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Model potential approach to elastic electron–helium scattering

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Abstract. Elastic scattering of electrons by helium atoms has been investigated using a model potential approach. The present model potential contains static, adiabatic polarisation and distortion potentials. A model exchange potential coupled with the orthogonality constraint for $l = 0$ has been employed to take account of the Pauli principle. The scattering parameters have been obtained in the energy range 2–19 eV. The present results are in good agreement with measured values and other theoretical estimates.

1. Introduction

The importance of low-energy electron–atom scattering data in different branches of physics is well known. Recently there has been a series of attempts by different workers to obtain scattering data either experimentally or theoretically in the low-energy region. The electron–helium system is the traditional proving ground of experimental and theoretical methods. Theoretically this is the simplest system after electron–hydrogen and one has to encounter first the basic difficulties that are embedded in the many-body problem. In other words, electron–helium scattering phenomena have taken the key position in the development of the quantum theory of scattering and many-body systems in general. In the last few years some good measurements of e^-–He low-energy scattering data have appeared (e.g. Golden and Bandel 1965, Andrick and Bitsch 1975, Kennerly and Bonham 1978, Williams 1979). Out of these measurements Andrick and Bitsch (1975) have given the results for the differential cross sections. A phaseshift analysis has been carried out by these authors and also by Williams (1979). Their results for the p- and d-wave phaseshifts differ by up to 10% including error bars in the overlapping energy region. There are some theoretical calculations (Callaway *et al* 1968, Burke *et al* 1969, Duxler *et al* 1971, Sinfailam and Nesbet 1972, Burke and Robb 1972) for e^-–He scattering in the low-energy region.

Here we have used a model (effective) potential method to calculate the e^-–He scattering data in the low-energy region. Apart from the short-range static potential, we have included the adiabatic and non-adiabatic polarisation potentials. The effect of the Pauli principle is also taken into account.

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The aim of this paper is not to suggest a better theoretical model than the existing ones but to demonstrate that this simple effective potential method predicts results that have been obtained by more sophisticated and rigorous calculations. This naturally encourages the testing of this method on more complex systems.

2. Theory

In the framework of the model (effective) potential scattering method the scattering equation can be written as

$$(T + V_{\text{eff}} - E + \varepsilon_0)F(r) = 0 \tag{1}$$

where T is the kinetic energy of the incident particle, V_{eff} is the effective potential, E the total energy of the system and ε_0 the binding energy of the atom in its ground state. It would be desirable if a way could be developed to incorporate the Pauli principle within the framework of the model potential method. Keeping this in mind we have introduced an inhomogeneous term (Lippman and Schey 1961, Valiron *et al* 1979) in equation (1) that reads

$$(T + V_{\text{eff}} - E + \varepsilon_0)F(r) = \lambda\phi_{1s} \tag{2}$$

where λ is an energy-dependent parameter and the helium ground-state wavefunction ϕ_{1s} is orthogonal to F, i.e.

$$\langle\phi_{1s}|F\rangle = 0. \tag{3}$$

This inhomogeneous term is similar to an exchange potential since it can be considered as equivalent to a non-local exchange operator operating on F.

After performing the partial-wave analysis equation (2) takes the form

$$\frac{d^2F_l}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} - 2V_{\text{eff}}\right)F_l = 2\lambda r\phi_{1s}\delta_{l0}. \tag{4}$$

One can see that for $l \geqslant 1$, equation (4) is purely homogeneous. In other words there is no orthogonality constraint for $l \geqslant 1$. This is not at all a desirable feature. There must be some other constraint consistent with the Pauli principle for $l \geqslant 1$. The simplest way is to take the exchange effect into account by including a local exchange potential for $l \geqslant 1$. Therefore we have to solve the following two equations

$$\frac{d^2F_l}{dr^2} + (k^2 + 2V_{\text{eff}})F_l = 2\lambda r\phi_{1s} \qquad l = 0 \tag{5}$$

$$\frac{d^2F_l}{dr^2} + (k^2 - 2V_{\text{eff}} - 2V_{\text{ex}})F_l = 0 \qquad l \geqslant 1 \tag{6}$$

where V_{ex} is the local exchange potential. Our effective potential V_{eff} is of the form

$$V_{\text{eff}} = V_s + V_p + V_d. \tag{7}$$

Here V_s is the static potential, obtained by using the helium ground-state wavefunction due to Roothaan *et al* (1960). The polarisation potential, V_p, consists of the sum of the first three multipole components ($l = 0, 1, 2$) of the adiabatic polarisation potentials while V_d is the distortion potential. This potential arises from the action of the kinetic energy operator of the scattered particle on the perturbed wavefunction. Our V_p and

V_d are identical to those of Callaway *et al* (1968). Hara (1967) has suggested an exchange potential using the free electron gas model which is of the form

$$V_{ex} = -2e^2\pi^{-1}k_F F(\eta) \tag{8}$$

where

$$F(\eta) = \frac{1}{2} + \frac{1-\eta^2}{4\eta}\ln\left(\frac{1+\eta}{1-\eta}\right) \tag{9}$$

and

$$\eta = k/k_F \quad \text{with} \quad k_F = (3\pi^2\rho(r))^{1/3} \tag{10}$$

and

$$k^2 = 2m(E+I)\hbar^{-2} + k_F^2. \tag{11}$$

Here I is the ionisation energy. This potential is less attractive than the desired one. k_F is the maximum momentum, corresponding to the surface of the Fermi sphere, in momentum space, k is the momentum of the electron considered, m is the mass of the electron and ρ is the total electron density. Hara's model is incorrect for large r. Asymptotically the electron energy tends to $\frac{1}{2}k^2 + I$ instead of $\frac{1}{2}k^2$. To have the correct asymptotic electron energy Riley and Truhlar (1975) have suggested the following form of equation (11)

$$k^2 = 2mE\hbar^{-2} + k_F^2.$$

This modification makes the potential more attractive at small separations than the desired one. We have used the exchange potential in which k^2 is redefined as

$$k^2 = \frac{2m}{\hbar^2}\left(E + \frac{I}{1+E}\right) + k_F^2.$$

One can see that our model exchange potential tends to that of Hara (1967) for small separations and to that of Riley and Truhlar (1975) asymptotically.

3. Validity of the proposed exchange potential

In order to examine the validity of our exchange potential we have considered the problem of e^-–He scattering. We have solved the following differential equation for e^-–He scattering

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V_s(r) + 2V_{ex}(r) + k_l^2\right) u_l(r) = 0$$

where $V_s(r)$ is the static potential as used by Riley and Truhlar (1975) and V_{ex} is the exchange potential given by equation (8). The s-, p- and d-wave phaseshifts for three different model exchange potentials are displayed in tables 1, 2 and 3, respectively, along with the corresponding exact static and static exchange results. It is evident from these tables that our phaseshifts nearly coincide with those of Hara (1967) at low energies and with those of Riley and Truhlar (1975) at comparatively higher energies. The present results also show that the potential used accounts for the exchange effect very satisfactorily.

Table 1. Electron–helium partial-wave phaseshifts (in radians) for $l = 0$.

Energy (eV)	k_0 (a_0^{-1})	Static	Exchange	Riley and Truhlar (1975)	Hara (1967)	Present
1.33	0.3	2.050	2.705	2.731	2.607	2.638
3.4	0.5	1.761	2.436	2.442	2.304	2.348
13.6	1.0	1.405	1.890	1.867	1.769	1.816
21.26	1.25	1.296	1.687	1.662	1.589	1.629
41.67	1.75	1.137	1.388	1.371	1.331	1.357
217.68	4.00	0.782		0.832	0.829	0.830

Table 2. Electron–helium partial-wave phaseshifts (in radians) for $l = 1$.

Energy (eV)	k (a_0^{-1})	Static	Exchange	AAFEGE†	HFEG†	Present
1.22	0.3	0.00242	0.0106	0.0268	0.00565	0.0071098
3.4	0.5	0.0104	0.0425	0.0680	0.0233	0.0295
13.60	1.0	0.0605	0.183	0.178	0.116	0.1397
21.26	1.25	0.0959	0.243	0.221	0.167	0.1945
41.67	1.75	0.166	0.3105	0.279	0.247	0.268
217.68	4.00	0.300		0.337	0.334	0.3367

† As quoted by Riley and Truhlar (1975).

Table 3. Electron-helium partial-wave phaseshifts (in radians) for $l = 2$.

Energy (eV)	k (a_0^{-1})	Static	Exchange	AAFEGE	HFEGE	Present
1.22	0.3	0.000 02	0.000 09	0.000 431	0.000 0603	0.000 0768
3.4	0.5	0.000 26	0.000 92	0.002 43	0.000 648	0.000 857
13.6	1.00	0.005 11	0.013 6	0.017 9	0.010 4	0.013 09
21.26	1.25	0.011 41	0.026 6	0.030 1	0.021 1	0.025 4
41.67	1.75	0.031 4	0.057 9	0.058 1	0.049 4	0.055 25
217.68	4.00	0.130 3		0.150	0.148	0.150 05

4. Results and discussions

Tables 4, 5 and 6 contain the present results for s-, p- and d-wave phaseshifts respectively, up to the incident energy 20 eV. The corresponding values of Andrick and Bitsch (1975) and Williams (1979) are also tabulated. The calculated phaseshifts due to Duxler *et al* (1971) and Sinfailam and Nesbet (1972) are also given for comparison. Figure 1 shows the s- and p-wave phaseshifts along with the corresponding experimental values. Our s-wave phaseshifts in the energy range given are in close agreement with the measured values. In the case of p-wave phaseshifts our results agree well with the corresponding theoretical and experimental values up to 13.6 eV. Our d-wave phaseshifts are in fair agreement with the theoretical prediction of Sinfailam and Nesbet

Table 4. s-wave phaseshifts for e^-–He scattering.

E (eV)	$k(a_0^{-1})$	Present	Williams (1979)	Andrick and Bitsch (1975)	Duxler *et al* (1971)	Sinfailam and Nesbet (1972)
1.23	0.3	2.752	2.745		2.7546	2.7459
2.0		2.6175		2.616		
2.176	0.4	2.265	2.613		2.6223	2.6142
3.4	0.5	2.472	2.464		2.4942	2.4836
4.91	0.6	2.356	2.332		2.3719	2.3638
5.0		2.3354	2.322†	2.323		
6.6	0.7	2.235	2.207		2.2564	2.2518
8.0	0.767	2.1532	2.134			
8.71	0.8	2.123	2.098		2.1479	2.0956
10.0	0.857	2.052	2.036			
12.0		1.977	1.968	1.985		
13.6	1.0	1.946			1.9530	1.89
16.0	1.085	1.876	1.857			
18.0	1.15	1.838	1.815			
19.0	1.18	1.8296	1.800	1.814		
20.0	1.21	1.801	1.784			

† This result is at 5.02.

Table 5. p-wave phaseshifts for e^-–He scattering.

E (eV)	$k(a_0^{-1})$	Present	Williams (1979)	Andrick and Bitsch (1975)	Duxler *et al* (1971)	Sinfailam and Nesbet (1972)
1.23	0.3007	0.0282	0.035		0.0327	0.0297
2.00		0.0487		0.052		
2.176	0.400	0.05374	0.060		0.0594	0.0539
3.40	0.500	0.0880	0.093		0.0926	0.0847
4.91	0.6008	0.1276	0.127		0.1302	0.1200
5.00		0.1298		0.135		
5.02			0.129			
6.66	0.700	0.1666	0.161		0.1696	0.1567
8.00	0.767	0.1913	0.186			
8.71	0.8002	0.2027	0.196			
10.0	0.857	0.2210	0.216			
12.0		0.2440	0.242	0.259		
13.0	0.978	0.2535	0.254			
13.6	1.0	0.2611			0.2749	0.2646
16.0	1.085	0.2761	0.289			
16.46					0.3016	0.2927
18.0	1.15	0.2873	0.305			
19.0	1.18	0.2920	0.311	0.325		
20.0	1.21	0.2962	0.315			

(1972) at low energies. Williams (1979) has claimed that the error in the d-wave phaseshift is 8%. Taking this into account one can see that our results lie within the experimental limit from 10 eV and onwards.

Table 6. d-wave phaseshifts for e^-–He scattering.

E (eV)	$k(a_0^{-1})$	Present	Williams (1979)	Duxler *et al* (1971)	Sinfailam and Nesbet (1972)
1.23	0.3007	0.0036	0.0031	0.00405	0.0036
2.0		0.0060			
2.176	0.4	0.0066	0.0056	0.00727	0.0064
3.40	0.5	0.0107	0.0087	0.0115	0.0097
4.91	0.6	0.0163	0.0132	0.0167	0.0141
5.00		0.0166			
5.02			0.0136		
6.66	0.7	0.0228	0.0188	0.0228	0.0197
8.00	0.76	0.0278	0.0228		
8.71	0.8002	0.0304			
10.0	0.857	0.0351	0.0302		
12.0		0.0422	0.0372		
13.6	1.0	0.0474		0.0458	0.0393
16.0	1.085	0.0553	0.0501		
18.0	1.15	0.0613	0.0556		
19.0	1.18	0.0642	0.0580		
20.0	1.21	0.0669	0.0602		

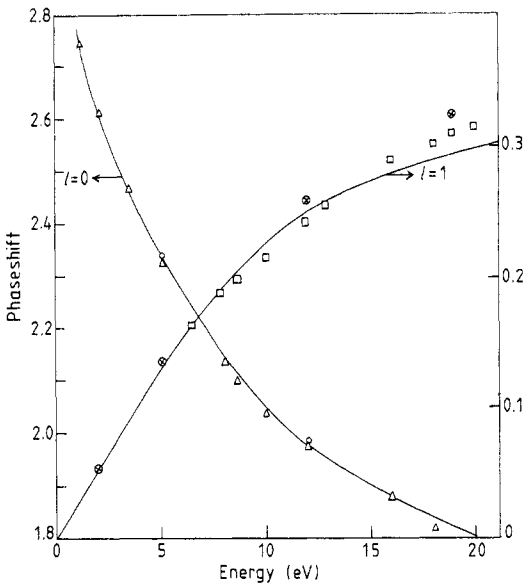

Figure 1. Phaseshifts for $l = 0$: ○, Andrick and Bitsch (1975); △, Williams (1979); ——, present calculations. Phaseshifts for $l = 1$: ⊗, Andrick and Bitsch (1975); □, Williams (1979); ——, present calculations.

In figure 2 we have presented our results for differential cross sections at four energies. The curves of Andrick and Bitsch (1975) are also shown in the same figure for comparison. The difference between the two sets of results is covered by the error limits

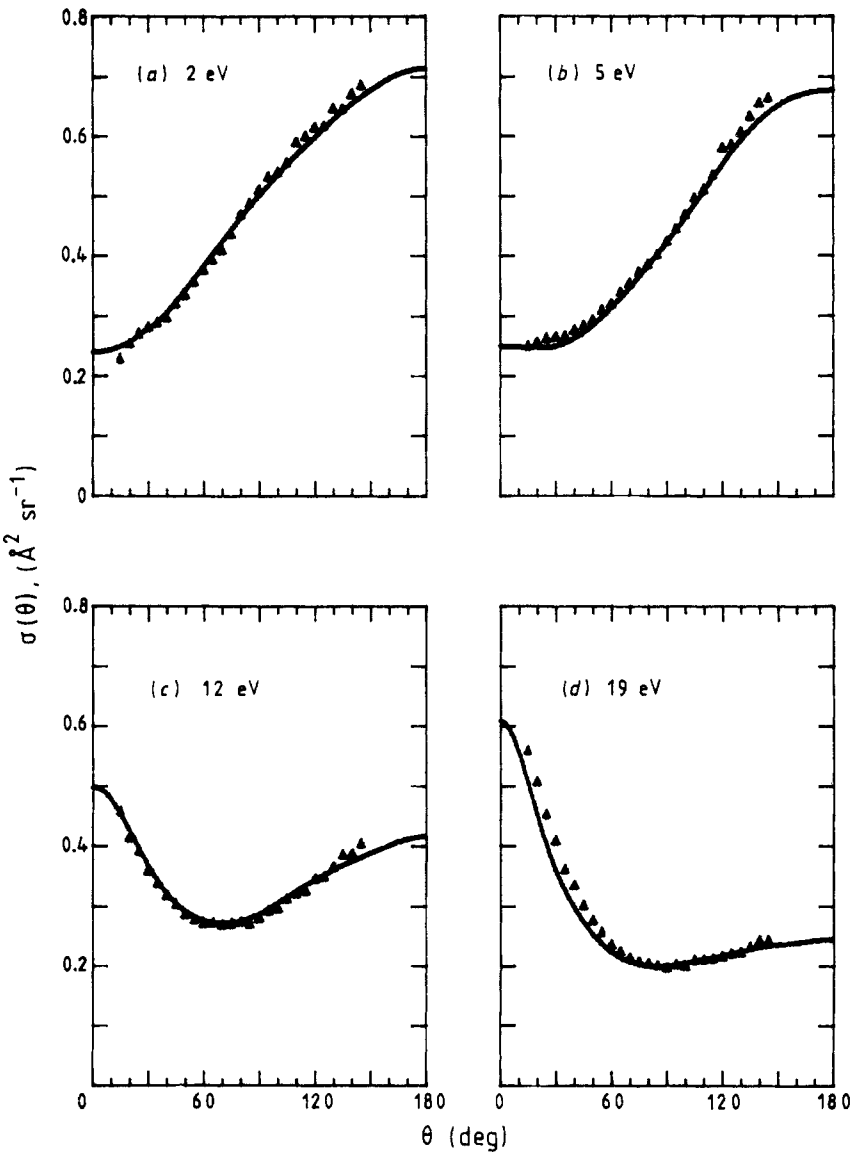

Figure 2. Differential cross sections for e^-–He scattering ($Å^2\,sr^{-1}$) Andrick and Bitsch (1975): ——, present calculations. The collision energies are (*a*) 2 eV, (*b*) 5 eV, (*c*) 12 eV and (*d*) 19 eV.

of the measured values. In table 7 we have given our results for total cross sections up to 20 eV along with the measured values of Andrick and Bitsch (1975) and Kennerly and Bonham (1978). At the highest energy the total cross section is obtained by taking the contribution up to $l = 6$. Our results always lie in between the two sets of measured values.

The effect of exchange is expected to influence the s- and d-wave phaseshifts. Considering the agreement between our results and more sophisticated theoretical predictions we conclude that our model exchange potential, along with the ortho-

Table 7. Total cross section for e^-–He scattering (up to $l = 6$).

E (eV)	Present	Kennerly and Bonham (1978)	Andrick and Bitsch (1975)
2.0	6.17	6.06	6.20
5.0	5.48	5.25	5.64
8.0	4.92	4.64	
10.0	4.455	4.30	
12.0	4.10	3.96	4.15
16.0	3.43	3.43	
19.0	3.04		3.19
20.0	2.94	3.03	

gonality constraints for the s wave, is a reasonably good choice. The present simple model, which can be extended to more complex atoms very easily, is reliable in predicting the scattering parameter at low incident energies. We hasten to add that one should be careful in choosing the potential of the system.

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