

An iterative perturbation solution of the inverse potential problem

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Abstract. A method is suggested for systematically obtaining model potentials that accurately reproduce spectroscopic or scattering data. Applications are made to atomic systems consisting of one electron outside a closed shell for the closed shells Li^+ , Na^+ , K^+ , He and Ne.

1. Introduction

The use of pseudopotential techniques for the calculation of atomic properties has a long history and has recently been the subject of intensified interest (cf Sheorey 1969, Callaway and Laghos 1969, Bardsley and Dorn 1969, Kutzelnigg 1969). In the model potential or pseudopotential method the interaction of an electron with a closed shell system is replaced by an empirically determined potential. Within this framework it is possible to formulate many different types of theory. The present approach is based on the simple assumption that the potential is a local function independent of angular momentum and energy (Caves and Dalgarno 1971, Dalgarno *et al.* 1970). The only practical difficulty which arises is that of determining a functional form of the potential which fits a wide range of experimental data. Since it is hoped to develop this method as a precise predictive tool it is desirable that the potentials be determined very accurately. With this object in view the present paper describes two algorithms for constructing the potentials.

2. Theory: bound state eigenvalues

We suppose that the potential for an electron outside a positively charged core can be written in the form

$$V(r) = U_0(r) + \sum_{j=1}^{N_c} c_j U_j(r) \quad (1)$$

where U_0 contains the correct form of $V(r)$ at large values of r ; the functions $\{U_j\}$ and linear parameters $\{c_j\}$ will be chosen to fit whatever data are available. In order to have a good initial estimate of the potential we incorporate the Hartree-Fock single particle interaction in U_0 ,

$$U_0 = V_{\text{HF}} - \frac{\alpha_d}{2r^4} [1 - \exp\{-(r/r_d)^6\}] - \frac{(\alpha_q - 3\beta_1)}{2r^6} [1 - \exp\{-(r/r_q)^8\}]. \quad (2)$$

The dipole and quadrupole polarizabilities are denoted by α_d and α_q ; β_1 is the dynamical correction discussed by Kleinman *et al.* (1968). For an electron outside several closed shells

$$V_{\text{HF}} = -\frac{(Z-N)}{r} + 2 \sum_{\alpha} (2l_{\alpha} + 1) \frac{\zeta_{\alpha}(r)}{r} \quad (3)$$

$$\zeta_{\alpha}(r) = \int_r^{\infty} \left(1 - \frac{r}{x}\right) P_{\alpha}(x)^2 dx \quad (4)$$

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where Z is the nuclear charge, N the number of electrons in the closed shells and $P_\alpha(r)$ is the Hartree-Fock orbital in the α th shell. Finally a choice must be made of the expansion set $\{U_j\}$; we took

$$U_j(r) = r^{m_j} \exp(-r/r_j). \quad (5)$$

The nonlinear parameters r_d , r_q and $\{r_j\}$ give the potential several extra degrees of flexibility.

Let us suppose that we know the experimental eigenenergies ϵ_α^x of the Rydberg states $n_\alpha l_\alpha$ ($\alpha = 1, \dots, N_\epsilon$) and that we have a potential $V(r)$ whose eigenenergies ϵ_α are not too different from ϵ_α^x ,

$$\left(\frac{d^2}{dr^2} - \frac{l_\alpha(l_\alpha+1)}{r^2} + 2(\epsilon_\alpha - V) \right) P_\alpha = 0. \quad (6)$$

If the potential V undergoes a slight change to $V + \delta V$ the energies undergo a corresponding change given by first order perturbation theory,

$$\delta\epsilon_\alpha = \int_0^\infty P_\alpha(r)^2 \delta V(r) dr. \quad (7)$$

By means of equation (7), δV may be chosen to make the energies closer to their experimental values. If the potential is only varied through the linear parameters defined in (1) we have

$$\delta\epsilon_\alpha = \sum_{j=1}^{N_c} U_{\alpha j} \delta c_j \quad (8)$$

$$U_{\alpha j} = \int_0^\infty P_\alpha(r)^2 U_j(r) dr. \quad (9)$$

Thus we have a set of linear equations which determine the δc appropriate to any set of $\delta\epsilon$. In particular if we set $\delta\epsilon_\alpha = \epsilon_\alpha^x - \epsilon_\alpha$ an improved set of coefficients $\{c_j^x\}$ is obtained by solving

$$\sum_{j=1}^{N_c} U_{\alpha j} (c_j^x - c_j) = \epsilon_\alpha^x - \epsilon_\alpha. \quad (10)$$

Since these equations are only exact in first order perturbation theory they must be solved iteratively; when a new set of c is obtained we re-evaluate ϵ_α , $P_\alpha(r)$ and $U_{\alpha j}$ and substitute them back in (10) until some convergence criterion is satisfied. It is perfectly possible to make the number of linear parameters N_c equal to the number of energies N_ϵ and thus to fit the data exactly. However no experimental data are free from random errors and it is better to smooth these out by overdetermining the coefficients, that is, by choosing $N_c < N_\epsilon$ and settling for a least squares solution of (10). By minimizing the function

$$\sum_{\alpha=1}^{N_\epsilon} \left(\sum_{j=1}^{N_c} U_{\alpha j} (c_j^x - c_j) - (\epsilon_\alpha^x - \epsilon_\alpha) \right)^2$$

we obtain the well-posed equations

$$\sum_{i=1}^{N_c} X_{ji} (c_i^x - c_i) = Y_j \quad (11)$$

$$X_{ji} = \sum_{\alpha=1}^{N_\epsilon} U_{\alpha j} U_{\alpha i} \quad Y_j = \sum_{\alpha=1}^{N_\epsilon} U_{\alpha j} (\epsilon_\alpha^x - \epsilon_\alpha). \quad (12)$$

Equation (10) is equivalent to a variational principle for the potential. From the Hellman–Feynman theorem (Feynman 1939),

$$\frac{\partial E}{\partial \lambda} = \left\langle \psi \left| \frac{\partial H}{\partial \lambda} \right| \psi \right\rangle \quad (13)$$

where λ is any parameter in the Hamiltonian, we deduce that

$$\delta \langle \psi_\alpha | V - \epsilon_\alpha | \psi_\alpha \rangle = 0. \quad (14)$$

The equations (11) may be derived from

$$\delta \sum_{\alpha=1}^{N_\epsilon} |\langle \psi_\alpha | V - \epsilon_\alpha | \psi_\alpha \rangle|^2 = 0. \quad (15)$$

3. Theory: scattering cross sections

To extend the method of § 2 to scattering data (electrons on neutral atoms) we need an analogue of equation (7). Suppose that instead of fitting energies we want to fit phaseshifts η_α^x in the angular momentum channels l_α at wavenumbers k_α . We begin with a potential $V(r)$ in which the phaseshifts are η_α

$$\left[\frac{d^2}{dr^2} + k_\alpha^2 - \frac{l_\alpha(l_\alpha+1)}{r^2} - 2V \right] P_\alpha = 0 \quad (16)$$

$$P_\alpha(r) \underset{r \rightarrow \infty}{\sim} \sin(k_\alpha r - \frac{1}{2} l_\alpha \pi + \eta_\alpha). \quad (17)$$

Let $\eta_\alpha^{\text{I}}, \eta_\alpha^{\text{II}}$ and $P_\alpha^{\text{I}}, P_\alpha^{\text{II}}$ denote the phaseshifts and wavefunctions in two different potentials $V^{\text{I}}, V^{\text{II}}$. From the differential equation (16) we can readily prove the identity,

$$\sin(\eta_\alpha^{\text{I}} - \eta_\alpha^{\text{II}}) = - \frac{2}{k_\alpha} \int_0^\infty P_\alpha^{\text{I}} (V^{\text{I}} - V^{\text{II}}) P_\alpha^{\text{II}} dr. \quad (18)$$

If $V^{\text{I}} = V, V^{\text{II}} = V + \delta V$ we have to first order in δV ,

$$\delta \eta_\alpha = - \frac{2}{k_\alpha} \int_0^\infty P_\alpha(r)^2 \delta V(r) dr. \quad (19)$$

The result of varying linear parameters in the potential is given by

$$\delta \eta_\alpha = \sum_{j=1}^{N_\epsilon} U_{\alpha j} \delta c_j \quad (20)$$

$$U_{\alpha j} = - \frac{2}{k_\alpha} \int_0^\infty P_\alpha(r)^2 U_j(r) dr. \quad (21)$$

One can easily write down equations analogous to (10) and (11). However phaseshifts are not directly accessible to observation so we have decided to utilize momentum transfer cross sections $Q_m(k)$ which probably provide the most accurate information on the interaction between low-energy electrons and the inert gases. These cross sections are given in terms of the phaseshifts by

$$Q_m(k) = \frac{4\pi}{k^2} \sum_{l=0}^\infty (l+1) \sin^2(\eta_l - \eta_{l+1}). \quad (22)$$

The sum over l converges very rapidly, even at several eV, so we will always truncate it at some small value of l , say L . Then we have

$$\delta Q_m(k) = \frac{4\pi}{k^2} \sum_{l=0}^L (l+1) \sin 2(\eta_l - \eta_{l+1}) (\delta\eta_l - \delta\eta_{l+1})$$

whence

$$\delta Q_m(k) = \sum_{j=1}^{N_e} U_{Qj} \delta c_j \quad (23)$$

$$U_{Qj} = \frac{4\pi}{k^2} \sum_{l=0}^L (l+1) (U_{lj} - U_{l+1j}) \sin 2(\eta_l - \eta_{l+1}) \quad (24)$$

$$U_{lj} = -\frac{2}{k} \int_0^\infty P_l(r)^2 U_j(r) dr. \quad (25)$$

We can fit experimental cross sections by treating equation (23) in the manner of § 2.

As in the theory developed for bound states the basic relation (19) can be regarded as a variational principle. In fact (19) leads directly to a theorem of the Feynmann type for continuum states,

$$\frac{\partial \eta_\alpha}{\partial \lambda} = -\frac{2}{k_\alpha} \int_0^\infty P_\alpha(r)^2 \frac{\partial H}{\partial \lambda} dr. \quad (26)$$

4. Applications to spectroscopic data

In fitting the term energies of the alkali metals we have arranged that the wavefunction of the lowest state $n_0 l$ of a given series has the correct number of nodes indicated by the aufbau principle. The states nl ($n < n_0$) are simply discarded as physically meaningless. This differs from the procedure of several other investigators (eg Callaway and Laghos 1969) who take $n_0 l$ to be the lowest eigenvalue. They force the wavefunction to have the correct number of nodes by projecting out the Hartree-Fock orbitals of the core.

In table 1 we list the best available values of the quantities α_d , α_q and β_1 for the systems studied in this paper. In all cases we took the values of α_d as they stood but

Table 1. Values of α_d , α_q and β_1 †

System	α_d	α_q	β_1	References
Li ⁺	0.1923	0.1134	0.0163	a, a, b
Na ⁺	0.9448	1.523	—	c, c
K ⁺	5.325	16.24	—	d, d
He	1.242	2.440	0.076	e, e, b
Ne	2.362	6.459	1.27	c, c, b

† atomic units throughout.

a, Dalgarno and Victor (1971, private communication)

b, Dalgarno *et al.* (1968)

c, Lahiri and Mukherji (1967a)

d, Lahiri and Mukherji (1967b)

e, Victor *et al.* (1968).

regarded $\alpha_q' = \alpha_q - 3\beta_1$ as an adjustable parameter. Because the model potential omits many physical effects (short range forces, higher multipoles, velocity dependence) one does not expect the value of α_q' which best fits the data to coincide with

the theoretical estimate. The nonlinear parameters for Li were taken from an earlier calculation (Dalgarno *et al.* 1970). In other cases we set r_d , r_a and $\{r_j\}$ equal (see (2) and (5)) and tried several values to find the best fit. The optimum value r_0 is always on the order of the atomic or ionic radius. If the value of r_d is too different from r_0 the method may fail to converge. To obtain convergence it was sufficient in most cases to try values of r_d separated by 0.1. The only exception was He (see § 5) where steps of 0.005 were needed. The convergence is not affected by the choice of Hartree-Fock potential or even whether it is omitted altogether. The Hartree-Fock potentials used in this work have been calculated using the analytic wavefunctions of Clementi (1965). It is interesting that the added exponential terms which presumably simulate the effects of exchange, fall off with r much more slowly than V_{HF} .

We begin with the spectrum of Li I. By fitting the five lowest energy levels to the term values of Johansson (1959) we have obtained the potential

$$\begin{aligned}
 V_{\text{Li}} = V_{\text{HF}} &- \frac{0.09615}{r^4} [1 - \exp\{- (r/0.47)^6\}] \\
 &- \frac{0.011589}{r^6} [1 - \exp\{- (r/0.44)^8\}] \\
 &+ 0.546266 \exp(-r/0.47) - 0.303243 r \exp(-r/0.47). \quad (27)
 \end{aligned}$$

The eigenvalues obtained from (27) are compared with experiment in table 2.

Table 2. Li I eigenenergies

State	Experiment	Calculation
2s	0.198158	0.198159
3s	0.0741878	0.0741863
2p	0.130245	0.130236
3p	0.0572390	0.0572458
3d	0.556102	0.0556214

Table 3. Na I eigenenergies

State	Experiment	Calculation
3s	0.18886	0.18899
4s	0.07158	0.07169
5s	0.03758	0.03764
3p	0.11155	0.11123
4p	0.05094	0.05082
5p	0.02919	0.02914
3d	0.05594	0.05621
4d	0.03144	0.03160
5d	0.02011	0.02020

In the case of Na I we fitted the nine lowest eigenenergies to the term values of Risberg (1956). Table 3 compares experimental results with those obtained from

the resulting potential,

$$\begin{aligned}
 V_{\text{Na}} = V_{\text{HF}} &- \frac{0.4724}{r^4} [1 - \exp\{-r/1.0\}^6] \\
 &- \frac{3.18006}{r^6} [1 - \exp\{-(r/1.0)^8\}] \\
 &+ 0.162339 \exp(-r/1.0) - 0.034902 r \exp(-r/1.0).
 \end{aligned} \quad (28)$$

Lastly we fitted the five lowest eigenenergies of K I to the term values of

Table 4. K I eigenenergies

State	Experiment	Calculation
4s	0.15952	0.15933
5s	0.06371	0.06440
4p	0.10018	0.10019
5p	0.04691	0.04767
3d	0.06139	0.05686

Risberg (1956). Table 4 shows the results obtained with the potential,

$$\begin{aligned}
 V_{\text{K}} = V_{\text{HF}} &- \frac{2.6625}{r^4} [1 - \exp\{-(r/1.2)^6\}] \\
 &- \frac{2.05132}{r^6} [1 - \exp\{-(r/1.2)^8\}] \\
 &- 1.07925 \exp(-r/1.2) + 0.34469 r \exp(-r/1.2).
 \end{aligned} \quad (29)$$

The potentials (27), (28) and (29) have been constructed to reproduce the positions of low lying energy levels with great accuracy, an essential precondition if we are interested in atomic interactions. It is not immediately obvious that they can be used to predict other physical quantities, for example, photoionization cross sections. However Weisheit and Dalgarno (1971) have shown that for higher members of the Rydberg series the quantum defects calculated with the potentials given above are in most cases accurate to better than 1%.

5. Application to scattering data

We have applied the technique of § 3 to obtain pseudopotentials for elastic scattering of electrons by helium and neon in the low energy range below 10 eV. It will be shown that potentials obtained by fitting momentum transfer cross sections can be used with confidence to predict other scattering properties.

For helium we adopted the momentum transfer cross sections of Crompton *et al.* (1967). The resulting potential is

$$\begin{aligned}
 V_{\text{He}} = V_{\text{HF}} &- \frac{0.621}{r^4} [1 - \exp\{1 - (r/0.355)^6\}] \\
 &- \frac{1.1614}{r^6} [1 - \exp\{-(r/0.355)^8\}] \\
 &+ 10.0564 \exp(-r/0.355).
 \end{aligned} \quad (31)$$

Table 5 compares the experimental and fitted momentum transfer cross sections Q_m . The total cross section Q_t is also compared with the results of Golden and

Table 5. Helium cross sections

E (eV)	$Q_t(a_0^2)$ expt	Q_t calc	Q_m expt	Q_m calc
0.03	—	19.6	19.6	19.6
0.05	—	19.9	20.2	20.4
0.07	—	20.2	20.6	20.8
0.09	—	20.4	20.9	21.1
0.12	—	20.6	21.3	21.4
0.18	—	21.0	22.0	22.0
0.25	—	21.3	22.5	22.5
0.4	19.3	21.7	23.2	23.2
0.6	—	22.0	23.8	23.8
0.8	—	22.1	24.2	24.2
1.0	20.0	22.1	24.5	24.4
1.5	—	22.1	25.0	24.7
2.0	19.6	21.8	25.0	24.7
3.0	19.3	21.1	24.6	24.3
4.0	18.6	20.3	23.6	23.5
5.0	17.1	19.5	22.4	22.5

Total elastic cross sections Q_t (Golden and Bandel 1965) and momentum transfer cross sections Q_m (Crompton *et al.* 1967) are compared with those calculated from the potential (31)

Table 6. Helium phaseshifts

E (eV)	η_0 (AEP)	η_0 (PP)	η_1 (AEP)	η_1 (PP)
0.034	3.0812	3.0790	0.00075	0.00067
0.136	3.0170	3.0129	0.00306	0.00267
0.50	2.8945	2.8867	0.0118	0.00996
0.85	2.8156	2.8050	0.0204	0.0170
1.00	2.7869	2.7752	0.0242	0.0200
2.00	2.6371	2.6175	0.0497	0.0401
2.50	2.5783	2.5545	0.0625	0.0500
3.40	2.4878	2.4565	0.0845	0.0677
5.00	2.3590	2.3137	0.1213	0.0986
7.65	2.1979	2.1284	0.1729	0.1479
10.00	2.0877	1.9960	0.2094	0.1890

Comparison of phaseshifts calculated by the adiabatic exchange polarization (AEP) method of Callaway *et al.* (1968) and the present pseudopotential (PP) method.

Bandel (1965) which seem to lie a little below all the theoretical calculations. In table 6 we compare our phaseshifts with those calculated by Callaway *et al.* (1968) using their adiabatic exchange polarization method. The agreement is excellent. The most sensitive test of theory and experiment is provided by the angular distribution of scattered electrons. Results for three energies (3.1, 7.1, 11.1 eV) are shown in figure 1 together with measurements by Gibson and Dolder (1969). The shapes of the angular distributions agree fairly well.

At very low energies the s wave phaseshift is given by

$$(\eta_0 - \pi)/k = -1.210 + 35.4k^2. \quad (32)$$

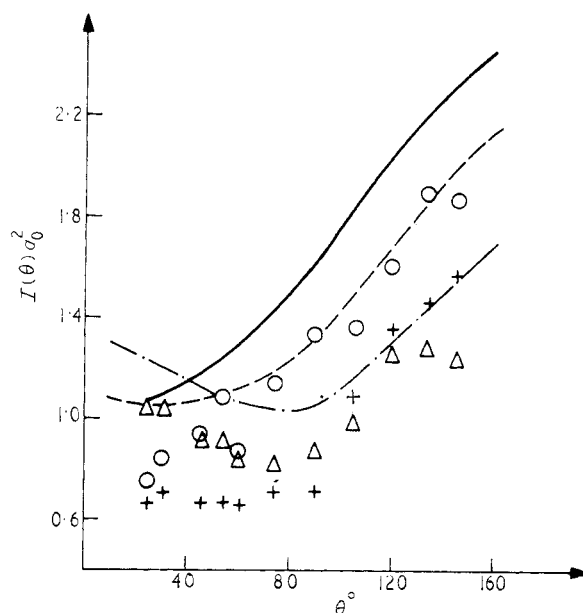


Figure 1. Angular distribution of scattered electrons in helium; ○, +, Δ measurements by Gibson and Dolder (1969) at 3.1, 7.1, 11.1 eV; —, — — —, — · — — calculations with model potential (31) at 3.1, 7.1, 11.1 eV.

The scattering length $A = -1.210$ is in excellent agreement with that obtained by other methods (cf Massey and Burhop 1969).

In the case of neon we used the momentum transfer cross sections of Gilardini and Brown (1957). The potential is

$$\begin{aligned}
 V_{\text{Ne}} = V_{\text{HF}} - \frac{1.181}{r^4} [1 - \exp\{-(r/0.9)^6\}] \\
 + \frac{0.22141}{r^6} [1 - \exp\{-(r/0.9)^8\}] \\
 - 0.76468 \exp(-r/0.9) + 0.087603 r \exp(-r/0.9). \quad (33)
 \end{aligned}$$

Table 7. Neon cross sections

E (eV)	$Q_t(a_0^2)$ expt	Q_t calc	Q_m expt	Q_m calc
0.0625	—	1.82	2.02	2.04
0.250	—	3.13	3.54	3.47
0.506	4.28	4.25	4.75	4.49
1.000	5.53	5.73	5.56	5.53
1.506	6.43	6.84	6.07	6.09
2.250	7.50	8.11	6.47	6.54
4.000	9.11	10.1	7.08	7.02
6.250	10.5	11.6	7.28	7.28
8.000	11.2	12.2	—	7.37
10.000	12.0	12.5	—	7.42

Experimental values of the total elastic cross section Q_t (Salop and Nakano 1970) and the momentum transfer cross section Q_m (Gilardini and Brown 1957) are compared with those calculated from the pseudopotential (33).

Table 7 shows the fitted momentum transfer cross sections Q_m together with total cross sections Q_t . The latter are in excellent agreement with the measurements of Salop and Nakano (1970). Table 8 demonstrates very close agreement between

Table 8. Neon phaseshifts

E (eV)	$\eta_0 - 2\pi$ (EP)	$\eta_0 - 2\pi$ (PP)	$\eta_1 - \pi$ (EP)	$\eta_1 - \pi$ (PP)
0.034	-0.0225	-0.0171	0.001	0.0010
0.136	-0.0533	-0.0438	0.002	0.0027
0.544	-0.132	-0.118	0.002	0.0029
1.224	-0.226	-0.213	-0.010	-0.0076
2.177	-0.328	-0.320	-0.033	-0.0315
3.401	-0.437	-0.434	-0.068	-0.0674
4.898	-0.548	-0.550	-0.111	-0.112
6.666	-0.660	-0.666	-0.158	-0.162
8.707	-0.771	-0.779	-0.210	-0.215
11.02	-0.880	-0.889	-0.263	-0.268
13.60	-0.986	-0.994	-0.318	-0.320

Phaseshifts calculated by the exchange polarization (EP) method of Thomson (1966) are compared with those calculated by the pseudopotential (PP) method.

the pseudopotential phaseshifts and those obtained from Thomson's (1966) exchange polarization calculation. In figure 2 we compare our predicted angular distributions at 1.15, 4.0 and 10.0 eV with the measurements of Ramsauer and Kollath (1932) which are rendered absolute using the values of $I(90^\circ)$. The agreement is not good, but improves slightly as the energy increases.

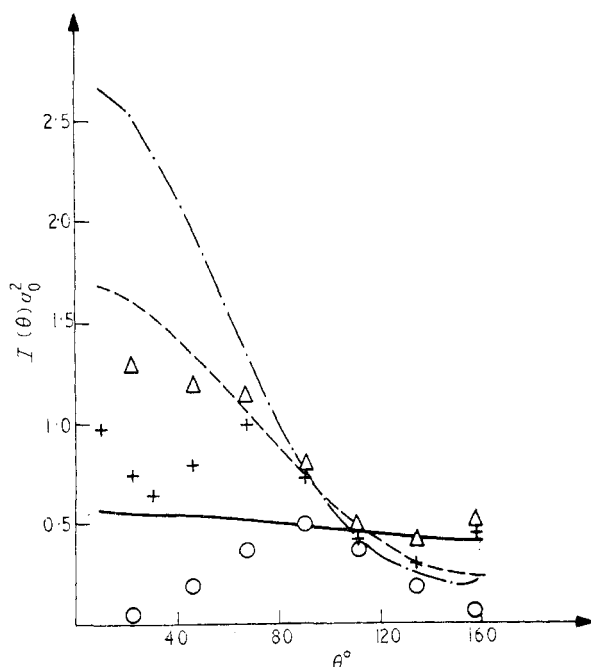


Figure 2. Angular distribution of scattered electrons in neon; \circ , $+$, \triangle measurements of Ramsauer and Kollath (1932) at 1.15, 4.0, 10.0 eV; —, — — —, — — — — calculations with model potential (33) at 1.15, 4.0, 10.0 eV.

The s wave phaseshift at very low energies is given by

$$(\eta_0 - 2\pi)/k = -0.2489 + 74.3 k^2. \quad (34)$$

The literature contains a wide range of values for the scattering length of neon (cf Massey and Burhop 1969). The present value of $A = -0.2489$ agrees with O'Malley (1963).

6. Conclusions

The procedures described above appear to provide a powerful means of investigating atomic properties and interpreting experimental data. It is hoped to extend the scattering calculations of § 5 to other systems, including molecules, in the near future.

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