Aust. J. Phys., 1993, **46**, 241–8

Some Remarks on the Use of Effective Charges in the Study of Electron Impact Ionisation Processes

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Abstract

The first-order effective charge description of the electron impact ionisation of H(1s) is considered. The effect of imposing the Peterkop relation on the charges occurring therein is discussed. A special case corresponding to high energy asymmetric geometry is considered and values for the effective charges deduced by comparison with the most accurate available theoretical and experimental data.

1. Introduction

At the present time a number of interesting studies of (e, 2e) and related processes have appeared which make use of the effective charge method, first introduced into ionisation physics by Peterkop (1962) and Rudge and Seaton (1965). We note in particular its use in problems of near-threshold ionisation (Pan and Starace 1991; Jones *et al.* 1992), (e, 3e) (Dal Cappello 1991), (e, 2e) in energy-sharing kinematics (Botero and Macek 1991), as well as in coplanar asymmetric geometries (Whelan *et al.* 1989, 1991; Jetzke *et al.* 1989). In this paper we investigate to what extent it is possible to have a successful effective charge description, within the context of first-order pertubation theory where the charges obey the Peterkop relation. For the particular case of the electron impact ionisation of H(1s) there are available the accurate experimental data of the Kaiserslautern group (Ehrhardt *et al.* 1986; Klar *et al.* 1987) for the highly asymmetric kinematics favoured by perturbation theory. The second Born calculations of Byron *et al.* (1985), and the coupled pseudo-state calculation of Curran *et al.* (1987, 1991) are in excellent accord with the measurements both as to the form and the absolute size of the triple differential cross section (TDCS). There are, however, some interesting calculations of Brauner *et al.* (1989) which are smaller in absolute size than some, though it should be emphasised not all, of the experimental cross sections. Brauner *et al.* have disputed the absolute normalisation, in the cases when their results are in poor accord, pointing out that they always reproduce a good shape for the TDCS. Curran *et al.* (1991) have considered the problem in some detail and have shown that the Brauner *et al.* data are also inconsistent with the relative normalisation of the data for

0004-9506/93/020241$05.00

different scattering angles, but the same impact and ejected energies. However, for an impact energy E_0 of 250 eV, ejection energy $E_s = 5$ eV and scattering angle $\theta_f = 3°$, we note that all theoretical calculations are in excellent accord with each other and the measurements of the Kaiserslautern group. The same is true for $E_0 = 150$ eV, $E_s = 5$ eV and $\theta_f = 4°$.

We therefore feel that these special cases can be used as a firm standard to judge the value of a simple effective charge approximation and indeed they present us with a means of empirically determining such charges. It is hoped that this study will help towards an understanding of how an effective charge approach could be used to advantage in the description of more complicated ionisation processes, where the use of higher-order theories is presently impracticable.

2. Theory

Suppose we have an electron with momentum $\boldsymbol{k}_0$ and energy E_0 which collides with a hydrogen atom in the ground state, and that after the collison two electrons, one fast (with momentum $\boldsymbol{k}_f$, energy E_f) and one slow ($\boldsymbol{k}_s, E_s$), are detected. Let $\Psi^+(\boldsymbol{r}_f, \boldsymbol{r}_s)$ be the desired solution of the Schrödinger equation, with outgoing wave boundary conditions, appropriate to the initial state

$$\Phi_i = \psi_0(\boldsymbol{r}_s)\, e^{i\boldsymbol{k}_0 \cdot \boldsymbol{r}_f}, \tag{1}$$

where $\psi_0(\boldsymbol{r}_s)$ is the hydrogen atom ground state wavefunction.

It was shown in Rudge and Seaton (1965) and Peterkop (1962) that the direct amplitude may be written as

$$f(\boldsymbol{k}_f, \boldsymbol{k}_s) = -\frac{e^{i\Delta}}{(2\pi)^{5/2}} \int \psi^{-*}(z_s, \boldsymbol{k}_s, \boldsymbol{r}_s)\, \psi^{-*}(z_f, \boldsymbol{k}_f, \boldsymbol{r}_f) \times \left(V_{sf} - \frac{1 - z_s}{r_s} - \frac{1 - z_f}{r_f} \right) \Psi^+(\boldsymbol{r}_f, \boldsymbol{r}_s)\, d\boldsymbol{r}_f\, d\boldsymbol{r}_s . \tag{2}$$

where $V_{sf} = ||\boldsymbol{r}_f - \boldsymbol{r}_s||^{-1}$ and

$$\Delta = \frac{2z_s}{k_s} \ln(k_s/X) + \frac{2z_f}{k_f} \ln(k_f/X),$$

with $X = \sqrt{k_s^2 + k_f^2}$. Here $\psi^-(z, k, r)$ defines a continuum Coulomb function with ingoing waves, where

$$\langle \psi^{\pm}(z, \boldsymbol{k}, \boldsymbol{r}) \,|\, \psi^{\pm}(z, \boldsymbol{k}', \boldsymbol{r}) \rangle = \delta(\boldsymbol{k} - \boldsymbol{k}')(2\pi)^3 . \tag{3}$$

The charges z_s, z_f are arbitrary, but must satisfy

$$\frac{z_s}{k_s} + \frac{z_f}{k_f} = \frac{1}{k_s} + \frac{1}{k_f} - \frac{1}{||\boldsymbol{k}_s - \boldsymbol{k}_f||}, \tag{4}$$

to avoid an indeterminate phase factor in (2). The Peterkop relation (4) is an inevitable consequence of taking the long-range Coulomb forces to infinity. It does have the physical interpretation that, asymptotically as the two electrons move away from the nucleus along straight lines defined by $\boldsymbol{k}_s, \boldsymbol{k}_f$, their potential energy in the effective field $-z_s/r_s - z_f/r_f$ should equal their true potential energy in the field (see Rudge 1965)

$$-\frac{1}{r_s} - \frac{1}{r_f} + \frac{1}{||\boldsymbol{r}_f - \boldsymbol{r}_s||}.$$

We note that in (2) no approximation has been made; in other words, even if

$$\psi^-(z_s, \boldsymbol{k}_s, \boldsymbol{r}_s)\,\psi^-(z_f, \boldsymbol{k}_f, \boldsymbol{r}_f)$$

is a poor representation of the final state, we will still arrive at the correct scattering amplitude if we use the exact wavefunction Ψ^+.

The simple model that we study here consists of taking Ψ^+ to be the unperturbed initial state Φ_i, and the direct amplitude will be given by

$$f(\boldsymbol{k}_f, \boldsymbol{k}_s) = -\frac{1}{(2\pi)^{5/2}} \int \psi^{-*}(z_s, \boldsymbol{k}_s, \boldsymbol{r}_s)\,\psi^{-*}(z_f, \boldsymbol{k}_f, \boldsymbol{r}_f) \times \left(V_{sf} - \frac{1-z_s}{r_s} - \frac{1-z_f}{r_f}\right) e^{i\boldsymbol{k}_0 \cdot \boldsymbol{r}_f}\,\psi_0(\boldsymbol{r}_s)\,d\boldsymbol{r}_f\,d\boldsymbol{r}_s, \quad (5)$$

and the exchange amplitude by

$$g(\boldsymbol{k}_f, \boldsymbol{k}_s) = \frac{1}{(2\pi)^{5/2}} \int \psi^{-*}(z_s, \boldsymbol{k}_s, \boldsymbol{r}_f)\,\psi^{-*}(z_f, \boldsymbol{k}_f, \boldsymbol{r}_s) \times \left(V_{sf} - \frac{1-z_f}{r_s} - \frac{1-z_s}{r_f}\right) e^{i\boldsymbol{k}_0 \cdot \boldsymbol{r}_f}\,\psi_0(\boldsymbol{r}_s)\,d\boldsymbol{r}_f\,d\boldsymbol{r}_s, \quad (6)$$

with the spin-averaged TDCS given by

$$\frac{d^3\sigma}{d\Omega_f\,d\Omega_s\,dE} = \frac{k_s\,k_f}{4k_0}(|f+g|^2 + 3|f-g|^2). \quad (7)$$

Note that when we exchange particles we also exchange the effective charges. Thus, the same z_s, z_f are used in the direct and exchange amplitudes, and therefore the factor $e^{i\Delta}$ occurring in (2) will in all cases disappear when we form the cross-section and may be neglected without loss of generality. We note that the value of approximating Ψ^+ by Φ_i in (2) implicitly affected by our choices of z_s, z_f.

A further simplification is possible. Using the well-known analytic expressions (see e.g. Coleman 1969) for the one-particle integrals occurring in (5), it is straightforward to show that the direct amplitude may be written as

$$f(\boldsymbol{k}_\mathrm{f}, \boldsymbol{k}_\mathrm{s}) = -\frac{1}{(2\pi)^{5/2}} \int \psi^{-*}(z_\mathrm{s}, \boldsymbol{k}_\mathrm{s}, \boldsymbol{r}_\mathrm{s}) \psi^{-*}(z_\mathrm{f}, \boldsymbol{k}_\mathrm{f}, \boldsymbol{r}_\mathrm{f}) \times \left(V_\mathrm{sf} - \frac{1}{r_\mathrm{f}}\right) \mathrm{e}^{\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{r}_\mathrm{f}} \psi_0(\boldsymbol{r}_\mathrm{s}) \, \mathrm{d}\boldsymbol{r}_\mathrm{f} \, \mathrm{d}\boldsymbol{r}_\mathrm{s} . \tag{8}$$

Now given (8) it is tempting to identify $\psi^-(z_\mathrm{s}, \boldsymbol{k}_\mathrm{s}, \boldsymbol{r}_\mathrm{s})\,\psi^-(z_\mathrm{f}, \boldsymbol{k}_\mathrm{f}, \boldsymbol{r}_\mathrm{f})$ with the final ionised state. However, it is worth noting that unless $z_\mathrm{s} = 1$ the initial and 'final' states are not orthogonal.

3. Discussion

In Whelan *et al.* (1989, 1991) we presented the TDCS for electron impact ionisation of atomic hydrogen (1s), calculated using a variety of effective charge prescriptions. In particular, we considered three approximations which used momentum-dependent effective charges chosen so that the Peterkop relation was satisfied. These were not satisfactory, yielding cross sections which differed little from the first Born approximation. Our results were consistent with those found in earlier calculations (Rudge and Schwartz 1966; Schulz 1973).

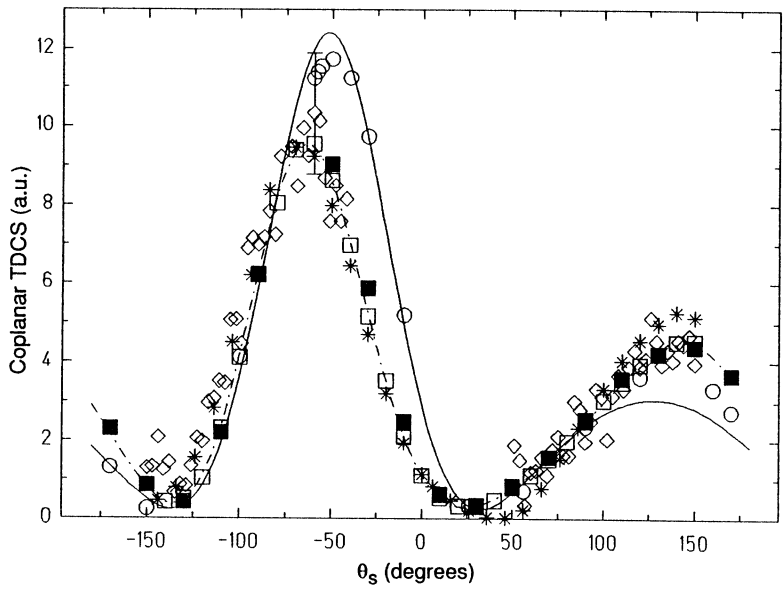

Fig. 1. Coplanar TDCS as a function of the ejected electron angle θ_s for $E_0 = 250$ eV, $E_\mathrm{s} = 5$ eV and $\theta_\mathrm{f} = 3°$:

Experiment: ◇ Ehrhardt *et al.* (1986), Klar *et al.* (1987)
Theory — First Born, ■ Second Born (Byron *et al.* 1985)
○ First-order perturbation theory with $\alpha = 3{\cdot}5$ (Jetzke *et al.* 1989)
-·-·-·-·- Pseudo-state approximation (Curran *et al.* 1991)
*, □ Effective charge approximation (a), (b)

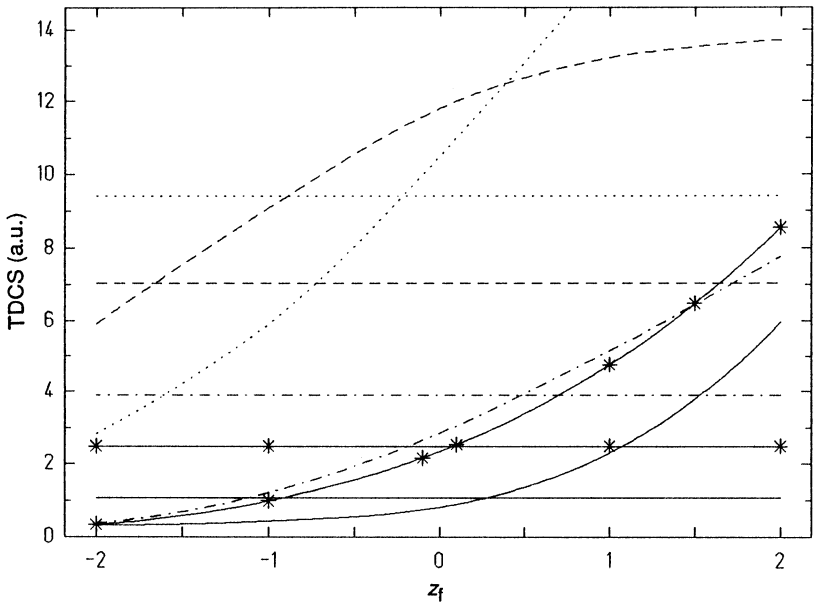

Fig. 2. Variation of the TDCS with z_f (with z_s fixed by equation 1) for: — $\theta_s = -120°$; ····· $\theta_s = -70°$; ----- $\theta_s = 40°$; * $\theta_s = 90°$; and -·-·- $\theta_s = 120°$. The pseudo-state TDCS is used to construct each of the corresponding horizontal lines.

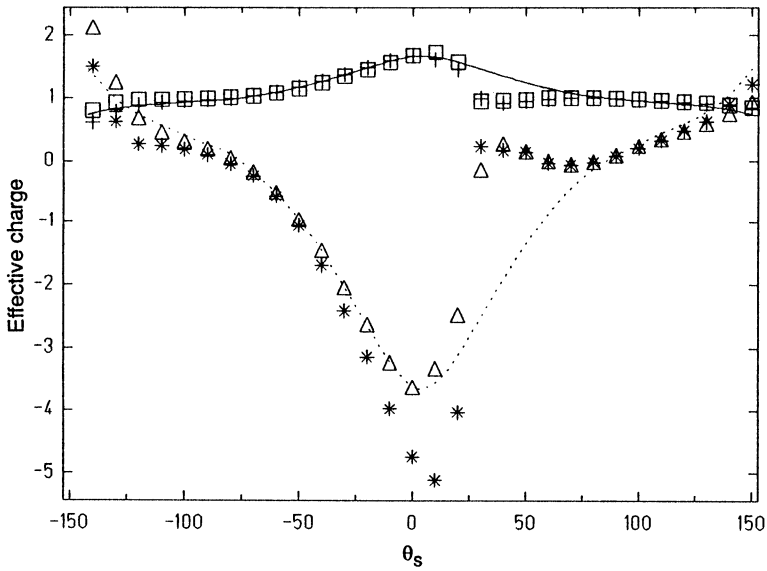

Fig. 3. Variation in charges z_f necessary to reproduce the pseudo-state results [i.e. choice (b) in Section 3] at:
(i) $E_0 = 250$ eV, $\theta_f = 3°$, $E_s = 5$ eV: □ z_s, * z_f
(ii) $E_0 = 150$ eV, $\theta_f = 4°$, $E_s = 5$ eV: + z_s, △ z_f.
Also shown is the variation corresponding to the choice (a) for the case (ii): — z_s, ···· z_f.

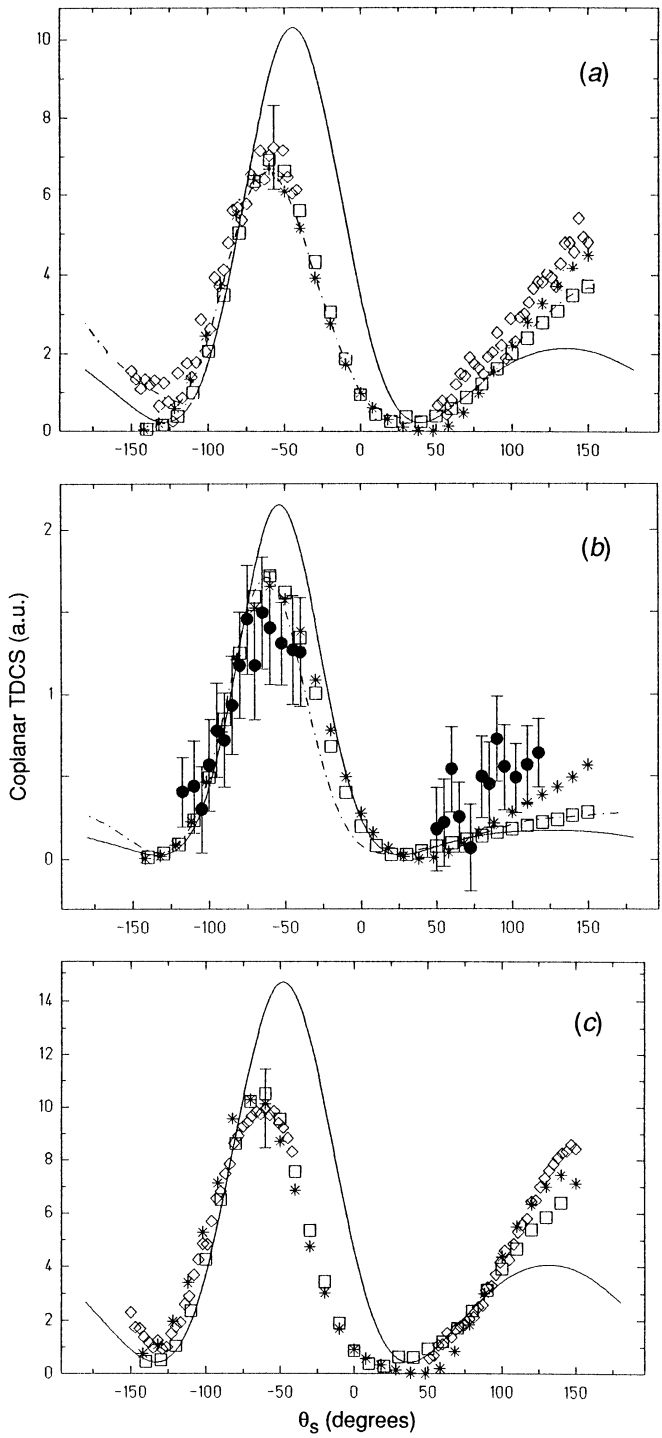

Fig. 4. Coplanar TDCS as a function of the ejected electron angle θ_s for (symbols are defined in Fig. 1): (*a*) $E_0 = 150$ eV, $E_s = 5$ eV, $\theta_f = 4°$; (*b*) $E_0 = 250$ eV, $E_s = 14$ eV, $\theta_f = 5°$; and (*c*) $E_0 = 150$ eV, $E_s = 3$ eV, $\theta_f = 4°$.

In Fig. 1 we show the results obtained using the recently published prescription of Jetzke *et al.* (1989), within our first-order approximation, for an impact energy of $E_0 = 250$ eV, where the slow electron has an energy of $E_s = 5$ eV and the fast electron is scattered through an angle of $\theta_f = 3°$. Again we see that there is little improvement over the first Born approximation. These results prompt the question: does there exist a first-order effective charge approximation, with charges z_s, z_f obeying the Peterkop relation, which gives good agreement with experiment?

We considered the special case, $E_0 = 250$ eV, $\theta_f = 3$, $E_s = 5$ eV, and looked to see what choices of z_s, z_f satisfying the Peterkop relation would reproduce the pseudo-state results. We proceeded as follows: z_f was varied over a wide range and z_s was fixed through (4). As can be seen from Fig. 2 there exists essentially a unique solution. The resulting effective charges are shown in Fig. 3.

Also in Fig. 3, we show the potential needed to fit the pseudo-state data at $E_0 = 150$ eV, $\theta_f = 4$, $E_s = 5$. We see that in both cases there is only a small variation in the values of z_s found. We consider two empirical potentials defined as follows:

(a) z_s is given by the solid curve shown in Fig. 3 for $\theta_s < \theta_f$ and by symmetry for $\theta_s > \theta_f$;

(b) z_s is given by the values shown in Fig. 3 for all θ_s.

The z_f values are, in both cases, deduced from (4). In Figs 1 and 4 we show some of our results obtained using these procedures. In Fig. 4*b* we compare results with the relative data of Lohmann *et al.* (1984) (solid circles), which we have normalized by taking the experimental TDCS at $\theta_s = 60°$ to be 1·4 a.u.

We remark that we have chosen to consider only cases where the magnitude and direction of the momentum transfer vector

$$\boldsymbol{K} = \boldsymbol{k}_0 - \boldsymbol{k}_f$$

remains essentially constant. It will be seen that the choice (b) tends to reproduce the pseudo-state results well in all cases, while (a) gives a better fit to the recoil peak as given by the absolute experimental results.

In summary, we have been able to derive effective charge prescriptions which allow us to reproduce to good accuracy the pseudo-state results of Curran *et al.* (1987, 1991) or the absolute experimental data. These prescriptions do not differ greatly from each other; however, the charges we use are somewhat surprising (see Fig. 3). It is our view that it would be misleading to try to interpret these charges in a simple physical way and that their form is a result of forcing a two-body description on what is a three-body problem. Indeed, the physics of the problem may well be contained in the rate of change of these charges, rather than the values of the charges themselves.

Acknowledgments

This work has been supported in part by the British–German Academic Research Collaboration Programme, the SERC and by a NATO collaborative research grant (CRG 920101).

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Manuscript received 2 June, accepted 20 November 1992