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Relativistic two-channel theory of elastic electron–atom scattering and application to He and Ne

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Abstract. Within the frame of relativistic Hartree–Fock theory, a two-channel model is proposed for the elastic scattering of electrons (in the energy range 10–200 eV) from noble-gas atoms. The coupling between the two channels is described by a dipole potential obtained from a charge polarisation potential of the Temkin type. Numerical results have been obtained for the differential and total scattering cross sections from He and Ne. We find excellent agreement with recent experimental data. Further, we compare our results with those from a one-pseudo-state calculation, from calculations using various local potential models and from one-channel relativistic Hartree–Fock calculations.

1. Introduction

In previous work on relativistic elastic scattering of slow electrons from Ar, Kr and Xe atoms (Kemper *et al* 1983, Awe *et al* 1983), in which we employed various effective local potential models, we concluded that in the energy range below 100 eV a more sophisticated treatment of exchange, charge polarisation and inelastic processes was required in order to improve, with respect to experimental data, the agreement of the differential cross section (intensity I) and the spin polarisation (P) as functions of the scattering angle (θ).

In principle, a most powerful approach is offered by relativistic multi-channel close-coupling theory. (For reviews on the non-relativistic theory see e.g. Callaway (1980) and Nesbet (1980); an analogous relativistic formulation has been given by Carse and Walker (1973)). However, calculations using such theory are, for larger target atoms, beyond the reach of present-day computing facilities. We therefore decided to explore an 'intermediate way', which consists of a two-channel close-coupling model based on relativistic Hartree–Fock (RHF) theory (for reviews on the latter see e.g. Grant (1970) and Walker (1971)), in which the channels are linked by a charge polarisation potential of the Temkin (1957) type. Our model thus incorporates dynamic charge polarisation, non-local exchange and inelastic scattering as well as relativistic effects.

While the goal of our theory is eventually the treatment of electron scattering from heavier atoms, an initial application to He and Ne appears useful as a test for the adequacy of the model and for the absence of errors in the computer code. Although relativistic effects are negligible for these light elements, a relativistic treatment of e–Ne scattering is further of interest in view of resolving a discrepancy, which was found

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between non-relativistic theory (Fon and Berrington 1981) and experiment with regard to an absolute minimum in the differential cross section.

In § 2, we put forward a relativistic Hartree–Fock two-channel theory for the elastic scattering of slow electrons from noble-gas atoms. Numerical results for differential and total cross sections from He and Ne atoms are, in § 3, presented and compared with experimental data and with other theoretical results. In particular, we make contact with recent theoretical work of Fritsche *et al* (1984), in which an appealing first-principles approach for the construction of a local exchange potential was proposed.

2. Theory

Our work is based on the relativistic close-coupling formalism, which was introduced by Carse and Walker (1973) and re-derived for the present study by means of the Hulthén–Kohn variational principle in analogy to the usual non-relativistic derivation (cf e.g. Burke 1969). Denoting by P/r and Q/r the 'large' and the 'small' components of the radial parts of the one-electron central-field spinors (see e.g. Grant 1970), the coupled integro-differential equations for the radial functions P_i, Q_i, where $i = 1, \ldots, N$ enumerates the energetically different channels taken into account, are (in atomic units $\hbar = 1$, $m_e = 1$, $e = 1$):

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa_i}{r}\right)P_i+\left[2c+\frac{1}{c}\left(\frac{Z}{r}+E_i\right)\right]Q_i=\frac{1}{c}\sum_j\left(V_{ij}Q_j+W_{ij}^{Q}+\sum_{A_j}\lambda_{ij}Q_{A_j}\right)$$

and (1)

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa_i}{r}\right)Q_i-\frac{1}{c}\left(\frac{Z}{r}+E_i\right)P_i=\left(-\frac{1}{c}\right)\sum_j\left(V_{ij}P_j+W_{ij}^{P}+\sum_{A_j}\lambda_{ij}P_{A_j}\right)$$

with $i, j = 1, \ldots, N$, where Z is the charge of the (point-like) nucleus and E_i the energy in the ith channel; the quantum numbers κ_i are related to the orbital and total angular momentum quantum numbers l_i and j_i by

$$j_i = |\kappa_i| - 1/2 \qquad l_2 = j_2 + \mathrm{sign}(\kappa_i)/2. \tag{2}$$

Within each channel, κ_i generally assumes several values corresponding to different coupled subchannels of the same energy E_i; the Lagrange multipliers λ_{ij} are determined such that the scattering states are orthogonal to the bound ones for the same values of the quantum numbers κ_i. Further, in equation (1) the direct potentials V are given as

$$V_{ij}(r)=\frac{1}{r}\sum_{A_iA_j}\sum_k c_k(S_iS_jA_jA_i)\,Y_k(A_i, A_j; r) \tag{3a}$$

and the exchange potentials $W^{P,Q}$ as

$$W_{ij}^{P,Q}(r)=\left(-\frac{1}{r}\right)\sum_{A_iA_j}\sum_k c_k(S_iA_jS_jA_i)\,Y_k(S_j, A_i; r)(P_{A_j}\text{ or }Q_{A_j}) \tag{3b}$$

with

$$Y_k(\alpha, \beta; r)=r\int_0^\infty \mathrm{d}s\; U_k(r, s)(P_\alpha(s)P_\beta(s)+Q_\alpha(s)Q_\beta(s)) \tag{4a}$$

$$U_k(r, s) = \begin{cases} r^k/s^{k+1} & \text{if } r \leqslant s \\ s^k/r^{k+1} & \text{if } r > s \end{cases} \tag{4b}$$

and

$$c_k(\alpha\beta\gamma\delta) = d^k(\alpha\,;\beta)d^k(\gamma\,;\delta)\delta(m_\alpha + m_\delta,\, m_\beta + m_\gamma) \tag{4c}$$

$$\begin{aligned} d^k(\alpha\,;\beta) &= d^k(j_\alpha m_\alpha\,;j_\beta m_\beta) \\ &= (-1)^{m_\alpha+1/2}[(2j_\alpha+1)(2j_\beta+1)]^{1/2}(2k+1)^{-1} \\ &\quad \times C(j_\alpha j_\beta k;\tfrac{1}{2},-\tfrac{1}{2})C(j_\alpha j_\beta k;-m_\alpha, m_\beta) \end{aligned} \tag{4d}$$

where A and S denote the sets of quantum numbers which define completely a one-electron bound or scattering state respectively; $C(abc;\, d,\, e)$ are Clebsch–Gordan coefficients (in the notation of Rose (1961)).

For closed-shell target atoms, the ground-state wavefunctions P_{A_1} and Q_{A_1} can be calculated by means of a relativistic Hartree–Fock method (Desclaux 1975). The first-channel potentials V_{11} and $W_{11}^{P,Q}$ are then readily obtained by numerical integration. Specialising equation (3*a*) to the closed-shell atoms under consideration we have

$$V_{11} = \left(-\frac{1}{r}\right)\sum_A q_A Y_0(A, A; r), \tag{5a}$$

where $q_A = 2j_A + 1$ is the occupation number of the target subshell A. For the exchange term W_{11} we obtain from equation (3*b*)

$$W_{11}^{P,Q}(r) = \left(-\frac{1}{r}\right)\sum_A \sum_k \tfrac{1}{2} q_A \Gamma_{j_A k j_s} Y_k(A, S; r)(P_A \text{ or } Q_A) \tag{5b}$$

where

$$\Gamma_{j_A k j_S} = \frac{2}{2k+1}[C(j_A j_S k;\tfrac{1}{2},-\tfrac{1}{2})]^2. \tag{5c}$$

However, for the channels involving an excited target atom, the energies E_i and wavefunctions P_{A_i} and Q_{A_i} are more difficult to come by, and so, therefore, are the potentials V_{ij} and $W_{ij}^{P,Q}$ (with $(i, j) \neq (1, 1)$), especially for large-Z atoms. We therefore adopt a two-channel model, in which the second channel is a 'pseudo-channel' (i.e. does not contain an eigenstate of the target), chosen so as to mimic the elastic scattering properties of the multichannel model. For the still unknown direct potentials $V_{12} = V_{21}$ and V_{22} and for E_2 and κ_2 we follow a plausible choice proposed by Onda and Truhlar (1980) in the context of a Schrödinger-equation-based local-potential theory:

$$V_{22} = V_{11} \tag{6a}$$

$$V_{12} = V_{21} = (|V^{\mathrm{Pa}}(r)\Delta E|)^{1/2} \tag{6b}$$

$$E_2 = E_1 - \Delta E \tag{6c}$$

and

$$\kappa_1 = \kappa_2 = \kappa \tag{6d}$$

where V^{Pa} is an adiabatic polarisation potential and ΔE an average excitation energy.

In contrast to Onda and Truhlar (1980) we calculated V^{Pa} within the Temkin approximation (Temkin 1957) along the lines of Walker (1970). The average excitation energy was obtained via Koopmans' theorem (1933) from RHF calculations (using the program of Desclaux 1975).

Having only knowledge of the target-atom ground state, the exchange potentials W_{22}, $W_{12} = W_{21}$ are still unknown. However, these quantities are, depending on the size of the target atom as well as on the energy of the incident electron, relatively small in comparison with the direct potentials. Further, $W_{12} = W_{21}$ will be much smaller than W_{22}, because the overlap of the orbitals, and thus the exchange effect between them, decreases, if the orbitals become more delocalised and diffuse, because of the charge polarisation effect. Since the unknown 'pseudo-channel' is to describe a dipole transition from the target's ground state, it has to account for an increased long-range behaviour as well as for a decay, in the vicinity of the nucleus, of the exchange potentials. The potentials W_{ij} (with $i, j \neq 1, 1$) are therefore certainly different from W_{11}. Also, a simple scaling, like $W_{ij} = \beta_{ij} W_{11}$ with $0 < \beta_{ij} < 1$, is not adequate. In the absence of quantitative knowledge, we therefore took, in the present work, the choice

$$W_{22} = W_{12} = W_{21} = 0. \tag{7}$$

For impact energies below the first ionisation energies (He: ~25 eV and Ne: ~23 eV, as obtained via Koopmans' theorem) our RHF two-channel model (RHFT) is not applicable, since there is no second open channel. Therefore, in this energy range, we performed calculations using a RHF one-channel model (RHFO), including a Temkin-type adiabatic polarisation potential (Walker 1970). Theoretically, this model for the description of 'closed channels', is founded on the adiabatic (i.e. low energy) limit of the close-coupling equations (e.g. Burke 1969). Our results (cf figure 2(*a*), this work) confirm that, in comparison with experimental data, this model is suited excellently to describe scattering processes below the first ionisation threshold.

Finally, in this section, we comment on numerical features of our calculations. The two-channel version of equation (1), (i.e.: $i, j = 1, 2$) is solved as follows: two linearly independent solutions of the system (1), which are regular at the origin, are constructed by the generalisation of a method, described by Allison (1970), to our case of four coupled first-order equations, using a five-point Adams predictor–corrector algorithm (Hildebrand 1974). The reaction matrices, and from these the intensities, are obtained by matching one of the wavefunctions, P or Q calculated by outward integration (both result in the same reaction matrix) with their analytical asymptotic forms in terms of spherical Bessel and Neumann functions.

3. Results and discussion

Using the two-channel (RHFT)—and below the first ionisation threshold, the one-channel (RHFO)—approximation including a Temkin-type charge polarisation potential, we calculated the differential and total cross sections for the relativistic scattering of electrons from the noble-gas atoms He and Ne in the energy range 10–200 eV. In the following, the intensities are given in units of $a_0^2\,\mathrm{sr}^{-1}$, where a_0 is the Bohr radius.

3.1. Helium

In figure 1 we present three of our own calculations in comparison with a non-relativistic ^{1}P pseudo-state calculation (Fon and Berrington 1981) which, like our RHFT model, considers only the dominating dipole term in the charge polarisation of the target, with experimental data. The overall excellent to good agreement of our and Fon's calculations with the experimental data indicates that our relatively simple model

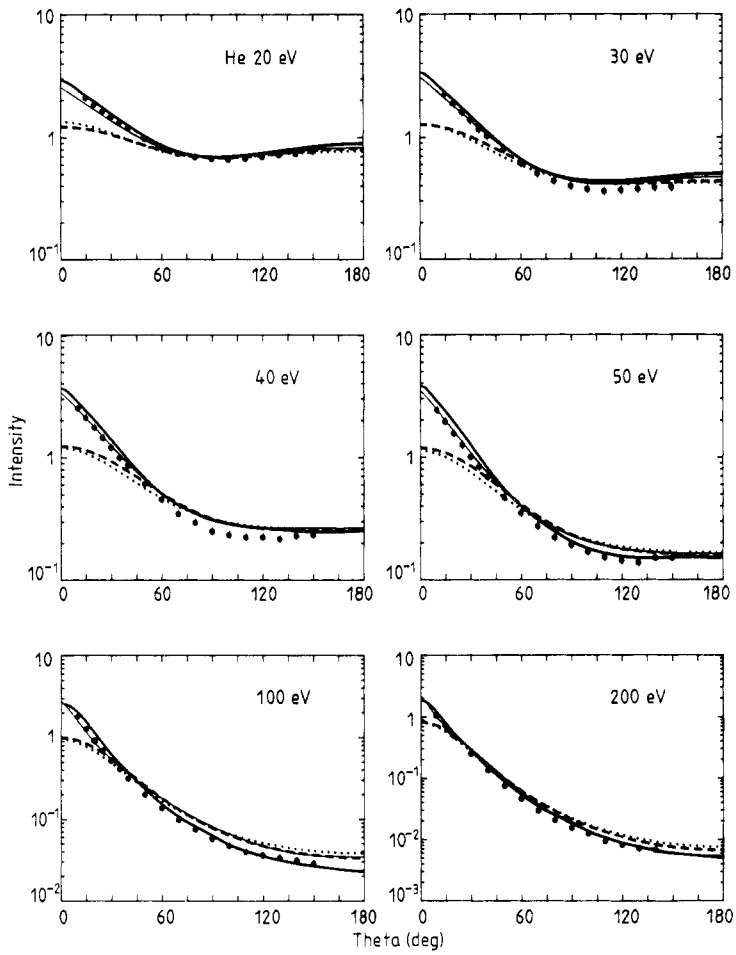

Figure 1. Thick full curve, our RHFT model (i.e. RHFO plus Temkin-type polarisation potential at 20 eV); broken curve, RHFO, present calculations; dotted curve, RLDA, present calculations; fine full curve, Fon and Berrington (1981); experiment: ●, Register *et al* (1980) (including error bars).

accounts well for the dipole selection rule (not included explicitly into our model) and also for exchange effects. Both of our one-channel calculations (RHFO and RLDA following Slater *et al* 1969), are shown to demonstrate the effect of the absence of long-range forces (charge polarisation) in these models. In the low-angle (i.e. forward) scattering regime, only calculations including long-range forces show an excellent agreement with the data. At 50 and 100 eV, the superiority of our RHFT model to the calculations of Fon and Berrington (1981) indicates that our method accounts in a better way for the influences of inelastic effects on the elastic channel. In tables 1–3 the total cross sections obtained from our calculations are displayed together with other theoretical results and with experimental and semiempirical data as well.

From table 1 we find that, for the total elastic cross sections for e^-/He-scattering, the theoretical values of Fon and Berrington (1981) show the best agreement with the experimental data. Considering tables 2 and 3 (i.e. for σ_{abs} and σ_{tot} respectively), we find the results of our own calculations in best agreement with the experiments.

Table 1. Values for the total *elastic* cross section (σ_{el}) for e^-–He scattering (in a_0^2).

	Theory					Experiment	
	Present calculations			Fon and Berrington (1981)	Onda and Truhlar (1980)	Register *et al* (1980)	de Heer and Jansen (1977)
E (eV)	RLDA	RHFO	RHFT				
20	11.45	11.36	11.35	10.81	11.62†	10.71	10.52
30	6.86	7.07	8.59	7.98	8.97	7.45	7.99
40	5.16	5.40	6.66	6.19	—	5.64	6.00
50	4.08	4.31	5.26	4.93	5.52	4.50	4.94
100	1.91	2.01	2.30	2.17	2.47	2.00	2.18
200	0.88	0.91	0.99	0.97	1.07	0.89	0.98

† Value for 19 eV.

Table 2. Values for the total *inelastic* cross sections (σ_{abs}) for e^-–He scattering (in a_0^2).

	Theory		Experiment
E (eV)	RHFT (this work)	Onda and Truhlar (1980)	de Heer and Jansen (1977)
30	0.79	0.99	0.81
40	1.03	—	1.27
50	1.63	2.13	1.52
100	2.01	2.47	1.89
200	1.15	1.98	1.65

Table 3. Values for the *total* cross sections (σ_{tot}) for e^-–He scattering (in a_0^2).

	Theory		Experiment	
E (eV)	RHFT (this work)	Onda and Truhlar (1980)	de Heer and Jansen (1977)	Register *et al* (1980)
30	8.78	9.96	8.79	8.36
40	7.69	—	7.27	6.93
50	6.89	7.65	6.47	6.04
100	4.31	4.93	4.07	3.89
200	2.14	3.05	2.63	2.53

3.2. Neon

For the case of e–Ne scattering, we first compare different theoretical results with experimental data (cf figures 2(*a*) and (*b*)). With regard to one of these calculations (McCarthy *et al* 1977) we mention that for the real part of the optical potential an adiabatic polarisation potential (Temkin and Lamkin 1961) and, above the first ionisation threshold, for the imaginary part a phenomenological absorption (Furness and McCarthy 1973), was used. Although this model is based on a completely different

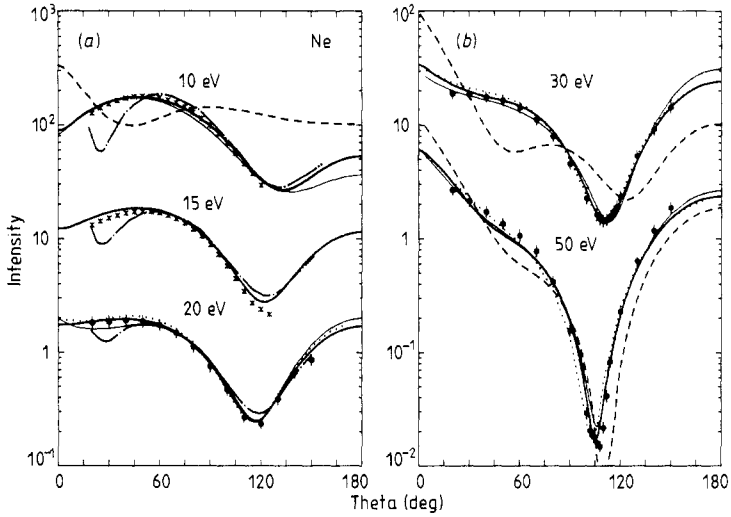

Figure 2. Calculations: thick full curve, our RHFT model (i.e. RHFO plus Temkin-type polarisation potential in figure 2(*a*)); thin full curve, Fon and Berrington (1981); broken curve, Thirumalai and Truhlar (1982b); dotted curve, McCarthy *et al* (1977); chain curve, Fritsche *et al* (1984) (in figure 2(*a*)). Experiments (including error bars): ⧗, Brewer *et al* (1981); ●, Williams and Crowe (1975).

description of the scattering process (in comparison with a two-channel theory), it yields an overall good agreement with the experimental data and with our RHFT model as well. The agreement of other two-channel calculations (Thirumalai and Truhlar 1982b) and of other local exchange (one-channel) calculations (Fritsche *et al* 1984) with the experiment is less satisfactory (especially with respect to forward scattering).

In figure 3 the results of three of our calculations, for 20–200 eV, are plotted in comparison with an (absolute) experiment. Unlike the He atom (figure 1), we conclude that now charge polarisation effects (for small scattering angles) play a less dominant role. Also, in contrast to the He case study, we find a pronounced minimum in the intensity near the scattering angle of 100°. Since such absolute minima are associated with extreme spin polarisation values changing from +100% to −100% within 0.1° (cf Bühring 1968), we performed calculations of the spin polarisation. Our results confirm the above correlation, and we used the ±100% P maxima to locate more precisely the position of the absolute intensity minimum. Table 4 shows our results in comparison with a non-relativistic calculation (Fon and Berrington 1981) together with experimental data. We find a striking agreement of our relativistic calculations (excluding the RLDA approach) with the non-relativistic ones. In contrast to Fon and Berrington (1981), we therefore conclude that the discrepancy between theory and experiment (concerning the location of this absolute minimum in I on the energy scale) is not a relativistic effect (as was suggested by Fon and Berrington 1981), but must have other, perhaps experimental, reasons.

Finally, in tables 5–7 we compare theoretical total cross section results with each other and with experimental data. In table 5 we find a fair agreement between experiments and theories (except for the calculation of Thirumalai and Truhlar 1982b). With respect to the experiments, our RHFT model yields good results (cf tables 6 and 7).

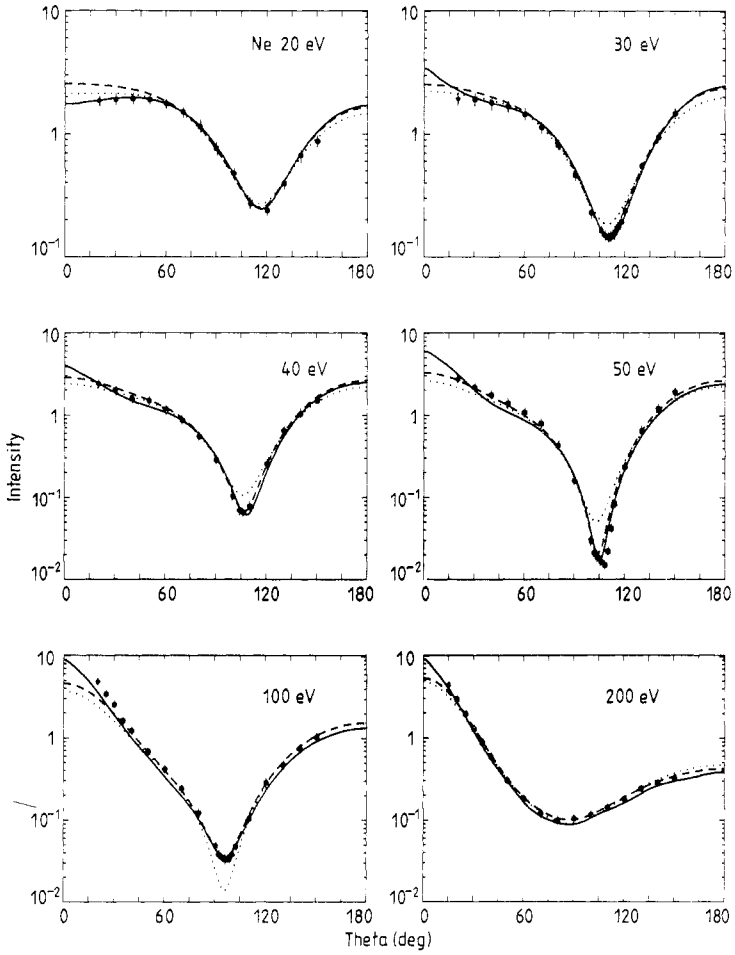

Figure 3. Full curve, our RHFT model (i.e. RHFO plus Temkin-type polarisation potential at 20 eV); broken curve, RHFO, present calculations; dotted curve, RLDA, present calculation; Experiment: ●, Williams and Crowe (1975) (including error bars).

Table 4. Position of complete spin polarisation and minimal intensity for the elastic e^-–Ne scattering.

	Theory				
	Present calculations			Fon and Berrington (1981)	Experiment Kollath and Lucas (1979)
	RLDA	RHFO	RHFT		
E (eV)	77.8	65.5	64.5	64	73
θ (deg)	97.8	101.25	102.5	103.6	103

Table 5. Values for the total *elastic* cross sections (σ_{el}) for e^-–Ne scattering (in a_0^2).

	Theory					Experiment	
	Present calculations			Fon and Berrington	Thirumalai and Truhlar	Williams and Crowe	de Heer *et al*
E (eV)	RLDA	RHFO	RHFT	(1981)	(1982b)	(1975)	(1979)
20	12.43	13.37	13.00	13.48	—	13.40	12.30
30	12.49	13.32	12.94	12.70	9.27	12.34	11.32
40	11.18	12.16	12.90	11.82	—	11.68	10.71
50	10.10	11.18	11.52	11.02	9.93	11.79	10.82
100	7.09	7.94	8.04	8.04	7.34	9.82	8.74
200	4.86	5.17	5.11	5.18	4.72†	5.64	4.99

† Thirumalai and Truhlar (1982a).

Table 6. Values for the total *inelastic* cross sections (σ_{abs}) for e^-–Ne scattering (in a_0^2).

	Theory		Experiment
E (eV)	RHFT (this work)	Thirumalai and Truhlar (1982b)	de Heer *et al* (1979)
30	0.66	2.13	0.75
40	1.06	—	1.35
50	1.80	3.40	1.85
100	2.34	3.85	2.92
200	1.38	3.23†	2.99

† Thirumalai and Truhlar (1982a).

Table 7. Values for the *total* cross sections (σ_{tot}) for e^-–Ne scattering (in a_0^2).

	Theory		Experiment		
E (eV)	RHFT (this work)	Thirumalai and Truhlar (1982b)	de Heer *et al* (1979)	Kaupilla *et al* (1981)	Wagenaar and de Heer (1980)
30	13.60	11.4	12.7	13.3	13.72
40	13.96	—	12.06	—	13.44
50	13.32	13.3	12.67	12.7	13.06
100	10.38	11.2	11.66	10.6	11.03
200	6.49	7.95†	7.98	7.08	8.45

† Thirumalai and Truhlar (1982a).

4. Conclusion and outlook

In conclusion, we would like to point out that the success of our relatively simple RHFT model especially in application to (closed-shell) systems of low electron numbers, is plausible for the following reasons.

(i) Exchange effects in the first channel, which are dominant, are treated exactly by the Hartree–Fock method.

(ii) For the atoms He and Ne, the influence of absorptive effects on the elastic channel is small. (This effect is stronger for the He than for the Ne atom, which may be seen by a synoptical view of tables 1, 2, 3, 5, 6 and 7. The reason is the low number of dominant discrete excitation energy levels for such 'small' atoms (see e.g. Callaway 1980).

(ii) The inclusion of dynamical charge polarisation effects seems to be essential (especially for low-angle, i.e. forward, scattering). This becomes obvious from our RHFT results in comparison with our (and other) calculations which do not take into account such long-range forces.

With regard to a possible optimisation of the energy differences ΔE by fitting to experimental data, this was not attempted, since we do not consider it to be in the spirit of our model.

The generally excellent to good agreement between various experimental data and our RHFT model, as presented in this work, shows that, at least for closed-shell targets of low electron number, the approximations we have made (in order to keep the computational effort as small as possible), are physically reasonable. Our model seems to account well for dynamical charge polarisation effects and for the influence of inelastic processes on the elastic scattering channel too. In order to investigate the adequacy of our model for targets with larger electron numbers, we are presently performing calculations for the elastic electron scattering from other noble-gas atoms.

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References

Allison A C 1970 *J. Comput. Phys.* **6** 378–91
Awe B, Kemper F, Rosicky F and Feder R 1983 *J. Phys. B: At. Mol. Phys.* **16** 603–12
Brewer D F C, Newell W R, Harper S F W and Smith A C H 1981 *J. Phys. B: At. Mol. Phys.* **14** L749–54
Bühring W 1968 *Z. Phys.* **208** 286–98
Burke P G 1969 *Lectures in Theoretical Physics, Atomic Collision Processes* ed S Geltman, K T Manhanthappa and W E Brittin (New York: Academic)
Callaway J 1980 *Adv. Phys.* **29** 771–867
Carse D G and Walker D W 1973 *J. Phys. B: At. Mol. Phys.* **6** 2529–44
Desclaux J-P 1975 *Comput. Phys. Commun.* **9** 31–45
Fon W C and Berrington K A 1981 *J. Phys. B: At. Mol. Phys.* **14** 323–34
Fritsche L, Noffke J and Gollisch H 1984 *J. Phys. B: At. Mol. Phys.* **17**
Furness J B and McCarthy I E 1973 *J. Phys. B: At. Mol. Phys.* **6** 2280–91
Grant I P 1970 *Adv. Phys.* **19** 747–811
de Heer F J and Jansen R H J 1977 *J. Phys. B: At. Mol. Phys.* **10** 3741–58
de Heer F J, Jansen R H J and van der Kay W 1979 *J. Phys. B: At. Mol. Phys.* **12** 979–1002
Hildebrand F B 1974 *Introduction to Numerical Analysis* (New York: McGraw-Hill)
Kaupilla W E, Stein T S, Smart J H, Dababneh M S, Ho Y K, Downing J P and Pol V 1981 *Phys. Rev.* A **24** 725–42
Kemper F, Awe B, Rosicky F and Feder R 1983 *J. Phys. B: At. Mol. Phys.* **16** 1819–25

Kollath K J and Lucas C J 1979 *Z. Phys.* A **292** 215–8
Koopmans T A 1933 *Physica* **1** 104
McCarthy I E, Noble C J, Phillips B A and Turnbull A D 1977 *Phys. Rev.* A **15** 2173–85
Nesbet R K 1980 *Variational Methods in Electron–Atom Scattering Theory* (New York and London: Plenum)
Onda K and Truhlar D G 1980 *Phys. Rev.* A **22** 86–100
Register D F, Trajmar S and Srivastava S K 1980 *Phys. Rev.* A **21** 1134–51
Rose M E 1961 *Relativistic Electron Theory* (New York: Wiley)
Slater J C, Wilson T M and Wood J W 1969 *Phys. Rev.* **179** 28–38
Temkin A 1957 *Phys. Rev.* **107** 1004–12
Temkin A and Lamkin J C 1961 *Phys. Rev.* **121** 788–94
Thirumalai D and Truhlar D G 1982a *Phys. Rev.* A **25** 3058–71
—— 1982b *Phys. Rev.* A **26** 793–807
Wagenaar R W and de Heer F J 1980 *J. Phys. B: At. Mol. Phys.* **13** 3855–66
Walker D W 1970 *J. Phys. B: At. Mol. Phys.* **3** 788–97
—— 1971 *Adv. Phys.* **20** 275–323
Williams J F and Crowe A 1975 *J. Phys. B: At. Mol. Phys.* **8** 2233–48