

Polarisation and exchange effects on elastic scattering of electrons from helium[†]

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Abstract. We examine the effects of the polarisation potential and of local exchange potentials in the adiabatic exchange approximation for low-energy elastic scattering of electrons from helium atoms. We conclude that the most reliable results are obtained by including only the dipole part of the polarisation potential and by treating exchange exactly. We present detailed results for phaseshifts, differential, total elastic and momentum transfer cross sections. These agree well with other calculations and with experimental measurements.

1. Introduction

Elastic scattering of electrons from noble gases has been of continuing interest to experimentalists and recent measurements have produced much detailed information. In the case of helium, in the last few years total cross sections have been measured by Charlton *et al* (1980), Kauppila *et al* (1981), Kennerly and Bonham (1978) and Stein *et al* (1978) and differential cross sections by Andrick and Bitsch (1975), Newell *et al* (1981) and Register *et al* (1980). In addition scattering phaseshifts have been extracted from experimental measurements of the angular distribution of the scattered electrons by Andrick and Bitsch (1975), Newell *et al* (1981) and Williams (1979).

Unlike the heavier noble gases, there has been a fair number of theoretical calculations of electron scattering from helium. Recently Nesbet (1979) has reported a matrix variational calculation for helium while O'Malley *et al* (1979) and Fon *et al* (1981) have carried out *R*-matrix calculations for this atom. There have been a number of polarised orbital type calculations by LaBahn and Callaway (1964, 1970), Callaway *et al* (1968), Duxler *et al* (1971) and Yau *et al* (1978).

In the work of Yau *et al* (1978, 1980) (to be referred to as I and II respectively) an adiabatic exchange approximation was used to calculate low-energy electron scattering from the noble gases. In this work exchange was described by a local potential and the polarisation potentials were those which had previously been used in a highly successful treatment of positron scattering by the noble gases (McEachran *et al* 1977a, 1978a, b, 1979, 1980). The results reported in I and II were in good agreement with experimental measurements for electron scattering from helium and neon. However, for scattering from argon, krypton and xenon the agreement was

[†] This paper is dedicated to Professor M J Seaton on the occasion of his 60th birthday.

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only satisfactory up to energies of a few electron volts. In an attempt to determine the cause of these discrepancies we investigate more thoroughly the effects of polarisation and exchange for these processes in the present paper. In particular we treat exchange exactly within the adiabatic exchange approximation and also study the effect of higher multipole moments in the polarisation potential.

2. The polarisation potential

We present here a brief description of the polarisation potential used in our calculations. For a more detailed treatment see paper I as well as McEachran *et al* (1977a, 1980).

The total atomic wavefunction is written as

$$\Psi = (N!)^{-1/2} \det |\psi_1, \psi_2, \dots, \psi_N| \quad (1)$$

where the orbitals ψ_i are the polarised orbitals of Temkin (1957, 1959). Thus we write

$$\psi_i(\mathbf{r}_i, \sigma_i, \mathbf{x}) = \phi_i^0(\mathbf{r}_i, \sigma_i) + \phi_i^1(\mathbf{r}_i, \sigma_i, \mathbf{x}) \quad (2)$$

where (\mathbf{r}_i, σ_i) are the position and spin coordinates of the i th bound electron and \mathbf{x} is the position coordinate of the incident electron. The ϕ_i^0 are the unperturbed Hartree-Fock atomic orbitals and the ϕ_i^1 are calculated via first-order Hartree-Fock perturbation theory where the perturbation is the interaction between the incident electron and the atom.

If the interaction between the incident electron and the atom is expanded in multipole moments then each such moment produces a corresponding term in the polarised orbital ϕ_i^1 and hence in the polarisation potential V_p (cf equation (19) of I). In I and II all multipole contributions were included in V_p whereas in the other polarised orbital calculations mentioned above only the dipole contribution was included or at most the first three multipole contributions. In the present paper we investigate the differences produced by these various approaches.

3. The scattering equation

The derivation of the integro-differential equation for the scattering of electrons from noble gases in the polarised orbital adiabatic exchange approximation has been given in I. We shall present here only a brief summary of the relevant theory. The total wavefunction $\tilde{\Psi}$ for the system of the atom plus incident electron is written as

$$\tilde{\Psi} = \mathcal{A} \Psi(\mathbf{r}, \sigma, \mathbf{x}) U(\mathbf{x}, \sigma) \quad (3)$$

where \mathcal{A} is the antisymmetrisation operator, Ψ is given by (1) and $U(\mathbf{x}, \sigma)$ represents the scattering wavefunction which, in turn, may be expanded in partial waves according to

$$U(\mathbf{x}, \sigma) = \sum_{ls} x^{-1} u_l(x) Y_{10}(\hat{\mathbf{x}}) \chi_s(\sigma) \quad (4)$$

where $Y_{10}(\hat{\mathbf{x}})$ and $\chi_s(\sigma)$ are normalised spherical harmonic and spin functions respectively.

In order to determine U the full Schrödinger equation is projected onto the ground state of the atom and the so-called polarisation exchange terms are neglected. The radial part of the scattering wavefunction, $u_l(x)$ then satisfies the equation

$$\left(\frac{d^2}{dx^2} - \frac{l(l+1)}{x^2} - 2V_s(x) - 2V_p(x) + k^2 \right) u_l(x) = \mathcal{H}_l(x) u_l(x) \quad (5)$$

where $V_s(x)$ and $V_p(x)$ are the static and polarisation potentials (cf equations (17) and (18) of I), $\frac{1}{2}k^2$ is the energy of the incident electron in au and the exchange terms are given by†

$$\mathcal{H}_l(x) u_l(x) = \sum_n (k^2 + 2\varepsilon_{nl}) \langle P_{nl} | u_l \rangle P_{nl}(x) - 2 \sum_{n'l'} g_{\nu}^{l'l} \frac{1}{x} Y_{\nu}(P_{n'l'}, u_l | x) P_{n'l'}(x) \quad (6)$$

Here P_{nl} is the usual radial part of an atomic Hartree–Fock orbital for the ground state of the atom and $2\varepsilon_{nl} > 0$ is the corresponding energy eigenvalue. The coefficients $g_{\nu}^{l'l}$ are given by, in terms of 3- j symbols (Edmonds 1957),

$$g_{\nu}^{l'l} = (2l' + 1) \begin{pmatrix} l' & \nu & l \\ 0 & 0 & 0 \end{pmatrix}^2. \quad (7)$$

The limits on the summation over n and l' in (6) are determined by which electron orbitals are present in the atom, while the limits for ν are those which give a non-zero value for $g_{\nu}^{l'l}$.

The remaining integral terms in equation (6) are defined by

$$\langle f | g \rangle = \int_0^{\infty} f(s) g(s) ds \quad (8)$$

and

$$Y_{\nu}(f, g | x) = x^{-\nu} \int_0^x f(s) g(s) s^{\nu} ds + x^{\nu+1} \int_x^{\infty} f(s) g(s) s^{-\nu-1} ds. \quad (9)$$

4. Method of solution

For computational purposes it is more convenient to re-express the exchange terms so that equation (5) can be written as

$$\mathcal{L}_l(x) u_l(x) = \sum_{n'l'} [(k^2 + 2\varepsilon_{nl}) \Delta_{n'l', -1}^l \delta_{ll'} \delta_{0\nu} - 2g_{\nu}^{l'l} \Delta_{n'l', \nu}^l] x^{\nu} P_{n'l'}(x) \quad (10)$$

where the operator $\mathcal{L}_l(x)$ is given by

$$\left(\frac{d^2}{dx^2} - \frac{l(l+1)}{x^2} - V(x) - K_l(x) + k^2 \right) \quad (11)$$

with

$$V(x) = 2(V_s(x) + V_p(x)) \quad (12)$$

$$K_l(x) u_l(x) = 2 \sum_{n'l'} \sum_{\nu} g_{\nu}^{l'l} \left(x^{\nu} \int_0^x \frac{dr}{r^{\nu+1}} P_{n'l'}(r) u_l(r) - \frac{1}{x^{\nu+1}} \int_0^x dr r^{\nu} P_{n'l'}(r) u_l(r) \right) P_{n'l'}(x) \quad (13)$$

† In both equations (21) and (22) of I there is an overall factor of -1 missing in the definition of the kernels and the ε_i in equation (21) are the negative of the ε_{nl} used here.

and

$$\Delta_{nl'\nu}^l = \int_0^\infty \frac{dr}{r^{\nu+1}} P_{nl'}(r) u_l(r). \quad (14)$$

Since the right-hand side of equation (10) explicitly contains definite integrals over the entire range of the unknown function $u_l(x)$ the direct solution of this equation would have to involve an iterative procedure. In order to avoid iterative techniques, together with their potential convergence problems, we re-cast equation (10) into the following series of differential equations, each of which can be integrated out directly from the origin (Marriot 1958),

$$\mathcal{L}_l u_l^0(x) = 0 \quad (15a)$$

$$\mathcal{L}_l u_l^{nl'\nu}(x) = x^\nu P_{nl'}(x). \quad (15b)$$

We note that equation (15b) is to be solved for each of the allowed combinations of the three parameters $l'\nu l$ which give rise to a non-zero value of $g_\nu^{l'l}$ in equation (7). If the scattering function $u_l(x)$ of equation (10) is now written as the following linear combination

$$u_l(x) = \alpha_0 u_l^0(x) + \sum_{nl'\nu} \alpha_{nl'\nu} u_l^{nl'\nu}(x) \quad (16)$$

then the coefficients $\alpha_{nl'\nu}$ are given by

$$\alpha_{nl'\nu} = (k^2 + 2\varepsilon_{nl'}) \Delta_{nl',-1}^l \delta_{ll'} \delta_{0\nu} - 2g_\nu^{l'l} \Delta_{nl'\nu}^l. \quad (17)$$

If we now let $p \equiv nl'\nu$ and $q \equiv n'l''\nu'$ then substituting our expansion (16) for $u_l(x)$ into the integrals $\Delta_{nl'\nu}^l$ leads to the following set of linear algebraic equations

$$\mathbf{A}\boldsymbol{\alpha} = \alpha_0 \mathbf{b} \quad (18)$$

where the elements of the matrices \mathbf{A} and \mathbf{b} are given by

$$A_{pq} = (k^2 + 2\varepsilon_{nl'}) \delta_{ll'} \delta_{0\nu} I_{pq,-1} - 2g_\nu^{l'l} I_{pq\nu} - \delta_{pq} \quad (19)$$

$$b_p = -[(k^2 + 2\varepsilon_{nl'}) \delta_{ll'} \delta_{0\nu} I_{p,-1}^0 - 2g_\nu^{l'l} I_{p\nu}^0] \quad (20)$$

and the vector $\boldsymbol{\alpha}$ includes all α except α_0 . The integrals introduced in equations (19) and (20) are defined as

$$I_{p\nu}^0 = \int_0^\infty \frac{dr}{r^{\nu+1}} P_{nl'}(r) u_l^0(r) \quad (21a)$$

and

$$I_{pq\nu} = \int_0^\infty \frac{dr}{r^{\nu+1}} P_{nl'}(r) u_l^{n'l''\nu'}(r). \quad (21b)$$

The system of equations (18) can now be solved for the vector $\boldsymbol{\alpha}' = \boldsymbol{\alpha}/\alpha_0$. If each of the solutions $u_l^0(x)$ and $u_l^{nl'\nu}(x)$ are determined such that their power series expansions about the origin begin with the identical first term, namely $[k^{l+1}/(2l+1)!!]x^{l+1}$, (as per equation (24) below) then the choice

$$\alpha_0^{-1} = 1 + \sum_q \alpha'_q \quad (22)$$

with the remaining coefficients given by $\alpha = \alpha_0 \alpha'$ ensures that the first term of u_l is the same as that of u_l^0 . The boundary conditions for elastic scattering which pertain to the solution $u_l(x)$ of equation (10) are

$$u_l(0) = 0 \quad (23a)$$

and

$$u_l(x) \underset{x \rightarrow \infty}{\sim} C_l [\sin(kr - \frac{1}{2}l\pi) + \tan \eta_l \cos(kr - \frac{1}{2}l\pi)] \quad (23b)$$

where η_l is the phaseshift.

Rather than solve the set of differential equations (15) we choose instead to solve the corresponding set of integral equations.

$$\begin{aligned} u_l^{nl'\nu}(x) = f_l(kx) - \frac{g_l(kx)}{k} \int_0^x dx' f_l(kx')(V(x') + K_l(x')) u_l^{nl'\nu}(x') \\ + \frac{f_l(kx)}{k} \int_0^x dx' g_l(kx')(V(x') + K_l(x')) u_l^{nl'\nu}(x') + G_{nl'l'}^\nu(x) \end{aligned} \quad (24)$$

where

$$G_{nl'l'}^\nu(x) = \frac{f_l(kx)}{k} \int_0^x dx' g_l(kx') x'^\nu P_{nl'l'}(x') - \frac{g_l(kx)}{k} \int_0^x dx' f_l(kx') x'^\nu P_{nl'l'}(x'). \quad (25)$$

The integral equation for $u_l^0(x)$ is the same as equation (24) except that the term $G_{nl'l'}^\nu(x)$ is omitted. The functions $f_l(\rho)$ and $g_l(\rho)$ are given by

$$f_l(\rho) = \rho j_n(\rho) \quad (26a)$$

$$g_l(\rho) = -\rho y_n(\rho) \quad (26b)$$

where $j_n(\rho)$ and $y_n(\rho)$ are the spherical Bessel functions of the first and second kinds respectively (Abramowitz and Stegun 1968). In order to determine the phaseshift η_l we first note that the asymptotic form of equation (10) can be written as

$$u_l(x) \underset{x \rightarrow \infty}{\sim} A_l f_l(kx) + B_l g_l(kx) \quad (27)$$

where A_l and B_l are constants. Then from equation (23b), it follows that

$$\tan \eta_l = B_l / A_l. \quad (28)$$

If we next define the integrals

$$A_l^0 = 1 + \frac{1}{k} \int_0^\infty dx g_l(kx)(V(x) + K_l(x)) u_l^0(x) \quad (29a)$$

$$B_l^0 = -\frac{1}{k} \int_0^\infty dx f_l(kx)(V(x) + K_l(x)) u_l^0(x) \quad (29b)$$

$$A_l^{nl'\nu} = 1 + \frac{1}{k} \int_0^\infty dx g_l(kx)[(V(x) + K_l(x)) u_l^{nl'\nu}(x) + x^\nu P_{nl'l'}(x)] \quad (29c)$$

and

$$B_l^{nl'\nu} = -\frac{1}{k} \int_0^\infty dx f_l(kx)[(V(x) + K_l(x)) u_l^{nl'\nu}(x) + x^\nu P_{nl'l'}(x)] \quad (29d)$$

then the constants A_l and B_l are given by

$$A_l = \alpha_0 A_l^0 + \sum_{nl'\nu} \alpha_{nl'\nu} A_l^{nl'\nu} \quad (30a)$$

and

$$B_l = \alpha_0 B_l^0 + \sum_{nl'\nu} \alpha_{nl'\nu} B_l^{nl'\nu}. \quad (30b)$$

The functions u_l^0 and the set $u_l^{nl'\nu}$ were all obtained by integrating equation (24) directly out from the origin by means of Simpson's one-third rule. In order to start such a procedure all the functions and integrals in these equations were evaluated at the origin $x = 0$ and, by power series expansions, at the first point $x_1 = h$, the interval of integration. This integration procedure was first continued to a point $x = x_n$ where the static potential $V_s(x)$ and the kernel $K_l(x)$ were zero i.e. all the radial Hartree-Fock functions $P_{nl}(x)$ had become effectively zero. The integrals from 0 to x_n in equations (29) were then known and the corresponding values from x_n to infinity were *estimated* by the asymptotic correction procedure described in the appendix. The constants A_l and B_l were calculated from equations (30) and a corresponding estimate of the phaseshift determined from equation (28). The integration procedure was then continued from x_n to $x_n + mh$ (m a positive integer) and a new estimate of the phaseshift was determined. This procedure was considered to have converged when the relative accuracy of consecutive estimates of the phaseshift differed by less than $(2l+1) \times 10^{-5}$. For helium the choices of $h = \frac{1}{32}$ and $m = 32$ proved satisfactory to determine η_l accurate to the number of figures given in table 1. The asymptotic correction procedure proved to be so successful that, except for the determination of the scattering length, the phaseshifts obtained when $x = x_n$ and $x = x_n + 1$ satisfied the above convergence criteria i.e. it is not necessary to integrate equations (24) more than one atomic unit beyond the range of the static potential and the exchange kernel. For the scattering length it is necessary to integrate to $x = x_n + 3$ before convergence is achieved. If the method due to Burgess (1963) is used instead then it is necessary to integrate the equations to approximately 5 au for large k and to approximately 60 au for small k beyond the range of the static potential and the exchange terms in order to achieve the same accuracy.

5. Results

In I we calculated the low-energy elastic scattering of electrons from helium. In this previous calculation the polarisation potential contained contributions from all multipole moments and the exchange kernel (equation (22) of I) was replaced by a local potential. The one-electron exchange term (equation (21) of I) was set equal to zero.

In the present work we have carried out three further calculations for this system which varied in their treatment of polarisation and exchange. In the first case we used a local exchange approximation (equation (24a) of I) and retained only the dipole contribution to the polarisation potential. As in I we set the one-electron exchange term equal to zero. In the other two cases exchange was treated exactly and we used the full polarisation potential as well as the dipole contribution only.

As part of our study we have tested the effect of arbitrarily setting the one-electron exchange term to zero in our full exchange treatment. If exchange is treated exactly

Table 1. Elastic scattering phaseshifts δ_l for helium.

k	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0	1.157 542 [†]						
0.1000	3.016 762	0.003 056	0.000 396	0.000 132	0.000 060	0.000 032	0.000 019
0.2000	2.883 129	0.013 286	0.001 594	0.000 528	0.000 240	0.000 129	0.000 077
0.3000	2.748 068	0.031 876	0.003 633	0.001 188	0.000 540	0.000 291	0.000 174
0.3834	2.637 200	0.054 004	0.006 028	0.001 944	0.000 881	0.000 474	0.000 285
0.4000	2.615 472	0.059 095	0.006 584	0.002 117	0.000 959	0.000 516	0.000 310
0.5000	2.487 696	0.093 990	0.010 536	0.003 321	0.001 500	0.000 807	0.000 484
0.6000	2.366 195	0.134 421	0.015 557	0.004 811	0.002 162	0.001 162	0.000 697
0.6063	2.358 773	0.137 088	0.015 910	0.004 915	0.002 208	0.001 187	0.000 712
0.7000	2.251 809	0.177 479	0.021 666	0.006 603	0.002 948	0.001 583	0.000 949
0.7426	2.205 351	0.195 869	0.024 589	0.007 461	0.003 321	0.001 782	0.001 068
0.8000	2.144 932	0.220 159	0.028 812	0.008 709	0.003 860	0.002 068	0.001 240
0.8575	2.086 914	0.243 529	0.033 345	0.010 067	0.004 444	0.002 378	0.001 425
0.9000	2.045 630	0.259 975	0.036 871	0.011 139	0.004 903	0.002 620	0.001 569
0.9393	2.008 646	0.274 453	0.040 250	0.012 183	0.005 349	0.002 856	0.001 710
0.9587	1.990 806	0.281 322	0.041 956	0.012 716	0.005 577	0.002 975	0.001 781
1.0000	1.953 731	0.295 303	0.045 663	0.013 892	0.006 079	0.003 239	0.001 938
1.0502	1.910 290	0.311 083	0.050 287	0.015 392	0.006 721	0.003 576	0.002 139
1.1000	1.868 905	0.325 403	0.054 976	0.016 955	0.007 392	0.003 926	0.002 347
1.1344	1.841 283	0.334 524	0.058 260	0.018 076	0.007 875	0.004 179	0.002 497
1.1503	1.828 777	0.338 531	0.059 787	0.018 606	0.008 104	0.004 298	0.002 567
1.1819	1.804 399	0.346 110	0.062 835	0.019 678	0.008 569	0.004 541	0.002 711
1.2000	1.790 719	0.350 225	0.064 587	0.020 304	0.008 842	0.004 683	0.002 795
1.2126	1.781 314	0.352 995	0.065 809	0.020 745	0.009 034	0.004 783	0.002 854
1.3555	1.681 180	0.379 336	0.079 641	0.025 997	0.011 364	0.005 999	0.003 572
1.4849	1.600 013	0.396 250	0.091 867	0.031 083	0.013 696	0.007 224	0.004 295
1.7146	1.474 904	0.414 423	0.112 073	0.040 568	0.018 289	0.009 681	0.005 746
1.9170	1.381 362	0.422 049	0.127 811	0.049 067	0.022 706	0.012 120	0.007 202

[†] Scattering length.

this approximation will only effect the S-wave equation and then only if a polarisation potential is included. (In the static-exchange approximation setting this term to zero is equivalent to requiring the scattered wave to be orthogonal to the bound state wavefunction (Riley and Truhlar 1975). This can be done without approximation only in cases where a particular bound state wavefunction P_{nl} is itself a solution of the scattering equation (5).)

We find the error introduced by this approximation in the S-wave phaseshift decreases with increasing energy as expected. It amounts to less than 5% for the scattering length and decreases to about 1% at 20 eV. Since only the S-wave phaseshift is affected, the error in the cross section is greatest for small energies and is about 10% at zero energy. Thus for helium this assumption is well justified except very close to zero energy. We remark that the inclusion of this term is a trivial matter in our full-exchange treatment of this problem.

In figure 1 we present the S-, P- and D-wave phaseshifts for the four cases mentioned above. In addition we include the results of the matrix variational calculation of Nesbet (1979). From these results we can draw the following conclusions.

Comparing the two calculations using a dipole polarisation potential we find the effects of using a local exchange approximation are very similar to those reported by Bransden *et al* (1976) for their adiabatic exchange model. Thus δ_0 is well represented

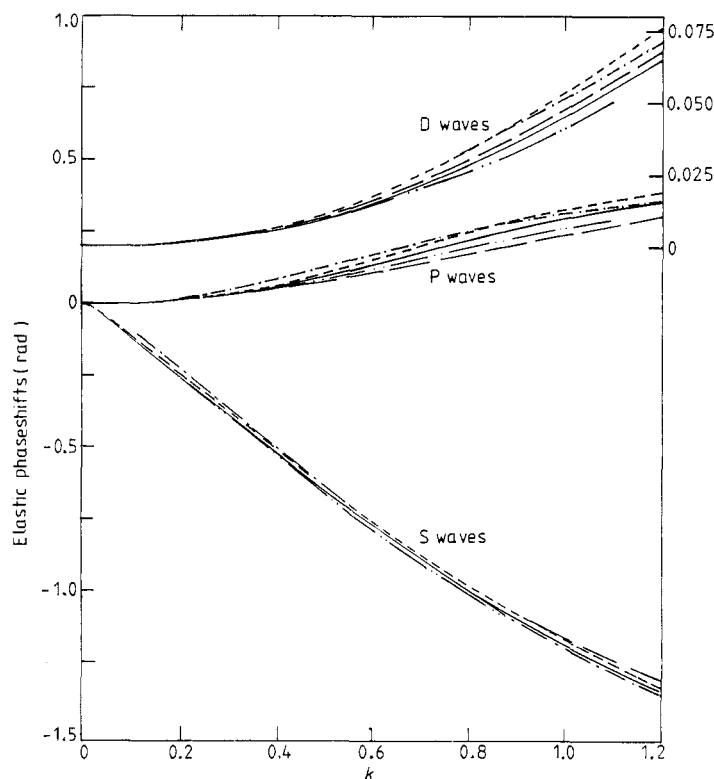


Figure 1. Phaseshifts for elastic scattering of electrons from helium: —, adiabatic exchange, dipole potential; ----, adiabatic exchange, all multipoles; - · -, adiabatic local exchange, dipole potential; — — —, adiabatic local exchange, all multipoles (Yau *et al* 1978), — · —, Nesbet (1979). The left-hand scale refers to S and P waves, the right-hand scale to D waves.

by the local exchange approximation which differs from the exact adiabatic exchange results by less than 1% for energies greater than 5 eV. The error increases as we go to lower energies however, reaching a maximum of 33% for the scattering length. For δ_1 the error is much larger, being over 50% at low energies and it is still over 10% at 10 eV while for δ_2 the error exceeds 10% for most of the elastic scattering range. Similar comments hold for the calculations employing the full polarisation potential. Therefore the local exchange approximation is not particularly good for low-energy elastic scattering.

If we compare our adiabatic exchange approximation with the two different polarisation potentials then, over the range of energies shown, we find differences of 2 to 3% in δ_0 , 5–10% in δ_1 and up to 16% in δ_2 . For higher partial-wave phaseshifts the maximum difference decreases with l but is still appreciable at the higher energies. Comparing the two local exchange approximation results we find even larger differences for δ_0 and δ_1 but somewhat smaller ones for δ_2 .

For most of the values calculated our adiabatic exchange results with the dipole polarisation potential are closer to the results of Nesbet (1979) than all our other calculations. Nesbet's results are also close to the *R*-matrix calculations of O'Malley

et al (1979) and Fon *et al* (1981). Thus we are led to the conclusion that only the dipole contribution to the polarisation potential should be retained in the adiabatic exchange approximation. This is, in fact, the usual approximation used (Drachman and Temkin 1972).

This conclusion is different from our experience in I where all multipole contributions were retained in the potential. From figure 1 we see that there is generally quite good agreement between the results of I and our present adiabatic exchange calculations with the dipole potential. Thus the effects of the local exchange approximation and the higher multipole contributions to the polarisation potential largely cancelled one another and led to the generally good results reported in I. This cancellation is presumably fortuitous.

Our present experience is also contrary to our previous experience for positron scattering (McEachran *et al* 1977a, 1978a) where retaining all multipole contributions consistently produced the most reliable results. This has also been noted in previous calculations (Drachman and Temkin 1972).

It is of some interest to investigate further this difference between electron and positron scattering. While it is not possible to give a definitive answer without more elaborate calculations, we can present qualitative arguments which throw some light on this subject.

The adiabatic exchange approximation involves two major approximations: the adiabatic approximation which assumes that the incident particle is at rest while the atomic polarised orbitals are calculated (or in other words the so-called dynamic terms are neglected) and the use of first-order perturbation theory in the calculation of the polarised orbitals. Within the framework of the adiabatic exchange approximation we would expect the interaction between the incident particle and the atom to contain contributions from all multipole moments. Thus we must consider why this is not so in the case of electron scattering.

If we analyse the terms of the perturbation expansion of the polarised orbital in powers of the interaction potential we find that they alternate in sign. The interaction potential itself is positive for electron scattering and negative for positron scattering. Hence the terms in the perturbation expansion are all of the same sign in the positron case but alternate in sign in the electron case. Thus in using first-order perturbation theory we produce a polarisation potential which is an underestimate of the full potential in the positron case but an overestimate in the electron case (assuming convergence of the perturbation series).

The neglected dynamic terms are repulsive for both electron and positron scattering. Asymptotically the leading dynamic term has the same radial dependence but the opposite sign to the quadrupole polarisation term and can actually produce a net repulsive effect for this term (Seaton and Steenman-Clark 1977). However there is no guarantee that the asymptotic forms for the adiabatic polarisation potential and the long-range dynamic terms are valid over the same interval of radial distances (Kleinman *et al* 1968). In fact there is evidence in scattering from hydrogen that the asymptotic form of the dynamic terms is not reached until such large distances that they have negligible effects on the long-range contribution to the scattering (Ali and Fraser 1977). One can argue further that these dynamic terms should be more significant for electron scattering than for positron scattering. This is because for electron scattering both the static and polarisation potential are attractive while for positrons the static potential is repulsive and the polarisation potential attractive. Hence during scattering the electrons will be accelerated more than positrons and

Table 2. Differential cross sections $d\sigma/d\Omega(a_0^2 \text{ sr}^{-1})$ for helium.

Energy (eV) Angle (deg)	2.0	5.0	7.5	10.0	12.0	12.5	15.0	17.5	18.0	19.0	20.0	25.0	30.0	40.0	50.0
0	0.625	0.870	1.361	1.842	2.170	2.243	2.557	2.796	2.835	2.909	2.974	3.207	3.337	3.444	3.466
5	0.652	0.856	1.305	1.746	2.045	2.111	2.392	2.601	2.635	2.698	2.753	2.940	3.030	3.072	3.040
10	0.688	0.841	1.237	1.628	1.890	1.948	2.189	2.364	2.391	2.442	2.485	2.619	2.665	2.638	2.553
15	0.729	0.832	1.175	1.516	1.744	1.793	1.997	2.139	2.161	2.200	2.233	2.321	2.332	2.252	2.130
20	0.772	0.828	1.120	1.415	1.609	1.651	1.821	1.934	1.951	1.980	2.004	2.055	2.038	1.922	1.777
25	0.819	0.830	1.073	1.323	1.486	1.521	1.660	1.748	1.760	1.781	1.797	1.818	1.780	1.640	1.485
30	0.869	0.839	1.035	1.241	1.375	1.403	1.513	1.579	1.587	1.601	1.610	1.606	1.553	1.399	1.241
35	0.922	0.854	1.005	1.170	1.276	1.298	1.382	1.427	1.433	1.440	1.443	1.419	1.355	1.194	1.039
40	0.978	0.876	0.984	1.111	1.191	1.208	1.267	1.294	1.296	1.298	1.297	1.256	1.185	1.022	0.873
45	1.037	0.906	0.974	1.063	1.119	1.130	1.167	1.178	1.178	1.175	1.169	1.115	1.038	0.877	0.737
50	1.099	0.942	0.972	1.027	1.060	1.067	1.083	1.079	1.076	1.069	1.059	0.994	0.913	0.756	0.624
55	1.164	0.985	0.980	1.003	1.015	1.016	1.014	0.996	0.991	0.980	0.967	0.892	0.809	0.655	0.533
60	1.231	1.035	0.998	0.990	0.982	0.979	0.958	0.928	0.921	0.906	0.891	0.807	0.722	0.573	0.459
65	1.300	1.091	1.025	0.988	0.961	0.954	0.916	0.874	0.865	0.847	0.829	0.737	0.650	0.506	0.399
70	1.371	1.153	1.060	0.996	0.951	0.941	0.887	0.833	0.822	0.801	0.780	0.680	0.592	0.451	0.350
75	1.443	1.220	1.102	1.014	0.952	0.938	0.868	0.803	0.791	0.767	0.743	0.636	0.545	0.407	0.312
80	1.516	1.293	1.152	1.040	0.962	0.944	0.860	0.784	0.770	0.743	0.717	0.601	0.508	0.372	0.280

85	1.590	1.369	1.208	1.074	0.981	0.959	0.860	0.774	0.759	0.728	0.699	0.576	0.479	0.343	0.255
90	1.664	1.448	1.270	1.115	1.007	0.982	0.869	0.772	0.755	0.721	0.690	0.557	0.457	0.320	0.235
95	1.738	1.530	1.335	1.161	1.039	1.011	0.884	0.777	0.757	0.721	0.686	0.545	0.440	0.302	0.218
100	1.810	1.613	1.405	1.211	1.076	1.045	0.904	0.787	0.766	0.726	0.689	0.537	0.429	0.288	0.204
105	1.882	1.697	1.476	1.266	1.117	1.083	0.929	0.801	0.778	0.735	0.695	0.534	0.420	0.276	0.193
110	1.952	1.781	1.549	1.322	1.161	1.123	0.957	0.819	0.795	0.748	0.706	0.535	0.416	0.268	0.185
115	2.020	1.864	1.622	1.380	1.206	1.166	0.987	0.839	0.813	0.764	0.718	0.538	0.413	0.261	0.178
120	2.084	1.945	1.694	1.438	1.253	1.210	1.019	0.861	0.834	0.781	0.733	0.542	0.412	0.256	0.172
125	2.146	2.022	1.764	1.495	1.299	1.254	1.051	0.884	0.855	0.800	0.749	0.548	0.413	0.253	0.167
130	2.204	2.097	1.831	1.550	1.345	1.297	1.083	0.907	0.877	0.818	0.765	0.555	0.415	0.250	0.163
135	2.258	2.166	1.895	1.603	1.388	1.338	1.114	0.930	0.898	0.837	0.781	0.562	0.417	0.248	0.160
140	2.307	2.231	1.955	1.652	1.429	1.377	1.143	0.951	0.918	0.855	0.796	0.570	0.419	0.246	0.157
145	2.352	2.290	2.009	1.698	1.466	1.412	1.170	0.972	0.937	0.871	0.811	0.577	0.422	0.245	0.155
150	2.391	2.342	2.058	1.738	1.500	1.445	1.195	0.990	0.955	0.887	0.825	0.583	0.425	0.244	0.154
155	2.425	2.387	2.100	1.774	1.530	1.473	1.217	1.006	0.970	0.900	0.837	0.590	0.427	0.244	0.152
160	2.453	2.424	2.135	1.803	1.555	1.496	1.235	1.020	0.983	0.912	0.847	0.595	0.430	0.244	0.152
165	2.475	2.454	2.163	1.827	1.575	1.516	1.250	1.031	0.993	0.921	0.855	0.600	0.432	0.244	0.151
170	2.491	2.476	2.183	1.844	1.589	1.529	1.260	1.039	1.001	0.928	0.861	0.603	0.434	0.245	0.151
175	2.501	2.489	2.195	1.854	1.597	1.537	1.267	1.044	1.006	0.932	0.865	0.605	0.435	0.245	0.151
180	2.504	2.493	2.200	1.858	1.601	1.541	1.270	1.047	1.008	0.934	0.867	0.606	0.436	0.245	0.152
$\sigma_e(a_0^2)$	20.732	18.971	17.450	16.020	14.957	14.702	13.502	12.422	12.222	11.830	11.457	9.830	8.534	6.650	5.379
$\sigma_{\text{mt}}(a_0^2)$	24.396	22.648	20.023	17.370	15.437	14.987	12.945	11.230	10.927	10.344	9.803	7.615	6.061	4.089	2.943

the adiabatic approximation could well break down at lower incident energies for electrons than for positrons.

The above arguments suggest that the full adiabatic polarisation potential will be too attractive in the case of electron scattering. Since this potential is dominant in the asymptotic region it is important to retain the leading term, viz the dipole part of the potential. The higher order terms are less important and dropping them compensates for the overattractiveness of the full potential. While there is no guarantee that this compensation will be of the right magnitude, previous experience and the fact that we have the correct leading term suggest that the dipole polarisation potential will produce good results for electron scattering. As we have seen, this is further confirmed in the present calculation.

6. Comparison with other work

In this section we compare our adiabatic exchange results using the dipole polarisation potential with previous calculations and with experiment. Our phaseshifts can be

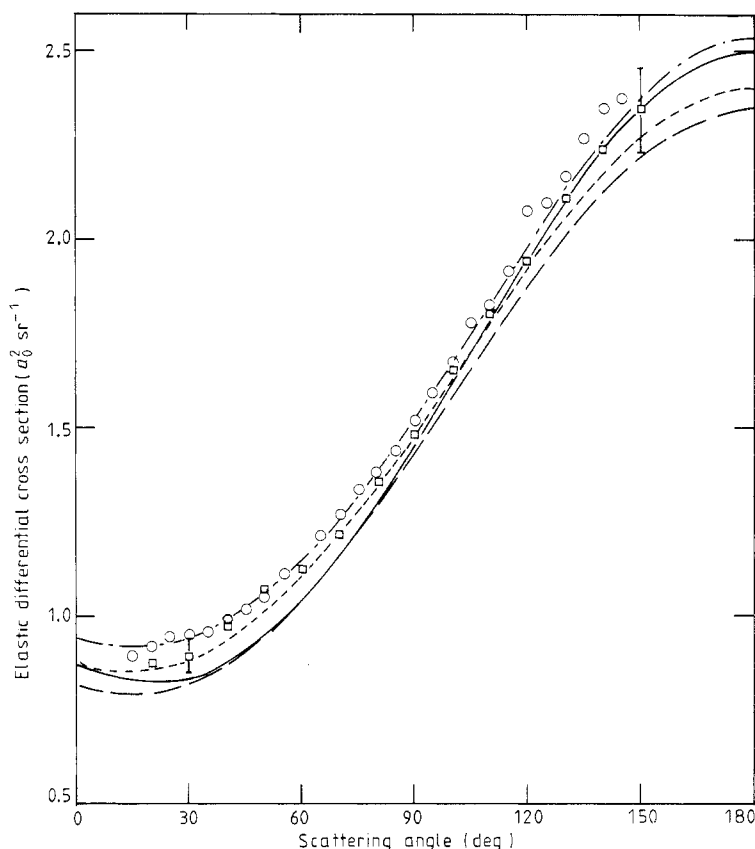


Figure 2. Differential cross sections for elastic scattering of electrons from helium at 5 eV: —, present results; ----, Nesbet (1979); — · —, LaBahn and Callaway (1970); · · ·, Williams (1979); ○, Andrick and Bitsch (1975); □, Register *et al* (1980). Representative error bars are shown.

compared with those similar calculations by LaBahn and Callaway (1964), Callaway *et al* (1968), Duxler *et al* (1971) and Williamson and McDowell (1964). For δ_0 all the various calculations, including the present one, yield very comparable values while for δ_1 and δ_2 there is greater variation among the various results (by as much as 20–30%).

We can also compare our phaseshifts with those of Nesbet (1979), O'Malley *et al* (1979) and Fon *et al* (1981). These latter two calculations yield essentially the same results. The δ_0 values of Nesbet and O'Malley *et al* agree to within 0.5% over the energy range considered whereas our results are between 1 and 2.6% higher (comparing values of $\delta_0 - \pi$). For δ_1 , the values of O'Malley *et al* lie 3–4% below Nesbet's while our results are 1–13% above the latter.

There have been a number of experimental measurements of the differential elastic cross sections and in some cases (Andrick and Bitsch 1975, Williams 1979, Newell *et al* 1981) scattering phaseshifts have been derived from these measurements. Our S-wave phaseshifts agree with all three sets of experimental values to within 5% over the energy range of our calculations. For the P wave we agree best with the results of Andrick and Bitsch where the differences are from 1 to 6% while the differences between our values and those of Williams and Newell *et al* range from 1–13% and 9 to 18% respectively. In the case of the D wave we have better general agreement with Newell *et al* than for the P wave whereas for Williams' data the differences are somewhat larger ranging from 6–18%.

Our differential cross sections were calculated using the phaseshifts of table 1 plus the analytic form

$$\tan \eta_l = k^2 \beta a_l + k^4 (\beta^2 b_l + \alpha c_l)$$

of Ali and Fraser (1977) where β and α are the dipole and quadrupole polarisabilities

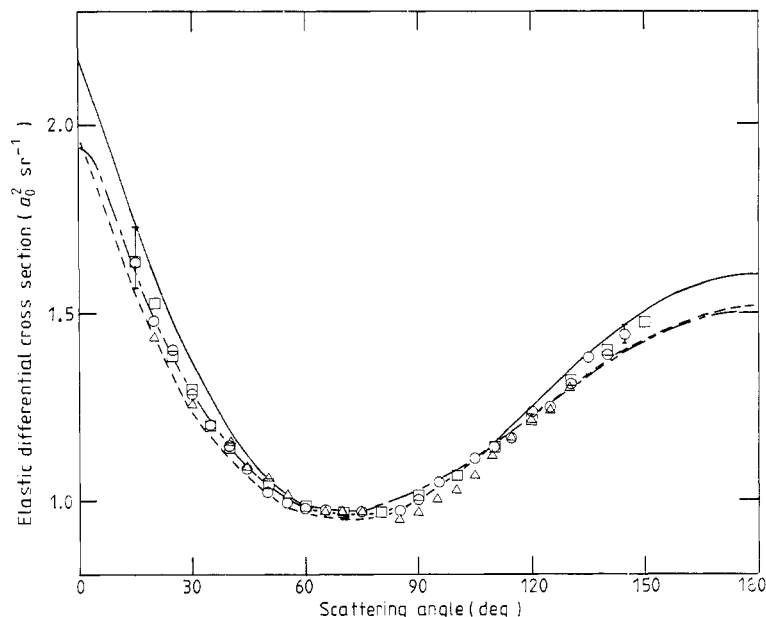


Figure 3. As for figure 2 at 12 eV with the addition of the results of Newell *et al* (1981), Δ , (scaled data) measured at 12.5 eV.

of the atom respectively and a_l , b_l and c_l are coefficients which are given analytically by Ali and Fraser. Normally only the first term of this expression is used for the higher-order phaseshifts. However, including the k^4 term gives substantially better agreement with calculated results at higher values of k . We use this form with values of α and β given by McEachran *et al* (1977b) for $l = 7$ to 50. No appreciable difference results if we include terms up to $l = 100$.

We compare our differential cross sections with other available data in figures 2, 3 and 4. In figure 2 we present our results at 5 eV along with the theoretical results of LaBahn and Callaway (1970) and Nesbet (1979). The results of O'Malley *et al* (1979) and Fon *et al* (1981) are close to those of Nesbet and we have omitted them. We also show the experimental measurements of Andrick and Bitsch (1975), Register *et al* (1980) and Williams (1979). The latter results are constructed from the phase-shifts given in the paper. The measurements of Andrick and Bitsch and Williams lie

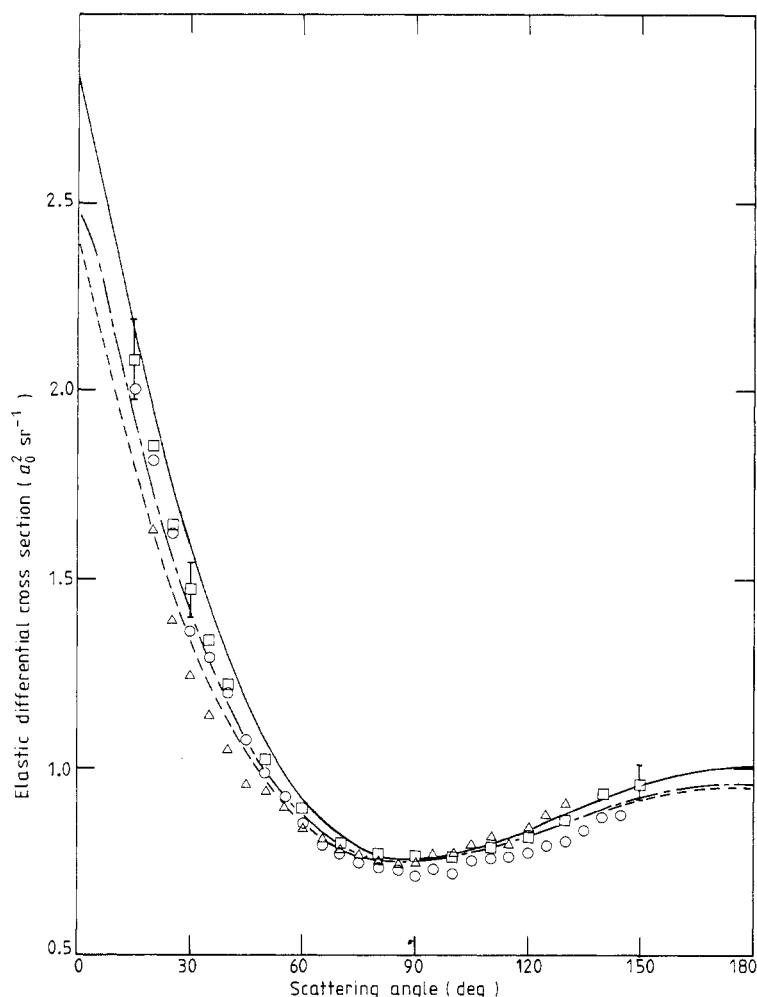


Figure 4. As for figure 2 at 18 eV except that ---- are the results of Fon *et al* (1981), the results of Newell *et al* (1981), Δ , are at 19 eV and those of Andrick and Bitsch, \circ , are at 17.5 eV.

above the theoretical results at all angles while those of Register *et al* agree quite well with the cross sections of Nesbet in the forward direction and with the present results in the backward direction. Figure 3 shows similar results at 12 eV except that the results of LaBahn and Callaway are not available at this energy and we have plotted the experimental measurements of Newell *et al* (1981) taken at 12.5 eV. In the forward direction the experimental results lie between the theoretical curves. In the backwards direction there is slightly more scatter but agreement is still good. Figure 4 shows our differential cross sections at 18 eV along with those of Fon *et al* (1981), Register *et al* (1980) and Williams (1979). In addition we have plotted the measurements of Andrick and Bitsch (1975) taken at 19 eV and of Newell *et al* (1981) taken at 17.5 eV. The pattern is similar to that at 12 eV though it should be noted that our results at 17.5 and 19 eV (not shown) agree well with the corresponding experimental values in the backward direction. In all cases the general shape of the experimental measurements is well reproduced by the theoretical calculations, including the location of the minimum.

Figure 5 shows the total elastic cross section for a number of theoretical and experimental investigations. In general there is good agreement among all these results with the variation among the theoretical results somewhat smaller than the experimental variation. Similarly in figure 6 we show the momentum transfer cross sections which exhibit similar behaviour to the total cross section. It should be noted

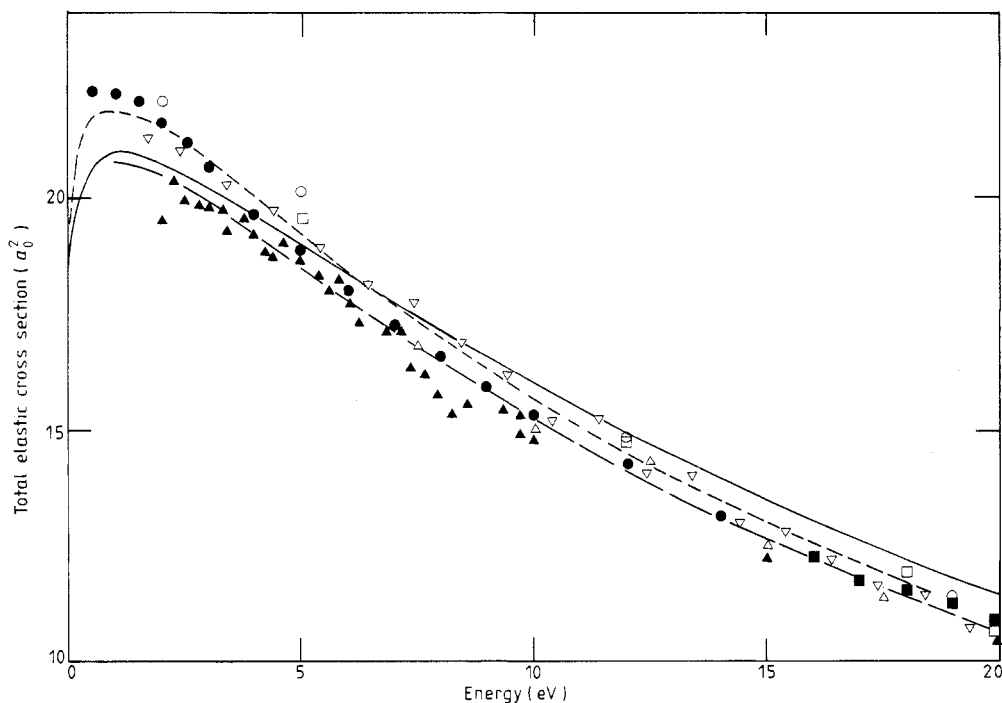


Figure 5. Total elastic cross section for elastic scattering from helium: —, present results; ----, Nesbet (1979); — —, LaBahn and Callaway (1970); ○, Andrick and Bitsch (1975); ■, Blaauw *et al* (1980), ▲, Charlton *et al* (1980), ▽, Stein *et al* (1978); ●, Kennerly and Bonham (1978) (identical to ■ above 16 eV); △, Newell *et al* (1981); □, Register *et al* (1980).

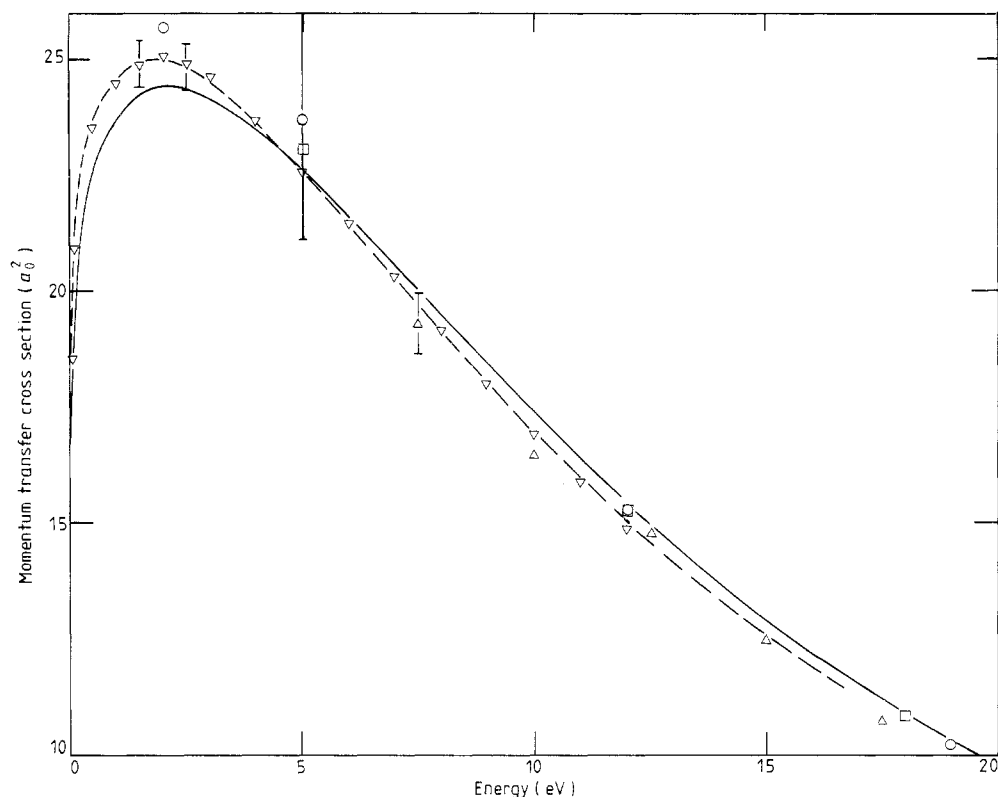


Figure 6. Momentum transfer cross section for electrons on helium. The legend is the same as for figure 5 except that ∇ represents the measurements of Crompton *et al* (1970) and Milloy and Crompton (1977).

that for the total elastic and momentum transfer cross sections the 'experimental' results of Andrick and Bitsch (1975), Newell *et al* (1981) and Register *et al* (1980) are not a direct measurement but are calculated from the phaseshifts which were derived from an analysis of differential cross section measurements.

We have included a few values in our tables at energies beyond the elastic scattering region. We do not expect our approximation to be particularly good in the intermediate energy range. Nevertheless the difference between our differential cross sections and the measurements of Register *et al* (1980) at these energies ranges from 10 to 25%. Thus even at intermediate energies the adiabatic exchange approximation gives reasonable results.

7. Conclusions

In this paper we have analysed the effects of the polarisation and local exchange potentials in the adiabatic exchange approximation for elastic scattering of electrons from helium. We conclude that only the dipole part of the polarisation potential should be used and further that the local exchange approximations are not particularly good at these low energies. Thus we have presented detailed calculations in the

adiabatic exchange model using the dipole polarisation potential and treating exchange exactly.

Comparison of differential cross sections with experimental measurements and other theoretical calculations is a severe test of any theory. We conclude from our present results that the adiabatic exchange approximation is capable of producing reliable results in the elastic scattering regime. We intend to extend these calculations to other noble gases.

Acknowledgments

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Appendix. Asymptotic correction for phaseshifts

In equation (29) it is necessary to determine integrals involving the scattering function over the entire range of integration from zero to infinity in order to determine the constants A_l^0 , B_l^0 , $A_l^{n'l'\nu}$ and $B_l^{n'l'\nu}$. We now let

$$A_l^0 = A_l^0(x_n) + \Delta A_l^0(x_n) \quad (\text{A.1})$$

$$A_l^{n'l'\nu} = A_l^{n'l'\nu}(x_n) + \Delta A_l^{n'l'\nu}(x_n) \quad (\text{A.2})$$

with similar expressions for B_l^0 and $B_l^{n'l'\nu}$. Here the quantities $\Delta A_l^0(x_n)$ and $\Delta A_l^{n'l'\nu}(x_n)$ are given by

$$\Delta A_l^0(x_n) = \frac{1}{k} \int_{x_n}^{\infty} dx g_l(kx) (V(x) + K_l(x)) u_l^0(x) \quad (\text{A.3})$$

and

$$\Delta A_l^{n'l'\nu}(x_n) = \frac{1}{k} \int_{x_n}^{\infty} dx g_l(kx) [(V(x) + K_l(x)) u_l^{n'l'\nu}(x) + x^\nu P_{n'l'}(x)] \quad (\text{A.4})$$

with corresponding expressions for $\Delta B_l^0(x_n)$ and $\Delta B_l^{n'l'\nu}(x_n)$. Thus the quantities $A_l^0(x_n)$, $A_l^{n'l'\nu}(x_n)$, $B_l^0(x_n)$ and $B_l^{n'l'\nu}(x_n)$ only involve integrals from 0 to x_n and hence can be determined at each point as the solutions to equations (24) are integrated out from the origin. If we now let x_n be chosen such that the radial Hartree-Fock functions are effectively zero for $x \geq x_n$ then the static potential $V_s(x)$ and the exchange kernel $K_l(x)$ will also be zero for $x \geq x_n$ and our expressions (A.3) and (A.4) reduce to

$$\Delta A_l^0(x_n) = \frac{1}{k} \int_{x_n}^{\infty} dx g_l(kx) V(x) u_l^0(x) \quad (\text{A.5})$$

and

$$\Delta A_l^{n'l'\nu}(x_n) = \frac{1}{k} \int_{x_n}^{\infty} dx g_l(kx) V(x) u_l^{n'l'\nu}(x) \quad (\text{A.6})$$

with correspondingly simplified expressions for $\Delta B_l^0(x_n)$ and $\Delta B_l^{n'l'v}(x_n)$. Here $V(x)$ is now given by just twice the polarisation potential $V_p(x)$ i.e.

$$V(x) = -\sum_{\nu} \frac{\alpha_{\nu}}{x^{2\nu+2}} \quad (\text{A.7})$$

where the α_{ν} are the multipole polarisabilities of the atom.

Then provided, for example, $u_l^0(x)$ can be adequately approximated by

$$u_l^0(x) = A_l^0(x_n) f_l(kx) + B_l^0(x_n) g_l(kx) \quad \text{for } x \geq x_n \quad (\text{A.8})$$

we can evaluate $\Delta A_l^0(x_n)$ and $\Delta B_l^0(x_n)$ analytically i.e.

$$\Delta A_l^0(x_n) = -A_l^0(x_n) \sum_{\nu} \alpha_{\nu} W_{2\nu+2}^l(k, x_n) - B_l^0(x_n) \sum_{\nu} \alpha_{\nu} V_{2\nu+2}^l(k, x_n) \quad (\text{A.9})$$

and

$$\Delta B_l^0(x_n) = A_l^0(x_n) \sum_{\nu} \alpha_{\nu} U_{2\nu+2}^l(k, x_n) + B_l^0(x_n) \sum_{\nu} \alpha_{\nu} W_{2\nu+2}^l(k, x_n) \quad (\text{A.10})$$

where

$$U_{2\nu+2}^l(k, x_n) = \frac{1}{k} \int_{x_n}^{\infty} \frac{dx f_l^2(kx)}{x^{2\nu+2}} \quad (\text{A.11})$$

$$V_{2\nu+2}^l(k, x_n) = \frac{1}{k} \int_{x_n}^{\infty} \frac{dx g_l^2(kx)}{x^{2\nu+2}} \quad (\text{A.12})$$

and

$$W_{2\nu+2}^l(k, x_n) = \frac{1}{k} \int_{x_n}^{\infty} \frac{dx f_l(kx) g_l(kx)}{x^{2\nu+2}}. \quad (\text{A.13})$$

These functions f_l and g_l can be conveniently expressed as (cf Abramowitz and Stegun 1968)

$$f_l(\rho) = c_l(\rho) \sin \rho + (-1)^{l+1} c_{-(l+1)}(\rho) \cos \rho \quad (\text{A.14})$$

$$g_l(\rho) = c_l(\rho) \cos \rho + (-1)^l c_{-(l+1)}(\rho) \sin \rho \quad (\text{A.15})$$

with the coefficients c_l given recursively by

$$c_{l+1}(\rho) + c_{l-1}(\rho) = \frac{2l+1}{\rho} c_l(\rho) \quad l = 0, \pm 1, \pm 2, \dots \quad (\text{A.16})$$

with $c_0(\rho) = 1$ and $c_1(\rho) = \rho^{-1}$.

Our expressions (A.11) to (A.13) can then be shown to reduce to

$$\begin{aligned} U_{2\nu+2}^l(k, x_n) = & \sum_{i=0}^{2l} \frac{2^i a_i^l}{(2k)^{1+i} (2\nu+1+i)} \frac{1}{x_n^{2\nu+1+i}} - (2k)^{2\nu} \sum_{i=0}^{2l} 2^i b_i^l h_{2\nu+2+i}(2kx_n) \\ & + (2k)^{2\nu} \sum_{i=0}^{2l-1} 2^i c_i^l i_{2\nu+2+i}(2kx_n) \end{aligned} \quad (\text{A.17})$$

$$\begin{aligned} V_{2\nu+2}^l(k, x_n) = & \sum_{i=0}^{2l} \frac{2^i a_i^l}{(2k)^{1+i} (2\nu+1+i)} \frac{1}{x_n^{2\nu+1+i}} + (2k)^{2\nu} \sum_{i=0}^{2l} 2^i b_i^l h_{2\nu+2+i}(2kx_n) \\ & - (2k)^{2\nu} \sum_{i=0}^{2l-1} 2^i c_i^l i_{2\nu+2+i}(2kx_n) \end{aligned} \quad (\text{A.18})$$

and

$$W_{2\nu+2}^l(k, x_n) = (2k)^{2\nu} \sum_{i=0}^{2l} 2^i b_i^l i_{2\nu+2+i}(2kx_n) + (2k)^{2\nu} \sum_{i=0}^{2l-1} 2^i c_i^l h_{2\nu+2+i}(2kx_n) \quad (\text{A.19})$$

where the constants a_i^l , b_i^l and c_i^l are defined implicitly by the relations

$$\sum_{i=0}^{2l} a_i^l \rho^{-i} = c_l^2(\rho) + c_{-(l+1)}^2(\rho) \quad (\text{A.20})$$

$$\sum_{i=0}^{2l} b_i^l \rho^{-i} = c_l^2(\rho) - c_{-(l+1)}^2(\rho) \quad (\text{A.21})$$

and

$$\sum_{i=0}^{2l-1} c_i^l \rho^{-i} = 2(-1)^{l+1} c_l(\rho) c_{-(l+1)}(\rho). \quad (\text{A.22})$$

The functions $i_\nu(x)$ and $h_\nu(x)$ in (A.17) to (A.19) are defined by

$$i_\nu(x) = \int_x^\infty dt \frac{\sin t}{t^\nu} \quad (\text{A.23})$$

and

$$h_\nu(x) = \int_x^\infty dt \frac{\cos t}{t^\nu} \quad (\text{A.24})$$

and can be determined recursively from the relations

$$i_\nu(x) = \frac{1}{\nu-1} \left(\frac{\sin x}{x^{\nu-1}} + h_{\nu-1}(x) \right) \quad \nu \geq 2 \quad (\text{A.25})$$

and

$$h_\nu(x) = \frac{1}{\nu-1} \left(\frac{\cos x}{x^{\nu-1}} - i_{\nu-1}(x) \right) \quad \nu \geq 2. \quad (\text{A.26})$$

The starting values $i_1(x)$ and $h_1(x)$ are given by

$$i_1(x) = \frac{1}{2}\pi - \text{Si}(x) \quad (\text{A.27})$$

and

$$h_1(x) = -\text{Ci}(x) \quad (\text{A.28})$$

where $\text{Si}(x)$ and $\text{Ci}(x)$ are the standard sine and cosine integrals respectively and can be determined numerically to any desired accuracy. Analytic values for $\Delta A^{nl\nu}(x_n)$ and $\Delta B_l^{nl\nu}(x_n)$ can be found in an identical manner.

When $k=0$ the analogous equation to (A.8) for $l=0$ is

$$\phi_0(x) = A_0^0(x_n)x + B_0^0(x_n) \quad \text{for } x \geq x_n \quad (\text{A.29})$$

where, for all x , $\phi_0(x) = \lim_{k \rightarrow 0} u_0(x)/k$. The corresponding equations for our expressions (A.9) and (A.10) are then simply

$$\Delta A_0^0(x_n) = -A_0^0(x_n) \sum_\nu \frac{\alpha_\nu}{2\nu} \frac{1}{x_n^{2\nu}} - B_0^0(x_n) \sum_\nu \frac{\alpha_\nu}{2\nu+1} \frac{1}{x_n^{2\nu+1}} \quad (\text{A.30})$$

and

$$\Delta B_0^0(x_n) = A_0^0(x_n) \sum_{\nu} \frac{\alpha_{\nu}}{2\nu-1} \frac{1}{x_n^{2\nu-1}} + B_0^0(x_n) \sum_{\nu} \frac{\alpha_{\nu}}{2\nu} \frac{1}{x_n^{2\nu}} \quad (\text{A.31})$$

with corresponding expressions for $\Delta A_0^{n'l'\nu}(x_n)$ and $\Delta B_0^{n'l'\nu}(x_n)$.

Although all the above expressions have been based upon the integral equation formulation of the problem, namely equations (24), all of the above formulae can be equally applied to each of the numerical solutions to the differential equations (15) provided each of the starting solutions of these equations is chosen so that the coefficient of x^{l+1} is also given by $k^{l+1}/(2l+1)!!$.

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