

Low-energy electron scattering from He, Ne and Ar atoms

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1988 J. Phys. B: At. Mol. Opt. Phys. 21 3753

(<http://iopscience.iop.org/0953-4075/21/22/013>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 132.166.200.210

The article was downloaded on 25/06/2012 at 09:04

Please note that [terms and conditions apply](#).

Low-energy electron scattering from He, Ne and Ar atoms

Jianmin Yuan

Applied Physics Department, National University of Defense Technology, Changsha, Hunan, The People's Republic of China

Received 6 January 1988, in final form 1 June 1988

Abstract. Modified static exchange calculations for the low-energy elastic scattering of electrons by He, Ne and Ar atoms are presented in the energy range 0.1–20 eV based on Roothaan–Hartree–Fock atomic wavefunctions. The exchange interaction is included exactly, while the correlation, distortion and polarisation effects are accounted for by a parameter-free correlation–polarisation potential. By comparing the calculated results with the experimental data, it is concluded that the correlation–polarisation potential can represent the interactions not included the static-exchange approximation adequately.

1. Introduction

A great deal of research work has been done on the scattering of electrons from noble-gas atoms both experimentally (for example Ramsauer and Kollath 1929, Brüche 1927, Brode 1925, Golden and Bandel 1965, Kennerly and Bonham 1978, Nickel *et al* 1985, Ferch *et al* 1985, Buckman and Lohmann 1986, Stein *et al* 1978, Salop and Nakano 1970) and theoretically (for example Nesbet 1979, O'Malley *et al* 1979, Fon *et al* 1981, Labahn and Callaway 1964, 1970, Yau *et al* 1978, 1980, McEachran and Stauffer 1983a, b, 1984, 1987, O'Connell and Lane 1983, Fon *et al* 1983, Bell *et al* 1984, Brewer *et al* 1981, Dasgupta and Bhatia 1984). The recent experimental results were summarised by Nickel *et al* (1985). Yau *et al* and McEachran *et al* have comprehensively studied the noble-gas atoms in the adiabatic exchange scheme which includes the polarisation potential in the calculations and obtained good results. Nevertheless, the procedure of including the polarisation potential in their calculations is too tedious and difficult to be applied to large atoms and molecules. O'Connell and Lane (1983) proposed a correlation–polarisation potential and applied it to the low-energy electron scattering from noble-gas atoms. According to the local density functional theory, Padial and Norcross (1984) modified O'Connell and Lane's potential. The correlation–polarisation potential of Padial and Norcross is less attractive than that of O'Connell and Lane. Although encouraging results have been obtained, most of the applications of the proposed correlation–polarisation potentials together with various local exchange potentials were insufficiently attractive to produce correct cross sections in low-energy electron scattering calculations (O'Connell and Lane 1983, Gianturco *et al* 1987, Yuan 1987a). Because of the approximation in the treatment of the exchange effect, it cannot be deduced clearly whether the weakness of the attraction is due to the correlation–polarisation potentials or the local exchange potentials.

In the present paper, modified static exchange calculations are applied to the low-energy scattering of electrons by He, Ne and Ar atoms, in which the exchange

interaction is included exactly and the correlation-polarisation effects are accounted for by means of Padial and Norcross's potential. By comparing our calculated results with experiments and other reliable calculations, the applicability of the correlation-polarisation potential is examined, taking advantage of the fact that no uncertainty exists in the treatment of the exchange effect.

2. Theoretical formalism

In the static exchange approximation, the set of equations for the continuum scattering wavefunction can be written as

$$(-\frac{1}{2}\nabla_r^2 + V_s(r) - \frac{1}{2}k^2)F(r) = \sum_i \left((\varepsilon_i - \frac{1}{2}k^2) \langle \phi_i | F \rangle + \left\langle \phi_i(r') \left| \frac{1}{|r' - r|} \right| F(r') \right\rangle \right) \phi_i(r) \quad (1)$$

where $V_s(r)$, k , $F(r)$, ε_i and ϕ_i are the static potential, the momentum of the incident electron, the scattering wavefunction, the one-electron eigenvalues and the one-electron orbitals of the target atom respectively.

Because of the closed-shell structure of the target atoms the radial equation set can be derived (McEachran and Stauffer 1983a) as follows:

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_s(r) + k^2 \right) U_l(r) = K_l(r) U_l(r) \quad (2)$$

where the exchange kernel, $K_l(r)U_l(r)$, can be written in terms of momentum, one-electron eigenvalues and one-electron orbitals of the atoms (cf equations (6), (7), (8) and (9) of McEachran and Stauffer (1983a)).

An improvement of the static exchange approximation is made by introducing the correlation-polarisation potential of Padial and Norcross (1984) in equation (2). Then, the final set of equations to be solved is

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_s(r) - 2V_{cp}(r) + k^2 \right) U_l(r) = K_l(r) U_l(r). \quad (3)$$

In the asymptotic region the potential V_{cp} can be written in terms of the dipole polarisability of the target in the form

$$V_p(r) \underset{r \rightarrow \infty}{\sim} -\alpha/2r^4. \quad (4)$$

Because equation (4) cannot be used at small r , an effective potential has to be developed to account for the short-range correlation effects. According to the density functional theory the effective potential arising from the correlation energy can be calculated from

$$V_c(r) = \frac{d}{d\rho} E_c(\rho) \\ = \begin{cases} 0.0311 \ln r_s - 0.0548 + 0.006r_s \ln r_s - 0.015r_s & r_s \leq 0.7 \\ -0.07356 + 0.02224 \ln r_s & 0.7 < r_s \leq 10.0 \\ -0.584r_s^{-1} + 1.988r_s^{-3/2} - 2.45r_s^{-2} - 0.0733r_s^{-5/2} & r_s > 10.0 \end{cases} \quad (5)$$

where, in local density functional theory, $E_c(\rho) = \int \rho(r) \varepsilon_c(r) dr$ is the correlation energy, $\varepsilon_c(r)$ is the correlation energy density of a free electron gas and $r_s = (3/4\pi\rho)^{1/3}$

is the density parameter. The short-range potential (5) is combined with the long-range potential (4) by joining them smoothly at their inner intersection point (Padial and Norcross 1984, O'Connell and Lane 1983):

$$V_{cp} = \begin{cases} V_c(r) & r < r_c \\ V_p(r) & r \geq r_c \end{cases} \quad (6)$$

Here r_c is determined by $V_c(r_c) = V_p(r_c)$.

The radial equation (3) is solved by iteration (Collins *et al* 1980) using Numerov's algorithm with a modified Hermann-Skillman radial mesh (Hermann and Skillman 1963) with the step size ranging from 0.0001 to $0.06 a_0$.

3. Results and discussion

In figure 1 the present calculated total cross sections for *e*-He scattering are presented and, for the convenience of comparison, McEachran and Stauffer's theoretical results using polarised orbitals and three sets of experimental data are also shown. Around 1 eV our results are lower than the experiments by 7%, while above 10 eV our results are about 6% higher than the experimental data. However, in the whole energy range the present results are in good agreement with the measured values and are very close to those of McEachran and Stauffer. Near 1.5 eV, the present results deviate slightly from those of McEachran and Stauffer, and we attribute these small discrepancies to the use of a different dipole polarisability in their calculations, which is 4.4% smaller than the accurate value. It can easily be seen that for *e*-He scattering the correlation-polarisation potential can adequately represent the correlation and polarisation interactions, although it is slightly too attractive.

In figure 2, the calculated results for *e*-Ne scattering are reported. The agreement of our theoretical results with the experiments is very good and is apparently better than that for *e*-He scattering. In this figure, our results are also quite close to those of McEachran and Stauffer (1983b, 1985), although the discrepancies of their original results appear relatively larger at very low energies. The small differences between the

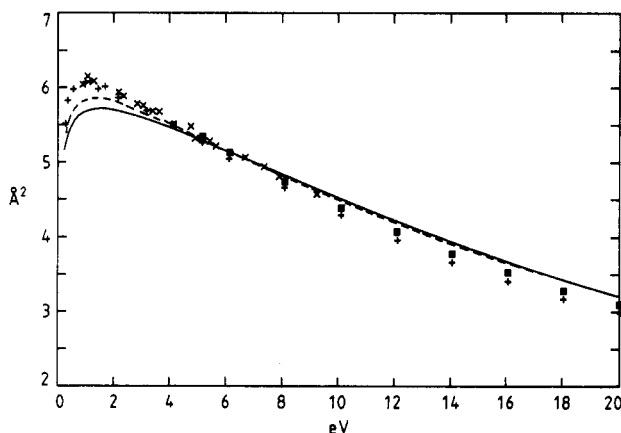


Figure 1. The total cross section for *e*-He scattering. —, present results; ---, McEachran and Stauffer (1983a); +, Buckman and Lohmann (1986); ×, Kumar *et al* (1987); ■, Nickel *et al* (1985).

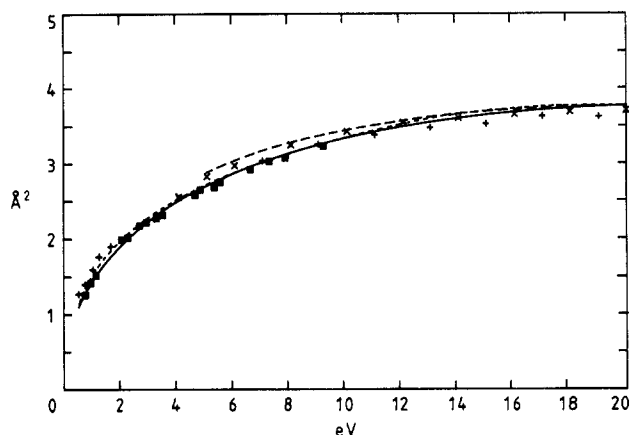


Figure 2. The total cross section for e-Ne scattering. —, present; ---, McEachran and Stauffer (1983b); - - -, McEachran and Stauffer (1985); ■, Kumar *et al* (1987); ×, Nickel *et al* (1985); +, Salop and Nakano (1970).

present work and McEachran and Stauffer's (1983b) original work are also mainly due to the use of different dipole polarisabilities. They made their calculations with the polarisation potential scaled to the correct asymptotic form using an accurate dipole polarisability. Their results are almost indistinguishable from the present results. The correlation-polarisation potential still shows slightly too strong an attraction; however it has been improved considerably compared with that of e-He scattering. In most of the energy region, the theoretical cross section curve lies within the error bars of the experiments.

The calculated cross sections for e-Ar scattering are reported in figure 3 together with the theoretical results of McEachran and Stauffer (1983b) and Bell *et al* (1984) using the R-matrix method and three sets of experimental data. Our calculation gives a Ramsauer-Townsend (RT) minimum of 0.29 Å^2 at 0.38 eV quite close to the recent experiments (Ferch *et al* 1985, Buckman and Lohmann 1986). The predicted broad maximum is at 12.8 eV with a maximum cross section of 24.5 Å^2 . The agreement of

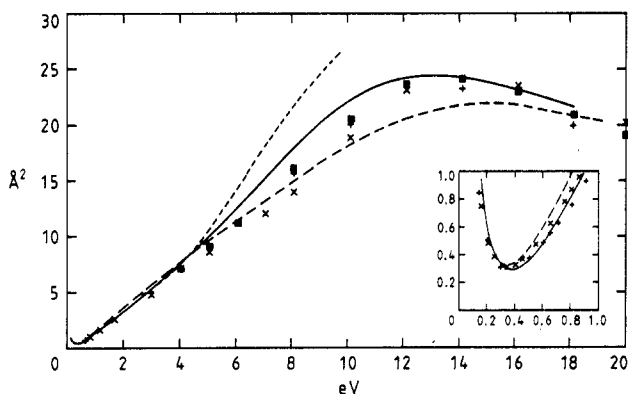


Figure 3. The total cross section for e-Ar scattering. —, present; ---, McEachran and Stauffer (1983b); — · —, Bell *et al* (1984); ■, Nickel *et al* (1985); +, Buckman and Lohmann (1986); ×, Ferch *et al* (1985).

our results with the experiments is apparently better than the polarised orbital calculation of McEachran and Stauffer (1983b) and the R-matrix calculation of Bell *et al.* McEachran and Stauffer's work gave a peak of 27 \AA^2 , which is about 4 \AA^2 above the measured values, at approximately 11 eV, which is about 2.5 eV below the measured position. The study of Bell *et al.* gave too low a maximum cross section of about 22 \AA^2 at too high an energy of 15 eV. Compared with the calculations of McEachran and Stauffer (1983a, b, 1985) the correlation-polarisation potential of Padial and Norcross works better for e -Ar than for e -He and e -Ne.

In the energy range 0–20 eV, the contributions to the total cross sections are dominantly elastic scattering. For He atoms, although the energies near 20 eV are above the first excitation threshold, the inelastic cross sections at these energies are very small compared with the elastic contribution. It has been shown by theory (Oberoi and Nesbet 1973, Berrington *et al.* 1975) as well as experiment (Spence *et al.* 1983) that the total inelastic cross sections for He is only some 0.03 \AA^2 at 20 eV, which is a mere 1% of the total cross section. In this energy region, it is then not necessary to consider the inelastic contributions when comparing our results with the experiments, even if the experiments were performed for the total cross sections without separating elastic from inelastic scattering.

In the applications of the correlation-polarisation potential together with local exchange potentials, the whole potentials were always too weak or too strong (O'Connell and Lane 1983, Gianturco *et al.* 1987, Yuan 1988a). Because approximations were also made for the exchange potentials it is not clear whether the inaccuracies of the whole potentials are due to the correlation-polarisation potential or to local exchange potentials. The relationship between the correlation potential of Padial and Norcross and the correlation potential of O'Connell and Lane is similar to that between the derivation of Slater (1960) and the variational treatment of Kohn and Sham (1965) of the exchange interaction. The correlation potential of Padial and Norcross is approximately $\frac{3}{5}$ the correlation potential of O'Connell and Lane, i.e. the former is weaker than the latter. In the present calculations, there is not any approximation in the evaluation of the exchange effect and we can conclude from the calculated results that the correlation-polarisation potential can represent the correlation and polarisation effects effectively when HF wavefunctions are used. Based on the calculated results we prefer to use Padial and Norcross's potential provided that exact exchange is included. However, O'Connell and Lane's potential should be used if it is combined with an insufficiently strong exchange potential (for example the HFEGE potential). It has been shown that the correlation potential works better for larger targets than for smaller targets, and further studies for other larger atoms (Xe, Kr) are needed. It can also be concluded that incorporating an adequate model correlation-polarisation potential into the exact static exchange calculations can give reliable results for the elastic cross sections of low-energy scattering, and our calculations also provide a simple way to calculate the low-energy elastic cross sections in an *ab initio* manner. The application of the present formalism to the scattering of e -CH₄ is given by Yuan (1988b).

References

- Bell K L, Scott N S and Lennon M A 1984 *J. Phys. B: At. Mol. Phys.* **17** 4757
Berrington K A, Burke P G and Sinfaiam A L 1975 *J. Phys. B: At. Mol. Phys.* **8** 1459

- 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
- Brode R B 1925 *Phys. Rev.* **25** 636
- Brüche E 1927 *Ann. Phys., Lpz* **84** 279
- Buckman S J and Lohmann B 1986 *J. Phys. B: At. Mol. Phys.* **19** 2547
- Collins L A, Robb W D and Morrison M A 1980 *Phys. Rev. A* **21** 488
- Dasgupta A and Bhatia A K 1984 *Phys. Rev. A* **30** 1241
- Ferch J, Granitzka B, Masche C and Raith W 1985 *J. Phys. B: At. Mol. Phys.* **18** 967
- Fon W C, Berrington K A and Hibbert A 1981 *J. Phys. B: At. Mol. Phys.* **14** 307
- Fon W C, Burke P G, Berrington K A and Hibbert A H 1983 *J. Phys. B: At. Mol. Phys.* **16** 307
- Gianturco F A, Jain A and Pantano L C 1987 *J. Phys. B: At. Mol. Phys.* **20** 571
- Golden D E and Bandel H W 1965 *Phys. Rev.* **138** A 14
- Herrmann F and Skillman S 1963 *Atomic Structure Calculations* (Englewood Cliffs, NJ: Prentice-Hall)
- Kennerly R E and Bonham R A 1978 *Phys. Rev. A* **17** 1844
- Kohn W and Sham L H 1965 *Phys. Rev.* **140** A1133
- Kumar V, Krishnakumar E and Subramanian K P 1987 *J. Phys. B: At. Mol. Phys.* **20** 2899
- Labahn R W and Callaway J 1964 *Phys. Rev.* **135** A1539
- 1970 *Phys. Rev. A* **2** 366
- McEachran R P and Stauffer A D 1983a *J. Phys. B: At. Mol. Phys.* **16** 255
- 1983b *J. Phys. B: At. Mol. Phys.* **16** 4023
- 1984 *J. Phys. B: At. Mol. Phys.* **17** 2507
- 1985 *Phys. Lett.* **107A** 397
- 1987 *J. Phys. B: At. Mol. Phys.* **20** 3483
- Nesbet R K 1979 *Phys. Rev. A* **20** 58
- Nickel J C, Imre K, Register D F and Trajmar S 1985 *J. Phys. B: At. Mol. Phys.* **18** 125
- Oberoi R S and Nesbet R K 1973 *Phys. Rev. A* **8** 2969
- O'Connell and Lane N F 1983 *Phys. Rev. A* **27** 1893
- O'Malley T F, Burke P G and Berrington K A 1979 *J. Phys. B: At. Mol. Phys.* **12** 953
- Padial N T and Norcross D W 1984 *Phys. Rev. A* **29** 1742
- Ramsauer C and Kollath R 1929 *Ann. Phys., Lpz* **3** 536
- Salop A and Nakano H H 1970 *Phys. Rev. A* **2** 127
- Slater J C 1960 *Quantum Theory of Atomic Structure* vol 2 (New York: McGraw-Hill)
- Spence D, Stuit D, Dillon M A and Wang R-G 1983 *Proc. 13th Int. Conf. on the Physics of Electronic and Atomic Collisions, Berlin* ed J Eichler *et al* (Amsterdam: North-Holland) Abstracts p 117
- Stein T S, Kauppila W E, Smart J H and Jesion G 1978 *Phys. Rev. A* **17** 1600
- Yau A W, McEachran R P and Stauffer A D 1978 *J. Phys. B: At. Mol. Phys.* **11** 2907
- 1980 *J. Phys. B: At. Mol. Phys.* **13** 377
- Yuan J 1988a *J. Phys. B: At. Mol. Opt. Phys.* **21** 2737
- 1988b *J. Phys. B: At. Mol. Opt. Phys.* **21** 3113