

The use of second order potentials in the theory of scattering of charged particles by atoms

VII. The partial wave formalism and elastic scattering of electrons by hydrogen and helium

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Abstract. The second order potential approximation of Bransden and Coleman is applied in a partial wave formalism to the elastic scattering of electrons from hydrogen and helium atoms. Differential, integrated, and total cross sections are presented for hydrogen in the energy range 100–200 eV and for helium in the range 50–500 eV. A one-channel approximation is used and the effect of exchange is included to first order in the potential. Conclusions are drawn as to the validity of the impact parameter approximation used in previous applications of the method.

1. Introduction

There has recently been considerable experimental interest in the scattering of electrons from hydrogen and helium atoms at intermediate energies. Absolute measurements have been made for helium by Crooks and Rudd (1973), and Jansen and de Heer (1973), and for hydrogen by Teubner *et al* (1973). In addition, relative measurements have been made for elastic scattering by McConkey and Preston (1973) and Suzuki and Takayanagi (1973).

For a theoretical description of scattering, the second order potential method of Bransden and Coleman (1972) may be used at energies above the ionization threshold. In previous applications of this method (Bransden *et al* 1972, Sullivan *et al* 1972, Berrington *et al* 1973), an impact parameter approximation has been used which has limited its validity to the higher intermediate energies. In the present work, the partial wave amplitudes T_l are obtained by solving numerically the radial equations resulting from a partial wave expansion of the equations of Bransden and Coleman (1972). It is to be expected that a large number of partial waves will contribute to the scattering amplitude, but it was found that the impact parameter approximation used previously is adequate for partial waves with l greater than 7. The results of preliminary calculations using a partial wave formalism have been presented by Winters *et al* (1973).

2. Theory

The total wavefunction for a system consisting of an electron with coordinates \mathbf{x} colliding with an atom whose electrons are collectively represented by the coordinates \mathbf{r} may be

expanded in the form

$$\psi(\mathbf{r}, \mathbf{x}) = \sum_n \phi_n(\mathbf{r}) F_n(\mathbf{x}) \quad (1)$$

where the sum over n includes integration over the continuum states of the target atom.

In the method of Bransden and Coleman (1972), when the first $N+1$ states are explicitly included in the expansion, the Schrödinger equation is replaced by the following set of equations:

$$(\nabla^2 + k_n^2) F_n(\mathbf{x}) = 2 \sum_{m=0}^N V_{nm}(\mathbf{x}) F_m(\mathbf{x}) + 4 \sum_{m=0}^N \int d\mathbf{x}' K_{nm}(\mathbf{x}, \mathbf{x}') F_m(\mathbf{x}') \quad (n = 0, \dots, N) \quad (2)$$

where

$$K_{nm}(\mathbf{x}, \mathbf{x}') = \sum_{m'=N+1}^{\infty} G(k_{m'}; \mathbf{x}, \mathbf{x}') V_{nm'}(\mathbf{x}) V_{m'm}(\mathbf{x}'). \quad (3)$$

$G(k_{m'}^2; \mathbf{x}, \mathbf{x}')$ is the free particle Green's function and

$$V_{nm}(\mathbf{x}) = \int \phi_n^*(\mathbf{r}) \left(-\frac{1}{x} + \frac{1}{|\mathbf{r} - \mathbf{x}|} \right) \phi_m(\mathbf{r}) d\mathbf{r}. \quad (4)$$

Replacing k_m^2 in the Green function by an average energy \bar{k}^2 , and using closure, equation (2) becomes, in a one channel approximation,

$$(\nabla^2 + k_0^2) F_0(\mathbf{x}) = 2V_{00}(\mathbf{x}) F_0(\mathbf{x}) + 4 \int d\mathbf{x}' K_{00}(\mathbf{x}, \mathbf{x}') F_0(\mathbf{x}') \quad (5)$$

where

$$K_{00}(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{\exp(i\bar{k}|\mathbf{x} - \mathbf{x}'|)}{|\mathbf{x} - \mathbf{x}'|} (V_{00}(\mathbf{x}, \mathbf{x}') - V_{00}(\mathbf{x}) V_{00}(\mathbf{x}'))$$

and

$$V_{00}(\mathbf{x}, \mathbf{x}') = \int \phi_0^*(\mathbf{r}) \left(-\frac{1}{x} + \frac{1}{|\mathbf{r} - \mathbf{x}|} \right) \left(-\frac{1}{x'} + \frac{1}{|\mathbf{r} - \mathbf{x}'|} \right) \phi_0(\mathbf{r}) d\mathbf{r}.$$

2.1. Partial wave expansion

Expanding the wavefunction $F_0(\mathbf{x})$ and the kernel $K_{00}(\mathbf{x}, \mathbf{x}')$ in partial wave series and substituting in (5) gives

$$\left(\frac{d^2}{dx^2} + k_0^2 - \frac{l(l+1)}{x^2} \right) f_l(x) = 2V_{00}(x) f_l(x) + 8\pi \int_0^\infty dx' h_l(x, x') x x' f_l(x') \quad (6)$$

$$h_l(x, x') = \int_{-1}^{+1} d(\hat{\mathbf{x}} \cdot \hat{\mathbf{x}}') K_{00}(\mathbf{x}, \mathbf{x}') P_l(\hat{\mathbf{x}} \cdot \hat{\mathbf{x}}'). \quad (7)$$

To include the effects of exchange we add to equation (6) the integral term that arises in the static exchange approximation. For hydrogen, for example, this term is

$$\frac{8\pi}{2l+1} (-1)^S \int_0^\infty dx' [\gamma_l(x, x') + (\epsilon_0 - \frac{1}{2}k_0^2)\delta_{l0}] \phi_0(x) \phi_0(x') x x' f_l(x') \quad (8)$$

where S is the total spin, ϵ_0 the ground state energy and

$$\gamma_l(x, x') = \frac{(r_<)^l}{(r_>)^{l+1}} \quad \text{with } r_< = \min(x, x') \quad r_> = \max(x, x').$$

When the equations of Bransden and Coleman (1972) are developed using a symmetrized wavefunction there are further second order terms which arise from exchange polarization. In the intermediate energy range it is considered that the effect of these terms is small.

The required solution $f_l^S(x)$ of equation (6) corresponding to a certain value of S has the asymptotic form

$$f_l^S(x) \sim x N_l [j_l(kx) - T_l^S(n_l(kx) - i j_l(kx))] \quad (9)$$

where $j_l(kx)$, $n_l(kx)$ are spherical Bessel and Neumann functions respectively, N_l is a constant and the partial wave amplitude T_l^S is related to the scattering amplitude $f(\theta)$ by

$$f^S(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) T_l^S P_l(\cos \theta) \quad (10)$$

and

$$|f(\theta)|^2 = \frac{1}{4} [|f^0(\theta)|^2 + 3|f^1(\theta)|^2]. \quad (11)$$

For helium there is only one spin state of the system, and the scattering amplitude is therefore given by only one set of partial wave amplitudes T_l .

2.2. The impact parameter T matrix

In the impact parameter approximation the scattering amplitude is given by McCarroll and Salin (1968), for a target with spherical symmetry.

$$f^{IP}(\theta) = -ik \int_0^{\infty} (a_0(b, \infty) - 1) J_0(2kb \sin \frac{1}{2}\theta) b \, db. \quad (12)$$

The transition amplitudes $a_0(b, \infty)$ have been calculated in the second order potential approximation by Bransden *et al* (1972) and Berrington *et al* (1973) for hydrogen and helium respectively.

Using the expansion

$$kb J_0(2kb \sin \frac{1}{2}\theta) = \sum_{l=0}^{\infty} (2l+1) J_{2l+1}(2kb) P_l(\cos \theta)$$

in equation (12) we find that the impact parameter partial wave amplitude T_l^{IP} is given by

$$T_l^{IP} = -ik \int_0^{\infty} (a_0(b, \infty) - 1) J_{2l+1}(2kb) b \, db \quad (13)$$

Hence, by calculating $f^{IP}(\theta)$ and T_l^{IP} for $l \leq 7$, the contribution to the scattering amplitude for $l > 7$ in the impact parameter approximation may be found.

2.3. Reduction of the kernel $h_l(x, x')$

The expression for the kernel $h_l(x, x')$ given by equation (7) may be easily reduced to a form more suitable for numerical calculations. Expanding the free particle Green's

function and the potential terms in the usual series of Legendre polynomials the integration over the variable $(\hat{\mathbf{x}} \cdot \hat{\mathbf{x}}')$ may be carried out. For hydrogen we obtain

$$h_n(x, x') = \frac{ik}{2\pi} \sum_{l=0}^{\infty} \sum_{\lambda=0}^{\infty} (2l+1) j_l(\bar{k}R_<) h_l^+(\bar{k}R_>) A_{nl\lambda}(x, x') \quad (14)$$

where

$$A_{nl\lambda}(x, x') = \frac{\delta_{nl}}{2n+1} Q(R_<) Q(R_>) - \frac{4}{2\lambda+1} \begin{pmatrix} n & \lambda & l \\ 0 & 0 & 0 \end{pmatrix}^2 X_\lambda(x, x')$$

$$X_\lambda(x, x') = \int_0^\infty \gamma_\lambda(r, x) \gamma_\lambda(r, x') r^2 e^{-2r} dr$$

$$Q(x) = \frac{1}{x} - \left(1 + \frac{1}{x}\right) e^{-2x} \quad \text{for } x \neq 0 \text{ and } Q(0) = 1$$

and $R_< = \min[x, x']$, $R_> = \max[x, x']$.

The limits on the λ summation, due to the properties of the Wigner $3-j$ symbol, reduce to $|n-l|$ and $n+l$. The integral $X_l(x, x')$ may be split into three integrals, each of which is found to satisfy a recurrence relation.

3. Numerical techniques

The second order integro-differential equation for the radial wavefunction was solved iteratively by the method of Austern (1969). This is a simplification of the nonlinear iterative formulation of Sasakawa (Sasakawa 1963). The zero-order trial function suggested by Austern (1969) was found to give rapid convergence of the iterative procedure for $l \geq 1$. For the $l = 0$ partial waves convergence was slow, but was improved by replacing the wavefunction at the p th iterate by a linear combination of the p th and $(p-1)$ th iterates, as discussed by Burke and Seaton (1971). It was also found to be useful to introduce a parameter $\lambda (\leq 1)$ multiplying the non-local terms in equation (6), such that at the start of the iterative procedure λ was small. The magnitude of λ was then increased at each successive iterate until, before iteration had converged, it was equal to one.

The infinite integrals in equation (6) were evaluated by the method of Clenshaw and Curtis (1960) in which the integrand is expanded in a series of Chebyshev polynomials and integrated term by term. The error estimates used were those of O'Hara and Smith (1968).

The integrals with integrands involving Bessel functions $J_\nu(x)$ were evaluated for $\nu = 0, 1$ by the gaussian quadrature formula of Piessens (1973) in which $J_\nu(x)$ is the weight function, and the limits of integration are successive zeroes of the Bessel function. For $\nu > 1$ a Romberg integration routine was used, and in both cases an Euler transformation was found to be useful in speeding up the convergence.

4. Partial wave amplitudes

The radial equations were solved for hydrogen and helium both with and without exchange. The choice of effective energy was that of Bransden *et al* (1972) for hydrogen and Berrington *et al* (1973) for helium.

We compare the values of $|T_l|^2$, without exchange, with the corresponding values $|T_l^{\text{IP}}|^2$ in the impact parameter approximation in table 1 for electron hydrogen scattering and table 2 for electron helium scattering. It can be seen that for helium at 50 eV, the $l = 0$ partial wave amplitude $|T_0^{\text{IP}}|^2$ in the impact parameter approximation is in error by 50 %. Even at 200 eV, this error is still greater than 30 %. A comparison of the values of $|T_l|^2$ calculated with and without exchange shows that at 50 eV the inclusion of exchange increases the $l = 0$ partial wave amplitude by 15 %.

Table 1. Electron-hydrogen elastic scattering

l	54.4 eV		100 eV		200 eV	
	(a)	(b)	(a)	(b)	(a)	(b)
0	0.269(0)†	0.391(0)	0.237(0)	0.295(0)	0.191(0)	0.213(0)
1	0.540(1)	0.736(1)	0.528(1)	0.670(1)	0.533(1)	0.611(1)
2	0.157(1)	0.188(1)	0.153(1)	0.202(1)	0.182(1)	0.205(1)
3	0.611(2)	0.696(2)	0.548(2)	0.552(2)	0.694(2)	0.767(2)
4	0.268(2)	0.309(2)	0.246(2)	0.266(2)	0.294(2)	0.314(2)
5	0.126(2)	0.147(2)	0.126(2)	0.134(2)	0.135(2)	0.142(2)
6	0.615(3)	0.718(3)	0.697(3)	0.750(3)	0.711(3)	0.720(3)
7	0.315(3)	0.367(3)	0.404(3)	0.435(3)	0.409(3)	0.403(3)

$|T_l|^2$ in (a) the impact parameter approximation and (b) partial wave treatment without exchange.

† The notation $X(n)$ implies that the number X must be divided by 10^n .

Table 2. Electron helium elastic scattering

l	50 eV			100 eV			200 eV		
	(a)	(b)	(c)	(a)	(b)	(c)	(a)	(b)	(c)
0	0.362(0)	0.762(0)	0.880(0)	0.361(0)	0.605(0)	0.713(0)	0.353(0)	0.464(0)	0.536(0)
1	0.680(1)	0.114(0)	0.196(0)	0.654(1)	0.962(1)	0.148(0)	0.710(1)	0.963(1)	0.124(0)
2	0.150(1)	0.218(1)	0.299(1)	0.157(1)	0.194(1)	0.273(1)	0.183(1)	0.221(1)	0.289(1)
3	0.399(2)	0.499(2)	0.591(2)	0.499(2)	0.592(2)	0.726(2)	0.581(2)	0.651(2)	0.813(2)
4	0.119(2)	0.125(2)	0.136(2)	0.197(2)	0.218(2)	0.246(2)	0.232(2)	0.244(2)	0.286(2)
5	0.386(3)	0.348(3)	0.362(3)	0.840(3)	0.880(3)	0.945(3)	0.108(2)	0.110(2)	0.122(2)
6	0.148(3)	0.111(3)	0.114(3)	0.381(3)	0.376(3)	0.392(3)	0.559(3)	0.556(3)	0.594(3)
7	0.633(4)	0.409(4)	0.411(4)	0.193(3)	0.173(3)	0.177(3)	0.300(3)	0.300(3)	0.313(3)

(a) and (b) as for Table 1; (c) $|T_l|^2$ in partial wave treatment including exchange.

5. Elastic scattering of electrons on hydrogen

In figure 1 we show differential cross sections for elastic scattering of electrons from hydrogen at 100 and 200 eV, in the angular range $0-30^\circ$. The present results are compared with the recent Eikonal-Born calculations of Byron and Joachain (1973), the Glauber approximation of Tai *et al* (1969) and the work of Bransden *et al* (1972). Our results are close to the Eikonal-Born results at 100 eV for $\theta > 15^\circ$ but fall below at smaller angles. The Glauber approximation lies closer to the curve of Bransden *et al* (1972) than to the present results. At 200 eV there is close agreement between all four approximations for $30^\circ < \theta < 50^\circ$.

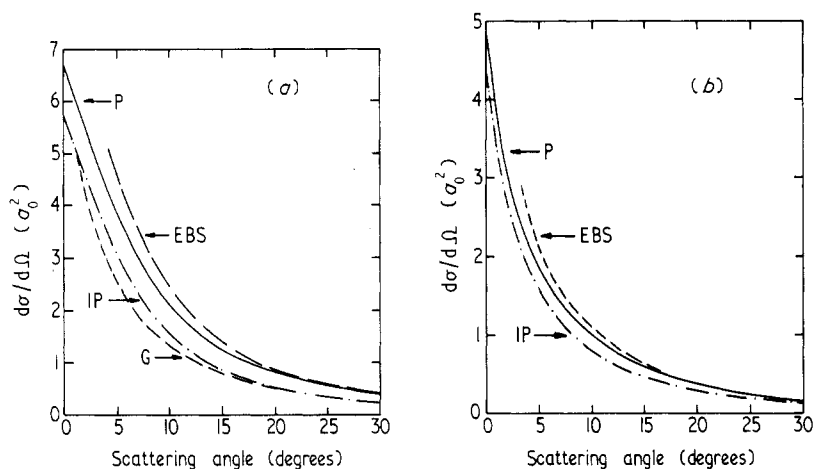


Figure 1. Differential cross sections for the elastic scattering of (a) 100 eV and (b) 200 eV electrons from hydrogen. Curve *P*, present results; curve *IP*, calculation of Bransden *et al* (1972); curve *EBS*, Eikonal-Born series results of Byron and Joachain (1973); curve *G*, Glauber approximation of Tai *et al* (1969).

In figure 2 we show cross section in the angular range 40–180° for the above energies. At these larger angles it can be seen that there is agreement between the impact parameter approximation and the present partial wave formulation only at 200 eV.

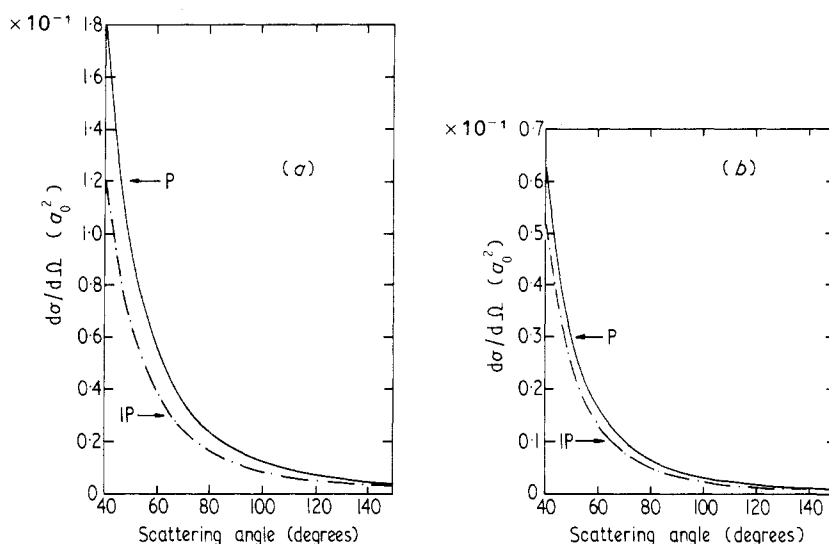


Figure 2. Large angle differential cross sections for the elastic scattering of (a) 100 eV and (b) 200 eV electrons from hydrogen. Curve *P*, present results; curve *IP*, calculation of Bransden *et al* (1972).

6. Elastic scattering of electrons on helium

In figure 3 we show differential cross sections for electron-helium scattering at 50, 300, 400 and 500 eV, in the angular range 0–30°.

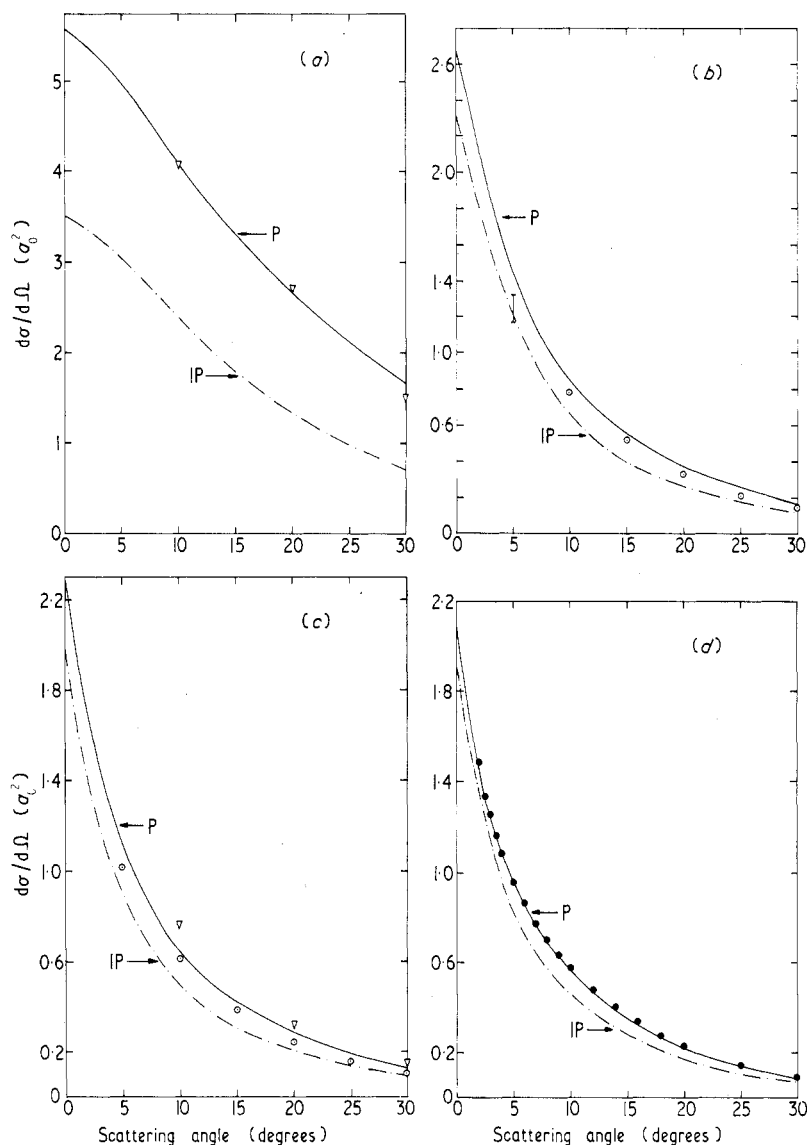


Figure 3. Differential cross sections for the elastic scattering of (a) 50 eV, (b) 300 eV, (c) 400 eV and (d) 500 eV electrons from helium. Curve P, present results; curve IP, calculation of Berrington *et al* (1973); ∇ Crooks and Rudd (1972); \bullet Bromberg (1969); \circ Vriens *et al* (1968) renormalized to Chamberlain *et al* (1970).

At 500 eV the agreement with the measurements of Bromberg (1969) are excellent, while at 400 eV our results lie between those of Crooks and Rudd (1973) and Vriens *et al* (1968) renormalized to Chamberlain *et al* (1970). In comparing with the experimental data it should be noted that the preliminary measurements of Jansen and de Heer (1973) have reproduced the results of Crooks and Rudd (1973) and Vriens *et al* (1968) rather than those of Chamberlain *et al* (1970).

The present results are found to be in exact agreement with the Eikonal-Born series results of Byron and Joachain (1973) in the angular range 0–30°.

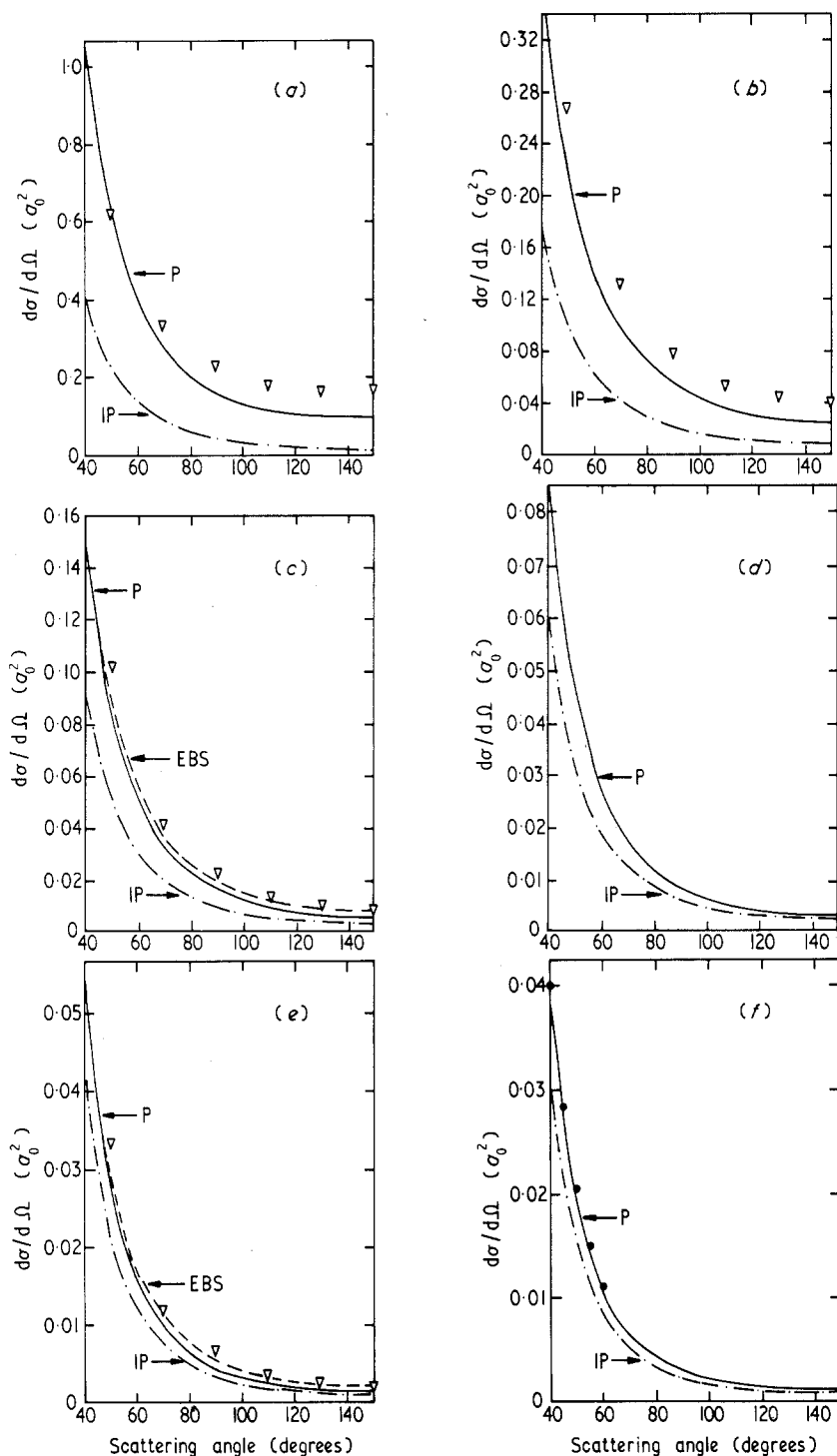


Figure 4. Large angle differential cross sections for the elastic scattering of (a) 50 eV, (b) 100 eV, (c) 200 eV, (d) 300 eV, (e) 400 eV and (f) 500 eV electrons from helium. Curve P, present results; curve IP, calculation of Berrington *et al* (1973); curve EBS, Eikonal-Born series results of Byron and Joachain (1973); ∇ Crooks and Rudd (1972); \bullet Bromberg (1969).

In figure 4 results are presented for large angle scattering at energies 50, 100, 200, 300, 400 and 400 eV. It can be seen that the results of the present approximation fall below the measurements of Crooks and Rudd (1973) particularly at the lower energies. In calculations at 50 eV for large angle electron hydrogen scattering (Winters *et al* 1973) a similar effect was observed in comparing with the absolute measurements of Teubner *et al* (1973).

The present results in addition to those of Winters *et al* (1973) clearly show the inadequacy of the impact parameter approximation used by Berrington *et al* (1973) for energies less than 300 eV.

The contribution from exchange to these cross sections was less than 10% for energies greater than 200 eV.

7. Integrated and total cross sections

In table 3 we tabulate integrated elastic scattering cross sections for electron on hydrogen and total cross sections calculated by means of the optical theorem. Also included for comparison are the results of Bransden *et al* (1972).

Table 3. Integrated and total cross sections in units of πa_0^2 for electron-hydrogen scattering

Energy (eV)	Integrated cross section		Total cross section	
	(a)	(b)	(a)	(b)
54.4	0.609	1.03	3.72	4.02
100	0.310	0.445	2.37	2.46
200	0.150	0.185	1.42	1.43

(a) Impact parameter approximation of Bransden *et al* (1972); (b) Present results.

Integrated cross sections for electron-helium scattering are given in table 4, and it can be seen that there is excellent agreement with the results of Vriens *et al* (1968). In table 5 we present results for the real part of the forward scattering amplitude and the

Table 4. Integrated cross section in units of πa_0^2 for electron-helium scattering

Energy (eV)	Present results	Experimental results
50	1.82	—
100	0.753	0.762
200	0.319	0.308
300	0.195	0.190
400	0.138	0.142
500	0.107	0.108

Experimental result at 500 eV that of Bromberg (1969), otherwise those of Vriens *et al* (1968) (not renormalized to Chamberlain *et al* 1970).

Table 5. Real part of forward scattering amplitude and total cross section (πa_0^2) for electron-helium scattering

Energy (eV)	$\text{Re}\{f(0, k^2)\}$			Total cross section	
	(a)	(b)	(c)	(a)	(b)
50	1.85	1.88	—	3.06	1.59
100	1.67	1.91	1.91	1.92	1.13
200	1.44	1.71	1.54	1.13	0.858
300	1.32	1.48	1.39	0.810	0.697
400	1.25	1.36	1.30	0.636	0.554
500	1.20	1.29	1.24	0.533	0.462

(a) Present results; (b) Values adopted by Bransden and McDowell (1970); (c) Eikonal-Born series results of Byron and Joachain (1973).

total cross section. It can be seen that the ratio of the imaginary to real parts of the scattering amplitude is in very poor agreement with the dispersion relation results of Bransden and McDowell (1970). The results of Byron and Joachain (1973) for the real part of $f(0, k^2)$ are in better agreement however with those of Bransden and McDowell (1970).

It should be noted that there is an apparent divergence of the forward scattering intensity with decreasing energy, common to all methods using an average energy. This is shown in figure 5.

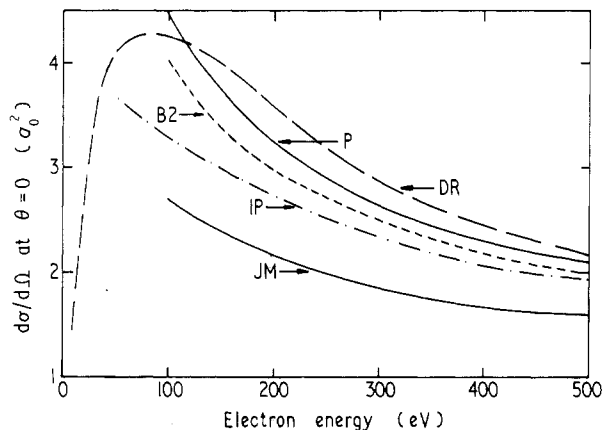


Figure 5. The forward scattered intensity for elastic electron-helium scattering. Curve P, present results; curve IP, calculation of Berrington *et al* (1973); curve B2, Second Born approximation of Holt *et al* (1971); curve JM, Eikonal approximation of Joachain and Mittleman (1971); curve DR, dispersion relation results of Bransden and McDowell (1970).

8. Conclusions

The very poor ratio of imaginary to real parts of the scattering amplitude in the forward direction at the lower energies would seem to be connected with our choice of effective energy. At present this is chosen so that the real part of the effective potential has the

asymptotic form of the adiabatic polarization potential. It would appear that an alternative prescription is required for the value of the effective energy in the imaginary part of the effective potential.

The present partial wave formulation of the second order potential method gives results that are a substantial improvement over those of the previous applications of the method. At angles $< 50^\circ$ differential cross sections obtained are in good agreement with the experimental measurements at intermediate energies. At large angles however the lack of agreement is somewhat disappointing.

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