$$

which is independent of $f_l(k, r)$, Eq. (33) is reduced to a one-dimensional integral equation:

$$f_l(k, r) = R(r) + \int_0^\infty K(r, r'; k^2) f_l(k, r')\, dr'. \tag{38}$$

The functions comprising the integrand of Eq. (37) are known so that one may proceed to simplify and evaluate this term.

Equation (38) is then integrated using a method described by Thomas [8]. Details of the numerical formulas are supplied by Thomas in his paper and no further development of the method to this problem need be given here.

To summarize, the solution of Eq. (20) proceeds in three steps:

(1) Compute the functions $a_\lambda(r)$ and $b_\lambda(r)$ comprising the Green's function $G_\lambda(r, r'; k_n^2)$ at each mesh point;

(2) compute the functions and integrals comprising $K(r, r'; k^2)$ of Eq. (37) at each mesh point;

(3) use the data of step (2) as input to a program to solve Eq. (38) based on the noniterative method of [8].

5. Application to Elastic Electron–Helium Scattering

Let us now use the methods described to compute elastic s-, p-, and d-wave phase shifts for electron–helium scattering. The summation over n, which in principle includes a discrete sum over the bound states and an integral over the continuum states of the target atom, is handled by the method of pseudostates such that by retaining just one state in the summation, the real part of the second-order potential will in the asymptotic region behave as $-\alpha/r^4$ where α is the static dipole polarizability of helium. To achieve this behavior, the pseudostate must be of P-symmetry; higher multipoles of the polarization potential may be derived by the further addition of states with $D, F, \ldots,$ symmetry.

Thus adopting the Hartree–Fock function of Green *et al.* [9] to describe the ground state function $R_{1s}(r)$, Eq. (8) is written as

$$\phi_{1s}(\mathbf{r}) = N(e^{-ar} + ce^{-br})\, Y_{00}(\hat{r}), \tag{39}$$

where $a = 1.4558$, $b = 2.9116$, $c = 0.6$, and N is a normalization constant. Based on the method of polarized orbitals [10], Eqs. (9) and (10) are taken to be of the form, denoting the pseudostate method by subscript p,

$$\phi_0(\mathbf{r}) = 2Z_0^{3/2} e^{-Z_0 r} Y_{00}(\hat{r}), \tag{40}$$

$$\phi_p(\mathbf{r}) = 4Z_0 \left(\frac{2Z_0}{129}\right)^{1/2} e^{-Z_0 r} \left[Z_0 r + \frac{1}{2}(Z_0 r)^2\right] Y_{1m}(\hat{r}). \tag{41}$$

In the adiabatic limit, assuming for α the value quoted by Teachout and Pack [11], namely, $\alpha = 1.383\ a_0{}^3$, $Z_0 = 1.2240$. Further details on this choice may be found in the papers by Scott and Taylor [2]. Use of a P-state implies that one takes $l' = 1$ in the formula for the optical potential given in Eq. (32). Consequently, from the properties of the Wigner 3-j symbols, the summation over λ reduces to one term for s-wave scattering ($\lambda = 1$) and to two terms otherwise ($\lambda = l \pm 1$).

Turning to the Green's function $G_\lambda(r, r'; k_p{}^2)$, the potential term appearing in Eq. (22) is expressed as

$$U(r) = V(r) + W(r) \tag{42}$$

with $V(r)$ defined in Eq. (36). Exchange effects are taken into account via $W(r)$. In the static-exchange approximation, $W(r)$ is an operator in the sense that

$$W(r)\, \psi_\lambda(k_p, r) = -\frac{2}{2\lambda + 1}\, rR_{1s}(r) \int_0^\infty \gamma_\lambda(r, x)\, \psi_\lambda(k_p, x)\, R_{1s}(x)\, x\, dx. \tag{43}$$

The regular component $a_\lambda(r)$ of the Green's function is in fact most easily obtained from this approximation (rather than in a model utilizing only local potentials) using an adaptation of the Numerov procedure incorporated into the program of

McDowell *et al.* [12]. For the component $b_\lambda(r)$, it is, however, more convenient to employ a local equivalent exchange potential for $W(r)$. In the present work, use is made of the (corrected) local potential originally due to Furness and McCarthy [13], viz.,

$$W(r) = \tfrac{1}{2}\{[k_p{}^2 - V(r)] - ([k_p{}^2 - V(r)]^2 + 8 \mid R_{1s}(r)|^2)^{1/2}\}. \tag{44}$$

This approximation to the static-exchange potential has been examined by Bransden *et al.* [14] and found to provide elastic phase shifts in close agreement with an exact treatment. Thus the resulting Green's function is expected to be a good approximation to the exact Hartree–Fock Green's function which would otherwise be considerably more complicated to compute [2]. Scattering functions have been computed using this approximation to the Hartree–Fock Green's function and also using the free-particle Green's function given by

$$a_\lambda(r) = k_p^{-1/2} \hat{j}_\lambda(k_p r) \qquad \text{and} \qquad b_\lambda(r) = -\hat{h}_\lambda(k_p r), \tag{45}$$

with $\hat{j}_\lambda(x)$ and $\hat{h}_\lambda(x)$ defined in connection with Eq. (23).

Apart from the free-particle Green's function, the Riccati–Bessel functions are required in the computation of the integrals arising from Eq. (37). Standard routines are readily available to evaluate these functions. The current program employs the method developed and programmed by Barnett *et al.* [15] and subsequently modified by Barnett [16].

In order to facilitate use of the Numerov method employed by [12] to compute the regular component $a_\lambda(r)$ of the Green's function, the set of mesh points used in this calculation is composed of 2000 points, divided into seven grids of 40, 40, 40, 40, 40, 800, and 1000 points. The initial step length is taken to be $h = 0.0005a_0$ and doubled at the end of each grid to yield a range of integration running from $r = 0$ to $r = 45.42a_0$. It is important that the initial step length be small so as to provide accurate starting values for the solutions using the method outlined by Thomas [8]. Stability of the program was tested by varying the initial step length and altering the number of points in each grid; accuracy to the fourth decimal place in each phase shift considered was maintained.

Incorporation of a switch into the program allowed results to be computed in the simpler first-order static-exchange approximation, though omitting the overlap term between $R_{1s}(r)$ and $f_0(k, r)$ arising in s-wave scattering. Additional switches enabled results from use of the full second-order potential to be computed employing either the Hartree–Fock approximation (G_{HF}) or the free-particle approximation (G_0) to the Green's function. Also, the second-order exchange term defined in Eq. (5c) could be omitted.

Because the Green's function defined in Eq. (21) incorporates outgoing wave boundary conditions, the optical potential will indeed possess both real and imaginary terms giving rise to complex phase shifts δ_l ($=\lambda_l + i\mu_l$, say). The imaginary component μ_l describes the effect of the inelastic channels upon the elastic scattering channel. If, however, one ignores μ_l (or takes no account of absorption as for example in the static-exchange approximation), the scattering becomes purely elastic described by the real component λ_l.

The real (elastic) components of the *s*-, *p*-, and *d*-wave phase shifts, computed at various incident energies in the above models, are presented in Tables I–III. Comparison of the phase shifts obtained by adopting the free-particle approximation to the Green's function reveals that the second-order many-body treatment is not particularly

TABLE I

Elastic *s*-Wave Phase Shifts (in Radians) for Electron–Helium Scattering

Energy (eV)	(a)	(b)	(c)	(d)	(e)
50	1.3113	1.3450	1.3466	1.3474	1.3499
100	1.0577	1.0696	1.0689	1.0698	1.0691
150	0.9334	0.9377	0.9377	0.9376	0.9375
200	0.8548	0.8561	0.8566	0.8561	0.8565
300	0.7559	0.7548	0.7558	0.7548	0.7557

[a] Static-exchange approximation.
[b] Many-body approximation with G_0 but omitting second-order exchange.
[c] Many-body approximation with G_{HF} but omitting second-order exchange.
[d] Many-body approximation with G_0.
[e] Many-body approximation with G_{HF}.

TABLE II

Elastic *p*-Wave Phase Shifts (in Radians) for Electron–Helium scattering

Energy (eV)	(a)	(b)	(c)	(d)	(e)
50	0.3219	0.3485	0.3407	0.3460	0.3351
100	0.3447	0.3510	0.3531	0.3497	0.3506
150	0.3467	0.3486	0.3515	0.3478	0.3501
200	0.3445	0.3448	0.3477	0.3443	0.3468
300	0.3372	0.3363	0.3388	0.3360	0.3384

[a] Static-exchange approximation.
[b] Many-body approximation with G_0 but omitting second-order exchange.
[c] Many-body approximation with G_{HF} but omitting second-order exchange.
[d] Many-body approximation with G_0.
[e] Many-body approximation with G_{HF}.

TABLE III

Elastic *d*-Wave Phase Shifts (in Radians)
for Electron–Helium Scattering

Energy (eV)	(a)	(b)	(c)	(d)	(e)
50	0.0682	0.0985	0.1004	0.0952	0.0969
100	0.1106	0.1185	0.1192	0.1179	0.1184
150	0.1340	0.1371	0.1383	0.1367	0.1378
200	0.1486	0.1500	0.1514	0.1497	0.1510
300	0.1656	0.1656	0.1669	0.1654	0.1667

[a] Static-exchange approximation.
[b] Many-body approximation with G_0 but omitting second-order exchange.
[c] Many-body approximation with G_{HF} but omitting second-order exchange.
[d] Many-body approximation with G_0.
[e] Many-body approximation with G_{HF}.

sensitive to the choice of propagator. At higher energies, the phase shifts within each table agree generally to two significant figures with the static-exchange results of column (a), demonstrating that the inelastic channels have a negligible effect on elastic scattering at these energies.

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