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Semiphenomenological optical model for electron scattering on atoms

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Abstract. It is shown that it is possible to derive from first principles a form for a local, central, complex potential that fits elastic electron scattering on hydrogen at various energies with two free parameters. The energy-dependence of the parameters is discussed. Understanding of the optical model based on hydrogen enables us to use published Hartree–Fock calculations to construct a potential that gives excellent fits to argon at several energies with no free parameters. In all cases the total reaction cross section, obtained from independent experimental information, is used to determine the strength of the imaginary part of the potential.

1. Introduction

With more-and-more accurate experimental cross sections becoming available for elastic, inelastic and breakup reactions initiated by electrons on atoms, the understanding of elastic scattering provided by the optical model is becoming necessary. Basically the optical model can give elastic differential cross sections, polarizations and total reaction cross sections, but it is necessary also for distorted-wave calculations of the non-elastic reactions. In the case of atomic hydrogen a large part of the optical model potential can be understood from first principles. It is necessary to understand the optical model for hydrogen in order to derive approximations for the various parts of the potential. These approximations can be extended to larger atoms. We will derive an approximate optical potential for hydrogen that depends on two adjustable parameters and examine its use in fitting differential elastic and total reaction cross sections. The understanding so obtained leads to an optical model that gives excellent fits to elastic electron scattering from argon at different energies with no free parameters.

The optical model potential can be derived as a formal solution of the close coupling equations (Feshbach 1958). It has the form of a complex nonlocal potential in a Schrödinger equation for the entrance channel wavefunction. One obtains an optical potential for each of a finite number of channels (in our case only the entrance channel) by formally eliminating channels of higher excitation energy. There is doubt about the convergence of this process when the total energy is above the breakup threshold (Newton 1966). Divergences could appear as infinities in the parts of the optical potential representing real and virtual excitations of breakup channels. However there is no doubt that experimental cross sections are finite, so the optical potential can be considered in any case as a renormalized potential in exactly the same sense as the renormalized coupling

constant in quantum electrodynamics where analogous infinities are due to real and virtual excitations.

These convergence difficulties could be understood as casting doubt on the validity of close-coupling calculations above the breakup threshold, especially if only a small number of low-excitation channels are included. In any case such calculations strictly involve renormalized potentials describing the process of truncating the total set of coupled equations. It is interesting to examine the phenomenological terms that describe real and virtual excitations in the case where the set of coupled equations is truncated to a single channel to see if they are significant in comparison with the average of the potential for the ground state. In practice the close coupling calculation of Scott (1965), which couples six channels and uses a unitarized Born approximation for higher partial waves, describes electron scattering on hydrogen at 30 and 50 eV very well (Teubner *et al* 1973), so it is not necessary to improve on this with renormalized potentials, so far as the description of elastic scattering on hydrogen is concerned. The main practical use of the present work is to obtain a basic understanding of the optical potential for extension to larger atoms in a form (local and central) that is suitable for easy application.

In the application to argon at 60 eV, 100 eV and 150 eV, we will show how excellent fits to elastic scattering, using as input independently-measured reaction cross sections and Hartree–Fock potentials and wavefunctions available in the literature, can be obtained with no free parameters.

2. The formal optical potential

The Schrödinger equation for electron scattering on hydrogen is

$$[E - K(x_1) - u(x_1) - K(x_2) - u(x_2) - v(x_1, x_2)]\Psi(x_1, x_2) = 0. \tag{1}$$

The electron co-ordinates $x_i (i = 1, 2)$ are the space and spin co-ordinates r_i, σ_i. The kinetic energy operator is denoted by K. The electron–proton potentials are $u_i(x_i)$ and the electron–electron potential is $v(x_1, x_2)$. For nonrelativistic energies we will neglect spin–orbit coupling. The electron spin comes into the calculation only through the Pauli exclusion principle. Singlet states are symmetric, triplet states are antisymmetric in the space co-ordinates r_1, r_2. Proton recoil is neglected.

The bound and continuum states of the hydrogen atom are denoted by a discrete notation $\phi_\mu(x)$ for simplicity. Sums over μ are understood as integrals over the electron energy when this is positive. The Schrödinger equation for the hydrogen atom is

$$[\epsilon_\mu - K(x) - u(x)]\phi_\mu(x) = 0. \tag{2}$$

The three-body wavefunction is expanded in terms of channel wavefunctions for singlet and triplet (space symmetric and antisymmetric) scattering

$$\Psi(r_1, r_2) = \tfrac{1}{2} \sum_\nu [\phi_\nu(r_1)\psi_\nu^{(+)}(r_2) + \phi_\nu(r_2)\psi_\nu^{(+)}(r_1)] - \tfrac{1}{2} \sum_\nu [\phi_\nu(r_1)\psi_\nu^{(-)}(r_2) - \phi_\nu(r_2)\psi_\nu^{(-)}(r_1)]. \tag{3}$$

This expansion includes the effect of the Pauli principle. Spin co-ordinates are now redundant in the notation and have been omitted.

Multiplying by $\phi_\mu^*(r)$ and integrating over the appropriate electron co-ordinate, we obtain two uncoupled sets of coupled equations, one for singlet and one for triplet scattering.

$$[E - \epsilon_\mu - K(r_1) - u(r_1)]\psi_\mu^{(\pm)}(r_1) - \sum_\nu \left[\int d^3r_2 \, \phi_\mu^*(r_2)v(r_1, r_2)\phi_\nu(r_2) \right]\psi_\nu^{(\pm)}(r_1)$$

$$\pm \sum_\nu (E - \epsilon_\mu - \epsilon_\nu)\left[\int d^3r_2 \, \phi_\mu^*(r_2)\psi_\nu^{(\pm)}(r_2) \right]\phi_\nu(r_1)$$

$$\mp \sum_\nu \left[\int d^3r_2 \, \phi_\mu^*(r_2)v(r_1, r_2)\psi_\nu^{(\pm)}(r_2) \right]\phi_\nu(r_1) = 0. \tag{4}$$

Ambiguities in the definition of $\psi_\mu^{(\pm)}$ have in fact been introduced by the expansion (3). They are removed by subsidiary conditions (Beregi *et al* 1970). The usual condition used in atomic physics (Walker 1971) is to define the $\psi_\mu^{(\pm)}$ so that the third term of equation (4) is equal to zero. This is the term involving the overlap of bound and scattering wavefunctions when μ is a two-body bound state. We will adopt this definition.

$$\sum_\nu (E - \epsilon_\mu - \epsilon_\nu)\left[\int d^3r_2 \, \phi_\mu^*(r_2)\psi_\nu^{(\pm)}(r_2) \right]\phi_\nu(r_1) = 0. \tag{5}$$

We will now rewrite equation (4) in terms of diagonal and off-diagonal nonlocal potentials $V_{\mu\mu}^{(\pm)}(r_1, r_2)$ and $V_{\mu\nu}^{(\pm)}(r_1, r_2)$.

$$[E - \epsilon_\mu - K - V_{\mu\mu}^{(\pm)}]\psi_\mu^{(\pm)} = \sum_{\nu \neq \mu} V_{\mu\nu}^{(\pm)}\psi_\nu^{(\pm)} \tag{6}$$

where

$$V_{\mu\mu}^{(\pm)}(r_1, r_2) = \left[u(r_1) - \int d^3r_2' \, \phi_\mu^*(r_2')v(r_1, r_2')\phi_\mu(r_2') \right]\delta(r_1 - r_2) \mp \phi_\mu^*(r_2)v(r_1, r_2)\phi_\mu(r_1) \tag{7}$$

$$V_{\mu\nu}^{(\pm)}(r_1, r_2) = - \int d^3r_2' \, \phi_\mu^*(r_2')v(r_1, r_2')\phi_\nu(r_2')\delta(r_1 - r_2) \mp \phi_\mu^*(r_2)v(r_1, r_2)\phi_\nu(r_1). \tag{8}$$

The notation $V_{\mu\nu}\psi_\nu$ in (6) means

$$V_{\mu\nu}\psi_\nu \equiv \int d^3r_2 \, V_{\mu\nu}(r_1, r_2)\psi_\nu(r_2). \tag{9}$$

The diagonal potential (7) contains the nuclear, screening and exchange terms. Its analogue for larger atoms, in the case where only the ground state is considered in the independent-particle approximation, is the Hartree–Fock potential (Walker 1971).

The off-diagonal potential is responsible for real and virtual excitations of channel ν, starting with channel μ.

Equation (6) is the starting point for the formal definition of the optical potential for the entrance channel $\mu = 0$. We write the $\mu = 0$ equation explicitly and the others in a condensed notation for $\mu, \nu \neq 0$. Repeated indices are summed over.

$$[E - K - V_{00}^{(\pm)}]\psi_0^{(\pm)} = V_{0\nu}^{(\pm)}\psi_\nu^{(\pm)} \tag{10}$$

$$[E - \epsilon_\mu - K - V_{\mu\nu}^{(\pm)}]\psi_\nu^{(\pm)} = V_{\mu0}^{(\pm)}\psi_0^{(\pm)} \qquad \mu, \nu \neq 0. \tag{11}$$

We can formally solve equation (11) for the vector $\psi_\nu^{(\pm)}$

$$\psi_\nu^{(\pm)} = [E - \epsilon_\mu - K - V_{\mu\nu}^{(\pm)}]^{-1}V_{\mu0}^{(\pm)}\psi_0^{(\pm)} \tag{12}$$

and substitute the solution in equation (10)

$$[E - K - V_{00}^{(\pm)} - V_{0v}^{(\pm)}(E - \epsilon_\mu - K - V_{\mu v}^{(\pm)})^{-1} V_{\mu 0}^{(\pm)}]\psi_0^{(\pm)} = 0. \tag{13}$$

The formal definition of the ground-state optical potential is

$$\tilde{V}^{(\pm)} = V_{00}^{(\pm)} - V_{0v}^{(\pm)}(E - \epsilon_\mu - K - V_{\mu v}^{(\pm)})^{-1} V_{\mu 0}^{(\pm)}. \tag{14}$$

The first term of (14) is the average of the direct and exchange potentials V_d, V_{exch} for the ground state. We will call it the ground state potential. The direct potential is obtained by straightforward evaluation of the screening integral for the ground state. The evaluation of V_{exch} will be discussed in § 3.

The second term of (14) represents virtual excitations of states μ and v and real excitations of these states when energetically possible. Virtual excitations are represented by a real term, real excitations by an imaginary term. They will be discussed in § 4. The strengths v and w of the phenomenological parts of these terms are parameters of the theory.

3. Equivalent local potential

In order to obtain a local, central potential, which is sufficiently simple for the purposes of an optical model, it is necessary to construct an equivalent local potential for the nonlocal parts of the potential (14). We will do this for the exchange term of the ground state potential. The method is easily generalized to larger atoms in the Hartree–Fock model, where the exchange term is simply a sum of terms similar to the one considered here. We will use an extension of the method of Perey and Buck (1962), which was very successful in finding a local potential equivalent to a nonlocal potential for nuclear elastic scattering. The equivalent local potential is of course energy-dependent.

We will assume that the entire potential is local except for the nonlocal term of equation (7). The Schrödinger equation for elastic scattering can then be written (omitting the singlet–triplet superscripts for simplicity)

$$\left[E + V_L(r_1) + \frac{\hbar^2}{2m}\nabla^2\right]\psi_N(r_1) = \mp \int d^3r_2\, \phi_0^*(r_2)\frac{e^2}{r_{12}}\phi_0(r_1)\psi_N(r_2). \tag{15}$$

The local part of the potential is attractive. We have reversed the sign and represented it by a positive number $V_L(r_1)$. Subscripts N and L on ψ refer to calculations with nonlocal and local potentials respectively.

The right hand side of (15) is now expanded in a Taylor expansion about r_1, putting $r_2 - r_1 = r'$.

$$\int d^3r_2\phi_0(r_1)\frac{e^2}{|r_1 - r_2|}\phi_0^*(r_2)\psi_N(r_2) = \phi_0(r_1)e^2\int d^3r'\frac{1}{r'}\exp[(\nabla_\phi + \nabla_\psi)\cdot r']\phi_0^*(r_1)\psi_N(r_1)$$

where the operators ∇_ϕ and ∇_ψ operate on ϕ_0^* and ψ_N respectively. Performing the integration over r', we have

$$4\pi e^2\phi_0(r_1)\frac{1}{|\nabla_\phi + \nabla_\psi|^2}\phi_0^*(r_1)\psi_N(r_1).$$

We now make the approximation that ϕ_0^* is a much smoother function of r_1 than ψ_N,

so that the gradient $\mathbf{V}_\phi$ can be neglected. This approximation proved quite accurate in the calculation of Perey and Buck, where the corresponding function was a Woods–Saxon form factor, considerably less smooth than ϕ_0^*. The validity of the approximation can be estimated after we find the equivalent local potential.

We assume that there is a local potential U_L, equivalent to the nonlocal potential in the sense that the solution ψ_L of the Schrödinger equation

$$\nabla^2 \psi_\mathrm{L}(r) = -\frac{2m}{\hbar^2}[E + V_\mathrm{L} - U_\mathrm{L}]\psi_\mathrm{L}(r) \tag{16}$$

is approximately identical to the solution ψ_N of (15).

$$\psi_\mathrm{N} = \psi_\mathrm{L} = \psi. \tag{17}$$

With this approximation, the operator ∇_ψ^2 can be replaced by its eigenvalue when operating on ψ. Combining equations (15) and (16) and using the two approximations, we have

$$\left(\frac{\hbar^2}{2m}\nabla^2 + E\right)\psi(r) = [U_\mathrm{L}(r) - V_\mathrm{L}(r)]\psi(r)$$

$$= \left(\frac{4\pi e^2 \hbar^2 \phi_0^2}{2m(E + V_\mathrm{L} - U_\mathrm{L})} - V_\mathrm{L}\right)\psi(r). \tag{18}$$

Thus,

$$U_\mathrm{L} = \frac{2\pi e^2 \hbar^2}{m}\phi_0^2 \frac{1}{E + V_\mathrm{L} - U_\mathrm{L}}$$

$$\equiv \frac{1}{4}\alpha^2 \frac{1}{E + V_\mathrm{L} - U_\mathrm{L}} \tag{19}$$

where

$$\alpha^2 = \frac{8\pi e^2 \hbar^2}{m}\phi_0^2 = 8\frac{e^4}{a_0^2}\mathrm{e}^{-2r/a_0}. \tag{20}$$

We have a quadratic equation (19) for U_L, whose physical solution is

$$U_\mathrm{L} = \tfrac{1}{2}[E + V_\mathrm{L} - \{(E + V_\mathrm{L})^2 - \alpha^2\}^{1/2}]. \tag{21}$$

This solution is physical, since $U_\mathrm{L} \to 0$ as $E \to \infty$.

Performing the integral in the screening term, we find that the equivalent local ground state potentials $V_{00}^{(\pm)}$ for the singlet and triplet cases are

$$V_{00}^{(\pm)} = -V_\mathrm{L} \pm \tfrac{1}{2}[E + V_\mathrm{L} - \{(E + V_\mathrm{L})^2 - \alpha^2\}^{1/2}] \tag{22}$$

where

$$V_\mathrm{L} = \frac{e^2}{a_0}\left(1 + \frac{a_0}{r}\right)\mathrm{e}^{-2r/a_0} \tag{23}$$

and a_0 is the Bohr radius.

We are now in a position to estimate the validity of neglecting $\mathbf{V}_\phi$ by comparing $\nabla^2\phi_0$ with $\nabla^2\psi$ at $r = a_0$.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r) = [E + V_{\rm L} - U_{\rm L}]\psi(r) = (13{\cdot}6\,{\rm eV} + E)\psi(r) \qquad r = a_0$$

$$-\frac{\hbar^2}{2m}\nabla^2\phi_0(r) = \left[\epsilon_0 + \frac{e^2}{r}\right]\phi_0(r) \cong (13{\cdot}6\ {\rm eV})\phi_0(r) \qquad r = a_0.$$

We will calculate elastic cross sections for $E \geqslant 30\,{\rm eV}$ where $\nabla^2\psi$ is several times $\nabla^2\phi_0$.

4. Nonelastic channels

The excitation of nonelastic channels is formally represented by the second term on the right hand side of equation (14). We can obtain some knowledge of the form of this term and represent the unknown aspects of it by parameters, whose values must make sense in terms of the phenomenology of fitting entrance-channel data at various energies.

One known aspect of virtual excitations is the polarization of the hydrogen charge distribution due to the presence of the incident electron. A local, central representation of this part of the potential has been given by Temkin (1957) and Mittleman and Watson (1959). At large distances it is γ/r^4, where γ is the (measured) polarizability of the atom. At short distances this term is only found by detailed evaluation of equation (14) (see for example Alton *et al* 1972). It is often cut off phenomenologically by introducing a range parameter βd_0^2. This will be a parameter of our theory.

$$V_{\rm pol}(r) = \gamma/(r^2 + \beta d_0^2)^2. \tag{24}$$
$$d_0^4 = \tfrac{1}{2}\gamma Z^{-1/3}.$$

We will represent any remaining short-range term for virtual excitations by $vf(r)$, where v is an adjustable parameter. The form factor $f(r)$ must be closely related to the ground state density $\phi_0(r)^2$ since this is the probability of finding an electron available for excitation. For simplicity of parametrization, however, we will choose $f(r)$ to be the same as the form factor for real excitations, which will now be discussed.

We may obtain a rough idea of the shape of the imaginary potential representing real excitations, by making the approximations that ionization is the only excitation, that the ionized states constitute a complete set, and that the eigenfunctions of the operator in parentheses in equation (14) are plane waves:

$$\chi(\mathbf{K}; r, r') = {\rm e}^{{\rm i}(k_0 - K).r}\,{\rm e}^{{\rm i}K.r'} \tag{25}$$

where k_0 is the incident momentum. These approximations clearly become more valid as the incident energy increases. We are representing the scattered electron by ${\rm e}^{{\rm i}K.r^1}$ and the state of the (ionized) hydrogen atom by ${\rm e}^{{\rm i}(k_0 - K).r}$.

The imaginary part of the potential is, of course, nonlocal. We will find an approximate local form factor $f(r)$ by a technique similar to that of § 3. The integral term in the Schrödinger equation for the wavefunction $\psi_{\rm N}$ is

$$\int {\rm d}^3r'\,{\rm Im}\,\tilde{V}(r, r')\psi_{\rm N}(r') \cong wf(r)\psi_{\rm L}(r). \tag{26}$$

Using the spectral representation in terms of $\chi(K)$ for the second term of (14), we have

$$wf(r)\psi_L(r) \cong -A \int d^3r' \int d^3r_2 \int d^3r_2' \int d^3K \phi_0^*(r_2) \frac{e^2}{|r_2 - r|} e^{i(k_0 - K).r_2} e^{iK.r}$$

$$\times e^{-iK.r'} e^{-i(k_0 - K).r_2'} \frac{e^2}{|r_2' - r'|} \phi_0(r_2')\psi_N(r').$$ (27)

Since the Coulomb potential occurs twice in this expansion, we apply the technique of § 3 twice to obtain

$$f(r) = \text{const } \phi_0^2[E + V_L - iwf(r)]^{-2}$$ (28)

where the constant will be included with the free parameter w, and V_L is the remaining (local) potential for the scattering problem. Making a binomial expansion of (28) for $wf(r) \ll E + V_L$, we arrive at the dimensionless form to be used for the imaginary form factor

$$f(r) = E^2[E + V_L(r)]^{-2} e^{-2r/a_0}.$$ (29)

5. Electron scattering by atomic hydrogen

The elastic differential cross section and total reaction cross section for electron scattering by hydrogen were calculated by solving the Schrödinger equation for the complex, local, central potential

$$V(r) = V_{00}^{(\pm)}(r) - V_{\text{pol}}(r) - (v - iw)f(r).$$ (30)

The individual terms in (30) are given as follows: $V_{00}^{(\pm)}(r)$ by (20), (22) and (23), $V_{\text{pol}}(r)$ by (24), $f(r)$ by (29). Differential cross sections for singlet and triplet cases are averaged with weights 1 and 3 respectively.

The parameter w was adjusted to give the correct total reaction cross section. The parameter v was adjusted to fit the differential cross section. Different values of the polarization range parameter β were also tried. For hydrogen we thus have two free parameters, v and β, and a parameter w whose value is determined by an independent experiment.

By varying the virtual excitation parameters v and β it is possible to obtain quite good fits to differential cross sections (including of course absolute magnitudes) at different energies. These are illustrated for 30 eV, 50 eV, 100 eV and 200 eV in figure 1. The virtual excitation term is in fact crucial for obtaining fits. It must be chosen so as to increase the magnitude of the cross section above that given by the ground state potentials $V_{00}^{(\pm)}$. This is exactly what happens when the virtual excitation term is calculated more explicitly by Alton *et al* (1972).

The parameters v and β are energy-dependent. The value of β decreases with increasing energy. The potential v is repulsive and its value is so large that the whole virtual excitation term is repulsive in the region where the charge density is appreciable. Both these effects increase with energy. The values of the parameters are given in table 1. Interpolation in this table should give a useful optical potential for applications such as distorted-wave reaction calculations.
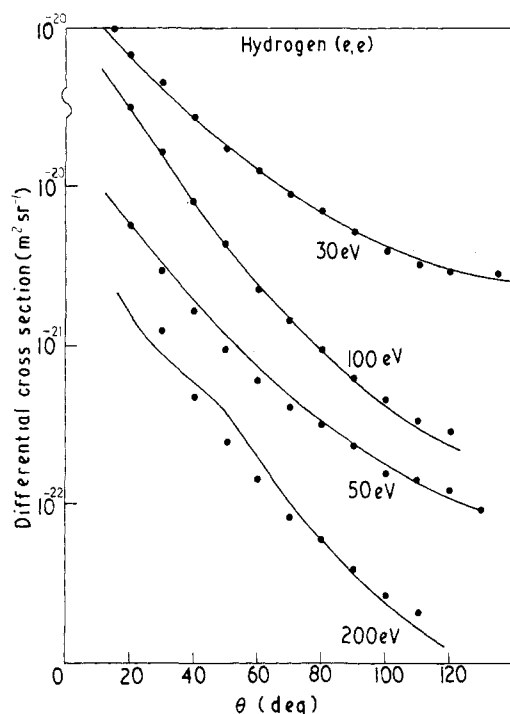
Figure 1. Optical model fits to the hydrogen elastic scattering data of Lloyd *et al* (1973).

Table 1. Total reaction cross sections and potential parameters used in the calculation of elastic electron scattering by hydrogen

E(eV)	w(eV)	v(eV)	β	$\sigma_R^{(exp)}(\pi a_0^2)$	$\sigma_R^{(h)}(\pi a_0^2)$
30	0·11	−0·89	1·1	1·40	1·36
50	0·16	−1·0	0·70	1·61	1·57
100	0·21	−1·4	0·52	1·50	1·51
200	0·19	−2·5	0·32	1·10	1·05

6. Electron scattering by argon

The ideas we have developed for hydrogen will now be extended to argon. We will construct an optical model potential analogous to (30). The analogue of the ground-state potential $V_{00}(r)$ is straightforward in the independent particle (Hartree–Fock) approximation. It has been previously discussed and used in computations, for example by Thompson (1971). Since we are not discussing polarization we will omit relativistic effects (spin–orbit coupling).

The direct part of the ground-state potential V_L is the Hartree–Fock potential for the target atom. In our calculations we use the Hartree–Fock potential and wavefunctions of Herman and Skillman (1963).

The exchange terms (one for each single particle state) are each reduced to local central potentials by the technique of § 3.

$$V_{exch} = \tfrac{1}{2} \sum_i N_i [(E + V_L) - \{(E + V_L)^2 - \alpha_i^2\}^{1/2}] \tag{31}$$

where N_i is the occupation number of the single particle state i,

$$\alpha_i^2 = \frac{8\pi e^2 \hbar^2}{m} u_i^2(r). \tag{32}$$

The Hartree–Fock radial wavefunction for the single particle state i is $u_i(r)$.

A numerical test of the approximation (31) is given by comparing phase shifts for $k^2 = 2\cdot 89$ with those of Thompson, who solved the integro-differential equations analogous to (15) numerically. This is done in table 2. Thompson used a different Hartree–Fock calculation to provide his central field V_L and radial wavefunctions u_i. In table 2 we therefore compare phase shifts for V_L and $V_L + V_{exch}$.

Table 2. Phase shifts for argon at $k = 2\cdot 89$ compared for the calculation of Thompson (1971) and the present work. Thompson's phase shifts are on the left in each column

	η_0		η_1		η_2		η_3		η_4	
V_L	0·380	0·402	1·127	1·387	1·227	1·479	0·166	0·158	0·040	0·021
$V_L + V_{exch}$	0·731	0·574	−1·523	−1·557	−1·395	−1·423	0·285	0·221	0·066	0·031

The imaginary potential is given by

$$W(r) = \sum_j N_j w_j f_j(r) \tag{33}$$

where

$$f_j(r) = u_j^2(r) E^2 / [E + V_L(r)]^2. \tag{34}$$

The sum over j includes only those single particle states from which real excitations are likely to occur. At the energies of our calculations we have included only the 3p state. The 3s state occupies essentially the same part of space. The parameter w_{3p} is fixed by fitting an estimate of the total reaction cross section arrived at by summing measured ionization cross sections (Kieffer 1966) and cross sections for inelastic scattering to certain states (which are much smaller than ionization cross sections). This estimate is a lower limit, but is believed to be close to the total value. It is possible that excitations can occur also from the 3s state. The corresponding radial wavefunction occupies the same general region of co-ordinate space as does the 3p wavefunction, and previous calculations (Furness and McCarthy 1973) have shown that cross sections are insensitive to assumptions about the proportion of 3s and 3p excitations in the model.

The real part of the potential representing virtual excitations of nonelastic channels is again represented at long range by the polarization potential.

$$V_{pol} = \gamma / (r^2 + d_0^2)^2 \tag{35}$$

where d_0^2 has its normal value, $d_0^4 = \tfrac{1}{2}\gamma Z^{-1/3}$.

At short range our experience with hydrogen has shown that this potential must be considerably reduced in the interior of the atom. We have chosen to cut the potential off at the atomic surface $r = r_0$. For hydrogen the surface is not well-defined but for argon the Hartree–Fock density falls extremely steeply at $r_0 = 1\cdot1$ Å. We have studied the effect of varying r_0 and found that the optimum value is $1\cdot1$ Å. Thus r_0 is not a free parameter. It is determined from the Hartree–Fock density.

Figure 2 shows the fit to the data of Vuskovic (1972) at 60 eV, 100 eV and 150 eV. Since the absolute values of the differential cross sections are somewhat uncertain within an overall factor, we have chosen this factor to normalize the data at 90° to those of
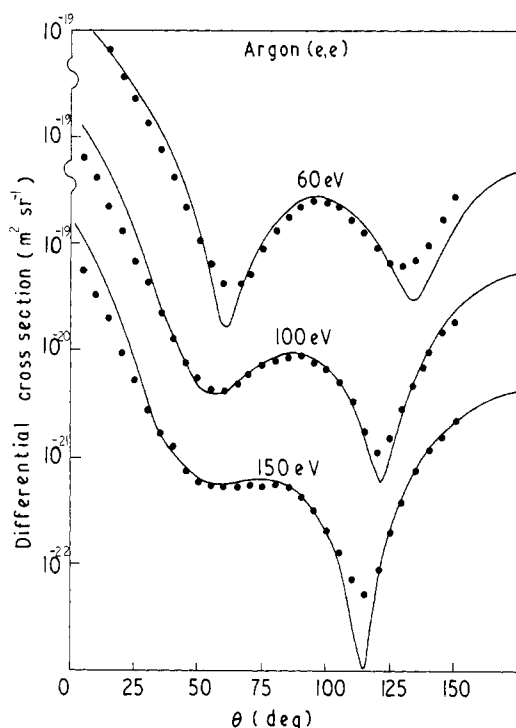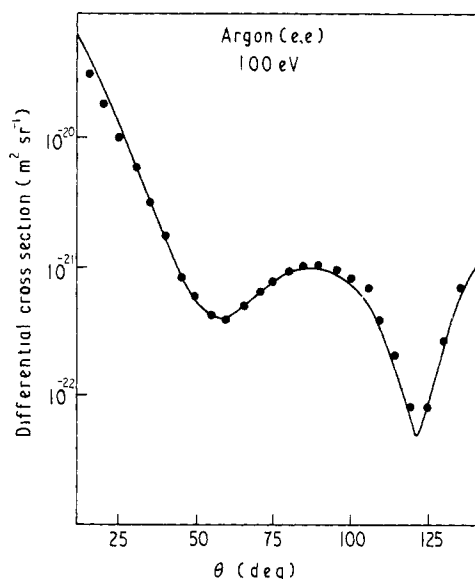

Figure 2. The present optical model compared with the argon elastic scattering data of Vuskovic (1972).

Bohm and Torop (1973) at 100 eV. Relative magnitudes for different energies and angles are significant. The values used for the total reaction cross section σ_R and the parameter w_{3p} are given in table 3. The gradual increase of w_{3p} with incident energy makes physical sense. One would expect the probability of exciting a non-elastic channel to increase as more channels become open.

In all the fits shown in figure 2 the theoretical curve comes below the data in sharp minima, as is usual with rather broad experimental angular resolution. In order to further check the shape of our theoretical curve we have compared it in figure 3 with the 100 eV data of Lloyd *et al* (1973), who put great effort into the angular resolution, but did not measure the absolute cross sections.

Table 3. The total reaction cross sections and imaginary potential parameters used in the calculation of elastic electron scattering by argon

E(eV)	w_{3p}(eV)	$\sigma_R^{(exp)}(\pi a_0^2)$	$\sigma_R^{(th)}(\pi a_0^2)$
60	5·55	2·90	2·83
100	7·5	3·04	3·02
150	8·0	2·88	2·83

Figure 3. The present optical model compared with the argon elastic scattering data of Lloyd *et al* (1973).

7. Conclusions

The first object of our work is to find out if it is possible to represent atomic elastic scattering by a local, central potential whose calculation is simple enough for application to more-detailed reactions such as inelastic scattering and $(e, 2e)$ in distorted-wave approximations.

Our study of hydrogen and argon has shown that this is possible at a wide range of energies.

The second object is to obtain sufficient understanding of the potential to make it easy to determine the values of its parameters for a given elastic scattering experiment.

For hydrogen we have observed the energy-dependence of the two free parameters v and β at several energies, so that interpolation should give reasonable starting values. To determine the parameter w it is always necessary to run the program two or three times in order to obtain a fit to the total reaction cross section. Each run takes $\frac{1}{7}$ second per partial wave on the CDC6400.

The understanding obtained for hydrogen has enabled us to construct a model for argon at various energies that has no free parameters. Only the value of w must be

found by a simple one-parameter search to fit the reaction cross section. The remainder of the input is obtained from published Hartree–Fock calculations.

In future work we will apply this potential to elastic scattering from other atoms and to the calculation of non-elastic reactions.

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