# High Energy Electron Impact Ionisation of H(1s) in Coplanar Asymmetric Geometry

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*Abstract*

Various effective charge approximations are explored for the high energy electron impact ionisation of H(1s) in coplanar asymmetric geometry, using a first order perturbative model. Our results are compared with other more sophisticated calculations and with experiment. It is found that effective charge prescriptions satisfying the requirement that, in the limit of zero ejection energy, the escaping electron sees the full nuclear charge while the scattered electron is totally screened, are unsuccessful. In contrast it is found that the Coulomb projected Born exchange approximation, where both electrons see the full nuclear charge, gives much better results. In general it reproduces the position and magnitude of the binary peak fairly well, although it is not so successful in the description of the recoil.

## 1. Introduction

This paper presents an investigation into the use of first order effective charge approximations in the theory of electron impact ionisation and as such is a sequel to the work of Rudge and Schwartz (1966) and Schulz (1973). Early investigations using this method were limited by the small amount of purely relative measurements with which one could compare the theoretical predictions. Very recently, accurate new experimental data both relative and absolute have become available for an energy regime not previously considered (Ehrhardt *et al.* 1986, 1989; Klar *et al.* 1987; Lohmann *et al.* 1984), where the kinematics are highly asymmetric and thus particularly favourable for a perturbative approach. The existence of these results together with the good agreement obtained by other more sophisticated approximations (Byron *et al.* 1983, 1985; Curran and Walters 1987) encourage us to believe that there is now a firm standard against which to judge the value of such simple effective charge approximations. We compare our calculations with both the new experimental data and the results of other more sophisticated theoretical approaches (Byron *et al.* 1983, 1985; Curran 1986; Curran and Walters 1987).

The purpose of the effective charge description is to represent in a simple way the essential physics of the interactions and correlations of the electrons

in the final ionised state; these complicated effects are viewed as giving rise to screening of the nuclear charge. Thus, an outgoing electron does not see the nucleus and the other electron but merely sees a nuclear Coulomb potential whose effective charge is different from the true nuclear charge. Such a view might be criticised because the effective Coulomb potential is spherically symmetric and so, it would seem, cannot represent angular correlation effects. However, these effects will be to some degree taken into account in that the effective charges will, in general, depend on the momenta of the outgoing electrons in the final state (see Coleman 1969; Geltman and Hidalgo 1974; Schulz 1971).

The use of effective charges should lead to simpler approximations; for example, in order to adequately describe the experimental data in asymmetric geometry it is necessary to go beyond the first Born approximation to the second. By using effective charges we hope to succeed with a first order approach. There is no unique way of selecting the effective charges and in this paper we experiment with some reasonable prescriptions. We look at several approximations which use momentum dependent effective charges chosen so that the Peterkop (1960, 1962) relation is satisfied. We also examine the case where the ejected electron totally screens the nucleus while seeing the full charge, i.e. the conventional first Born approximation (B1), and where no screening takes place, i.e. both electrons see a nuclear charge of unity, the Coulomb projected Born (CPB) approximation (Geltman and Hidalgo 1974). With the exception of the CPB, all approximations satisfy the usual constraint that in the limit of zero velocity for one of the outgoing electrons this electron sees the full nuclear charge, while the other is totally screened. As will be seen from our calculations this constraint seems to lead to poor results. In stark contrast the CPB performs relatively well in the binary direction.

We start in Section 2 with an outline of our approximation. Section 3 discusses the selection of effective charges. Section 4 gives calculational details. Our results are presented in Section 5 and conclusions in Section 6. In addition, we have thought it worth while to include, mainly in the appendices, a novel derivation of the scattering amplitude and triple differential cross section (TDCS). Some of the results presented here have already appeared in a preliminary communication (Whelan *et al.* 1989). Atomic units in which $h/2\pi = m_e = e = 1$ are used throughout.

## 2. Theory

*Preliminaries*

Suppose we have an electron with momentum $k_0$, energy $E_0$, which collides with a hydrogen atom in the ground state and that after the collision two electrons, one fast with momentum $k_f$, energy $E_f$, and one slow $k_s, E_s$, are detected. The total energy and momentum are conserved:

$$k_0^2 = k_f^2 + k_s^2 - 2\epsilon_0 + 2E_{\text{recoil}}, \tag{1}$$

$$k_0 = k_f + k_s + k_{\text{recoil}}, \tag{2}$$

where $\epsilon_0$ is the energy of the ground state ($-0\cdot5$ a.u. for 1s) and $\boldsymbol{k}_{\mathrm{recoil}}, E_{\mathrm{recoil}}$ are the momentum, energy of the recoiling ion. We define the momentum transfer as

$$\boldsymbol{K} = \boldsymbol{k}_0 - \boldsymbol{k}_{\mathrm{f}}. \tag{3}$$

Because of the large mass difference between the proton and the electron, we may neglect $E_{\mathrm{recoil}}$ in (1). From (2) we have

$$\boldsymbol{k}_{\mathrm{recoil}} = \boldsymbol{K} - \boldsymbol{k}_{\mathrm{s}}. \tag{4}$$

Therefore we see that for fixed $\boldsymbol{K}$, $\|\boldsymbol{k}_{\mathrm{s}}\|$ we have maximal recoil of the nucleus when $\boldsymbol{k}_{\mathrm{s}}$ lies in the $-\boldsymbol{K}$ direction and minimal when $\boldsymbol{k}_{\mathrm{s}}$ is parallel to $\boldsymbol{K}$. The proton has on average a momentum of one atomic unit prior to the collision (Bethe and Salpeter 1957), and therefore if the magnitude of $\boldsymbol{k}_{\mathrm{recoil}}$ is significantly greater than unity then it must follow that the nucleus has experienced a force during the collision. As we will see below, the TDCS becomes very small in the recoil direction in those cases where

$$\|\boldsymbol{k}_{\mathrm{recoil}}\| > 1.$$

Because we include exchange in our formalism we have found it convenient to adopt the operationally sound definitions of 'slow' and 'fast' detected electrons. We use this notation throughout this paper, i.e. anything with the subscript s applies to the slow electron, anything with f applies to the fast. It should be noted, however, that all our theoretical results are quite general and can be equally well applied to symmetric and asymmetric geometries. We assume that before the collision the system is in a state $i$ and after in a state $j$.

*General Formalism*

The Hamiltonian for the system may be written as

$$H = T_{\mathrm{f}} + T_{\mathrm{s}} + V_{\mathrm{f}} + V_{\mathrm{s}} + V_{\mathrm{sf}}, \tag{5}$$

where $T_{\mathrm{f}} = -\frac{1}{2}\nabla_{\mathrm{f}}^2$, $T_{\mathrm{s}} = -\frac{1}{2}\nabla_{\mathrm{s}}^2$, $V_{\mathrm{s,f}} = -1/r_{\mathrm{s,f}}$ is the interaction between the $s,f$th electron and the nucleus, $V_{\mathrm{sf}}$ is the electron–electron interaction $1/\|\boldsymbol{r}_{\mathrm{s}} - \boldsymbol{r}_{\mathrm{f}}\|$. Let $\Psi^+$ be the desired solution of the Schrödinger equation, i.e. $H\Psi^+ = E\Psi^+$, with outgoing wave boundary conditions, appropriate to the initial state:

$$\Phi_{\mathrm{i}} = \psi_0(r_{\mathrm{s}}) \exp(\mathrm{i}\,\boldsymbol{k}_0 \cdot \boldsymbol{r}_{\mathrm{f}}), \tag{6}$$

where $\psi_0(r_{\mathrm{s}})$ is the hydrogen atom ground state wavefunction.

Ionisation may be considered as being a rearrangement collision and from the general theory for such a process (Goldberger and Watson 1964) it follows that the direct amplitude may be written as

$$f(\boldsymbol{k}_{\mathrm{f}}, \boldsymbol{k}_{\mathrm{s}}) = -\frac{1}{(2\pi)^{5/2}} \langle \Phi_j | V_j | \Psi^+ \rangle, \tag{7}$$

where

$$\Phi_j = \exp(\mathrm{i}\, \mathbf{k}_\mathrm{s} . \mathbf{r}_\mathrm{s}) \exp(\mathrm{i}\, \mathbf{k}_\mathrm{f} . \mathbf{r}_\mathrm{f}), \tag{8a}$$

$$V_j = V_\mathrm{s} + V_\mathrm{f} + V_\mathrm{sf}. \tag{8b}$$

Here $\Phi_j$ is the final state which is an eigenvector of the reduced Hamiltonian

$$H_j = T_\mathrm{s} + T_\mathrm{f}, $$

i.e. we assume $V_j$ to be negligible in the final state. The corresponding exchange amplitude $g(\mathbf{k}_\mathrm{s}, \mathbf{k}_\mathrm{f})$ is obtained from (7) on interchanging the coordinates $\mathbf{r}_\mathrm{f}$ and $\mathbf{r}_\mathrm{s}$ in $\Psi^+$. From (7) and (8) it is clear that

$$g(\mathbf{k}_\mathrm{s}, \mathbf{k}_\mathrm{f}) = f(\mathbf{k}_\mathrm{f}, \mathbf{k}_\mathrm{s}). \tag{9}$$

In the formulation of (7) it has been tacitly assumed that the interactions between the particles tend to zero sufficiently rapidly at large separation. However, in reality $V_\mathrm{f}$, $V_\mathrm{s}$ and $V_\mathrm{sf}$ are long range pure Coulomb potentials. Our attitude is that we regard the Coulomb potentials as being cutoff to zero at some very large but finite distance. It would indeed be a serious matter if this viewpoint were invalid, i.e. if the physical results of interest were dependent on the environment outside the experimental apparatus.

It is useful to write the basic matrix element (7) in a form in which some interaction $W_j$ is absorbed into the left-hand side state. It is shown in Appendix A that

$$f(\mathbf{k}_\mathrm{f}, \mathbf{k}_\mathrm{s}) = -\frac{1}{(2\pi)^{5/2}} \langle \chi_j^- | (V_j - W_j) | \Psi^+ \rangle - \frac{1}{(2\pi)^{5/2}} \langle \chi_j^- | (V_\mathrm{i} - V_j + W_j) | \Phi_\mathrm{i} \rangle, \tag{10}$$

where

$$V_\mathrm{i} = V_\mathrm{f} + V_\mathrm{sf}, \tag{11}$$

and $\chi_j^-$ is the scattering state, with ingoing scattered waves, resulting from $\Phi_j$ in the presence of the interaction $W_j$.

We assume that $W_j$ is separable, i.e. that

$$W_j = V_\mathrm{a}(\mathbf{r}_\mathrm{f}) + V_\mathrm{b}(\mathbf{r}_\mathrm{s}), \tag{12}$$

where $V_\mathrm{a}(\mathbf{r}_\mathrm{f}), V_\mathrm{b}(\mathbf{r}_\mathrm{s})$ are potentials which act upon the fast and slow electrons respectively. For the choice (12), $\chi_j^-$ has the form

$$\chi_j^- = \zeta_\mathrm{a}^-(\mathbf{k}_\mathrm{f}, \mathbf{r}_\mathrm{f})\, \zeta_\mathrm{b}^-(\mathbf{k}_\mathrm{s}, \mathbf{r}_\mathrm{s}), \tag{13}$$

where

$$\left( T_\mathrm{f} + V_\mathrm{a}(\mathbf{r}_\mathrm{f}) - \frac{k_\mathrm{f}^2}{2} \right) \zeta_\mathrm{a}^-(\mathbf{k}_\mathrm{f}, \mathbf{r}_\mathrm{f}) = 0, \tag{14}$$

with $\zeta_a^-$ having ingoing scattered waves and originating from the state $\exp(i\,\boldsymbol{k}_f\cdot\boldsymbol{r}_f)$ of $\Phi_f$, and similarly for $\zeta_b^-$. With the choice (12) we show in Appendix B that the second term in (10) vanishes and so

$$f(\boldsymbol{k}_f,\boldsymbol{k}_s) = -\frac{1}{(2\pi)^{5/2}}\langle \zeta_a^-(\boldsymbol{k}_f,\boldsymbol{r}_f)\,\zeta_b^-(\boldsymbol{k}_s,\boldsymbol{r}_s)\mid V_s + V_f + V_{sf} - V_a(\boldsymbol{r}_f) - V_b(\boldsymbol{r}_s)\mid \Psi^+\rangle. \qquad (15)$$

Again $g(\boldsymbol{k}_f,\boldsymbol{k}_s)$ is obtained from (15) on interchanging the coordinates $\boldsymbol{r}_f,\boldsymbol{r}_s$ in $\Psi^+$. Formula (15) is the starting point for the approximations considered in this paper.

Suppose now that we take $V_a$ and $V_b$ to be Coulomb potentials with effective charges $z_f, z_s$ respectively, i.e.

$$V_a(\boldsymbol{r}_f) = -\frac{z_f}{r_f}, \qquad V_b(\boldsymbol{r}_s) = -\frac{z_s}{r_s}. \qquad (16)$$

Then (16) becomes

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

$$\times \Psi^+(\boldsymbol{r}_f,\boldsymbol{r}_s)\,\mathrm{d}\boldsymbol{r}_f\,\mathrm{d}\boldsymbol{r}_s, \qquad (17)$$

where $\psi^-(z,k,r)$ defines a continuum Coulomb function with ingoing waves, and where

$$\langle \psi^\pm(z,\boldsymbol{k},\boldsymbol{r})\mid \psi^\pm(z,\boldsymbol{k}',\boldsymbol{r})\rangle = \delta(\boldsymbol{k}-\boldsymbol{k}')(2\pi)^3. \qquad (18)$$

We note that in (17) we have made no approximation other than the assumption that $V_j$ may be treated as short range. 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 approximation to the final state and we use the exact wavefunction $\Psi^+$, we will arive at the correct scattering amplitude.

The simple model that we study here consists of taking $\Psi^+$ to be the unperturbed initial state $\Phi_i$. Given this perturbative approach it is then reasonable to identify $\psi^-(z_s,\boldsymbol{k}_s,\boldsymbol{r}_s)\,\psi^-(z_f,\boldsymbol{k}_f,\boldsymbol{r}_f)$ with the final ionised state which is now described through the potentials (16). These potentials represent an average screening of the nucleus by the other electron in the final state; $z_{s,f}$ being the effective nuclear charge visible to each electron. The charges $z_{s,f}$ will in general be functions of $\boldsymbol{k}_f$ and $\boldsymbol{k}_s$. Therefore, the direct amplitude is given by

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

$$\times \exp(i\,\boldsymbol{k}_0\cdot\boldsymbol{r}_f)\,\psi_0(r_s)\,\mathrm{d}\boldsymbol{r}_f\,\mathrm{d}\boldsymbol{r}_s \qquad (19a)$$

and the exchange amplitude by

$$g(\boldsymbol{k}_f, \boldsymbol{k}_s) = -\frac{1}{(2\pi)^{5/2}} \int \psi^{-*}(z_s, \boldsymbol{k}_s, \boldsymbol{r}_f)\, \psi^{-*}(z_f, \boldsymbol{k}_f, \boldsymbol{r}_s) \left( V_{sf} - \frac{(1-z_f)}{r_s} - \frac{(1-z_s)}{r_f} \right)$$

$$\times \exp(i\,\boldsymbol{k}_0 \cdot \boldsymbol{r}_f)\, \psi_0(r_s)\, d\boldsymbol{r}_f\, d\boldsymbol{r}_s. \tag{19b}$$

Note that when we exchange the particles we also exchange the effective charges; the same $z_s, z_f$ being used in the direct and exchange amplitudes. Given the amplitudes (19) the spin averaged triple differential cross section is given by

$$\frac{d^3\sigma}{d\Omega_f\, d\Omega_s\, dE} = \frac{k_s k_f}{4k_0} (|f+g|^2 + 3|f-g|^2). \tag{20}$$

## 3. Choices of Effective Charges

In the formalism given above the potentials $V_s, V_f, V_{sf}$ have been treated as finite range potentials, albeit of very long extension. A theory of ionisation in which the Coulomb potentials are treated exactly to infinity has been developed (Peterkop 1960, 1962; Rudge and Seaton 1965). Apart from an overall phase factor, which disappears on forming the cross section (20), the results so obtained are in agreement with (15) and (19). However, this analysis (Peterkop 1962) requires that $z_s, z_f$ be chosen to satisfy

$$\frac{z_s}{k_s} + \frac{z_f}{k_f} = \frac{1}{k_s} + \frac{1}{k_f} - \frac{1}{\|\boldsymbol{k}_s - \boldsymbol{k}_f\|}, \tag{21}$$

in order to avoid an indeterminate phase factor in (15). The Peterkop relation (21) is an inevitable consequence of the long range treatment and 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 fields (16) should equal their true potential energy in the field $V_j$ (Rudge 1968). However, in (19) when we approximated $\Psi^+(\boldsymbol{r}_f, \boldsymbol{r}_s)$ by

$$\Phi_i = \psi_0(r_s) \exp(i\,\boldsymbol{k}_0 \cdot \boldsymbol{r}_f),$$

we lost the correct asymptotic form for an ionisation problem:

$$\lim_{r_s \to \infty, r_f \to \infty} \Phi_i = 0.$$

Here $\Phi_i$ is zero almost everywhere on the hypersphere $\rho = (r_s^2 + r_f^2)^{1/2}$ (see Rudge and Seaton 1965) and we no longer need the Peterkop relation (21) to avoid indeterminate phase factors.

In these circumstances it is not clear *a priori* whether (21) is an important condition to impose on the effective charges, especially as we have seen that it plays no role in an entirely consistent formulation in terms of short range potentials. We will discuss the significance of imposing the Peterkop condition within the limits of first order perturbation theory in a latter communication

(Whelan *et al.* 1990). However, (21) does present a criterion for the selection of $z_s, z_f$. In the calculations below we consider the following choices for the effective charges: $z_s = 1, z_f = 0$, i.e. the first Born approximation; $z_s = 1, z_f = 1$, the Coulomb projected Born approximation (CPB); and also

(i)

$$z_s = 1,$$

$$z_f = 1 - \frac{k_s}{\| \mathbf{k}_s - \mathbf{k}_f \|},$$

i.e. the slow electron sees the full nuclear charge at all times.

(ii)

$$z_s = 1 - \frac{k_s \, \mathbf{k}_s \cdot (\mathbf{k}_s - \mathbf{k}_f)}{\| \mathbf{k}_s - \mathbf{k}_f \|^3},$$

$$z_f = 1 - \frac{k_f \, \mathbf{k}_f \cdot (\mathbf{k}_f - \mathbf{k}_s)}{\| \mathbf{k}_s - \mathbf{k}_f \|^3},$$

see Schulz (1973, approximation A6).

(iii)

$$z_s = 1 - \frac{k_s^{n+1}}{(k_s^n + k_f^n) \| \mathbf{k}_s - \mathbf{k}_f \|},$$

$$z_f = 1 - \frac{k_f^{n+1}}{(k_s^n + k_f^n) \| \mathbf{k}_s - \mathbf{k}_f \|},$$

see also Schweitzer and Klapish (1987). We only consider $n = 1$ here.

All five approximations satisfy the physically reasonable requirement that as

$$k_s \to 0,$$

then

$$z_s \to 1.$$

The approximations (i), (ii) and (iii) satisfy the Peterkop relation (21), while B1 and CPB do not. Of course if $k_s \to 0$ or $k_f \to \infty$ then (21) reduces to $z_s = 1$ which is obeyed by all the approximations. However, the Rudge–Seaton–Peterkop scattering amplitude contains an indeterminate phase factor for all finite values of $k_s$ and $k_f$ if either the B1 or CPB choices of $z_s$ and $z_f$ are employed. It is frequently assumed that in the limit of zero ejection energy that the slow electron should totally screen the fast electron from the nucleus, i.e. when $k_s \to 0$ we should have

$$z_s \to 1, \quad z_f \to 0. \tag{22}$$

It should be noted that the CPB differs from the other choices of effective charges in respect that (22) is not valid; it assumes that both escaping electrons always see the full nuclear charge. Both (ii) and (iii) have the advantage that they are symmetric in $k_s$ and $k_f$, i.e.

$$z_s(k_s, k_f) = z_f(k_f, k_s).$$

We include exchange as in (19b) for the Coulomb projected Born approximation, hereafter denoted CPBX, and in (i), (ii) and (iii).

## 4. Evaluation of Integrals

The evaluation of (19) essentially reduces to the evaluation of integrals of the form

$$I_n = \int \exp(-\lambda r_s) \exp(-i\, k_s \cdot r_s) \exp\{i\,(k_0 - k_f) \cdot r_f\} A(n)$$

$$\times\, _1F_1(a_s, 1, i(k_s r_s + k_s \cdot r_s))\, _1F_1(a_f, 1, i(k_f r_f + k_f \cdot r_f))\, dr_s\, dr_f, \qquad (23)$$

with

$$A(1) = -(1 - z_s)/r_s, \qquad A(2) = -(1 - z_f)/r_f,$$

$$A(3) = \frac{1}{\| r_f - r_s \|},$$

$$a_s = i\frac{z_s}{k_s}, \qquad a_f = i\frac{z_f}{k_f}.$$

Well known analytic expressions exist when $n = 1, 2$ (Coleman 1969). The case $n = 3$ is much more difficult and there have been a number of alternative approaches to its computation proposed (Geltman and Hidalgo 1974; Schulz 1971). We have chosen to follow the analyses of Sinha and Sil (1979) and Roy *et al.* (1980).[*] It can be shown that $I_3$ may be written as a single integral over the real variable $v$:

$$I_3 = \text{constant} \int_0^\infty dv\, N(v), \qquad (24)$$

where

$$N(v) = \lim_{\sigma \to 0} \frac{\partial^2}{\partial\lambda\,\partial\sigma} \left\{ \frac{1}{U} \exp(i\,\pi a_f)\left(\frac{U}{Y}\right)^{a_f}\left(\frac{Y}{Y+W}\right)^{a_s}\right\}\, _2F_1\left(1 - a_f, a_s, 1, \frac{UW - VY}{U(Y+W)}\right), \quad (25)$$

[*] Unfortunately the Roy *et al.* paper, which is the most detailed account of the method, contains a confusing series of misprints: on p. 3446 they define the quantities $\{X_i, Y_i, Z_i\}_{i=1,4}$ which apparently depend on $y$, a variable which should have disappeared in an earlier integration. Throughout their 12 definitions, $y$ should be replaced by $\lambda$.
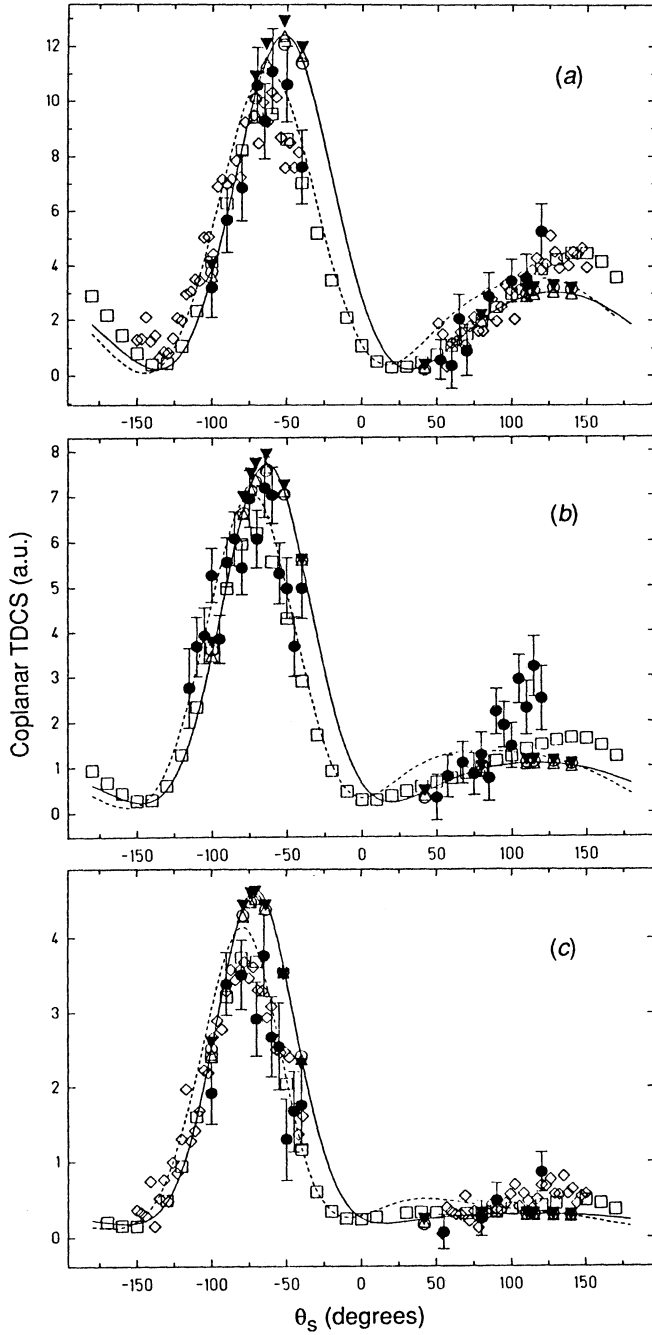
**Fig. 1.** Coplanar triple differential cross section as a function of the ejected electron angle $\theta_S$ for $E_0 = 250$ eV and $E_s = 5$ eV; (a) $\theta_f = 3°$, (b) $\theta_f = 5°$ and (c) $\theta_f = 8°$ :

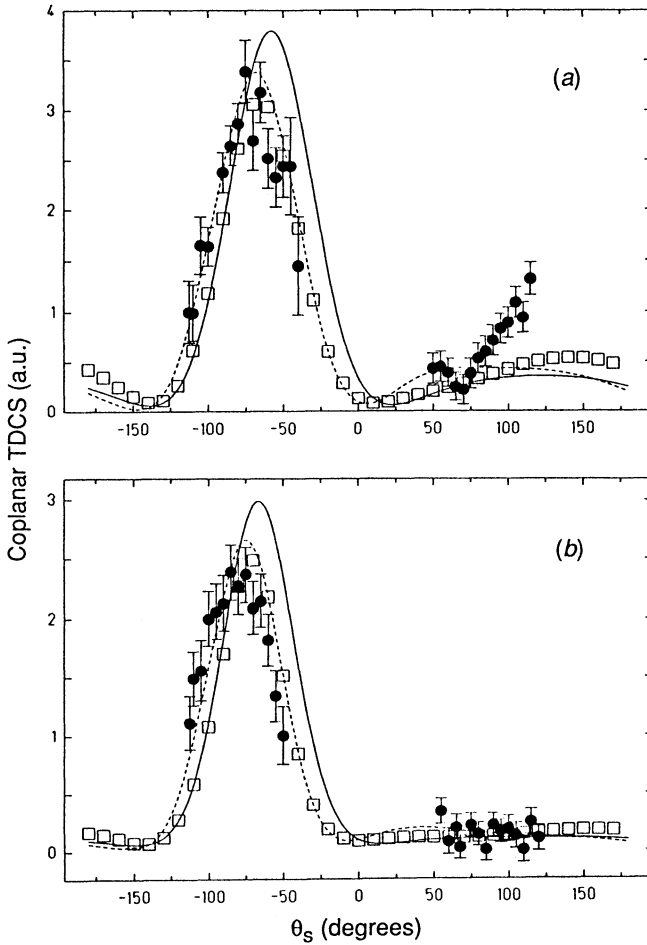Experiment:  ◇ Erhardt *et al.* (1986, 1989)   ● Lohmann *et al.* (1984)

Theory:        —— B1      ---- CPBX

△, ○, ▼ Effective charge approximation (i), (ii), (iii)

□ Pseudo state approximation (Curran and Walters 1987)

■ EBS (Byron *et al.* 1983, 1985)

**Fig. 2.**  As for Fig. 1 but with $E_0 = 250$ eV, $E_s = 10$ eV: (*a*) $\theta_f = 5°$ and (*b*) $\theta_f = 8°$.

and where $U, V, W, Y$ are polynomials of the form $\alpha v^2 + \beta v + \gamma$ with $\alpha, \beta, \gamma$ complex depending on $k_0, k_f, k_s, \sigma, \lambda$. Therefore $N(v)$ is simply a sum over algebraic terms multiplied by hypergeometric functions; recall that $(d/dz)_2F_1(a, b, c, z) = {}_2F_1(a+1, b+1, c+1, z)$. The hypergeometric functions were evaluated by direct expansion using the linear transformations specified in Abramowitz and Stegun (1972) and the complex gamma functions using the method of Lanczos (1964). The one dimensional integral over $v$ in (24) was evaluated numerically.

## 5. Results

In this section we compare our theoretical predictions with the experimental results of the Kaiserslautern group (Ehrhardt *et al.* 1986, 1989; Klar *et al.* 1987). These experiments considered events where the incident, scattered and ejected electron lie in a single plane. It will be convenient to introduce polar
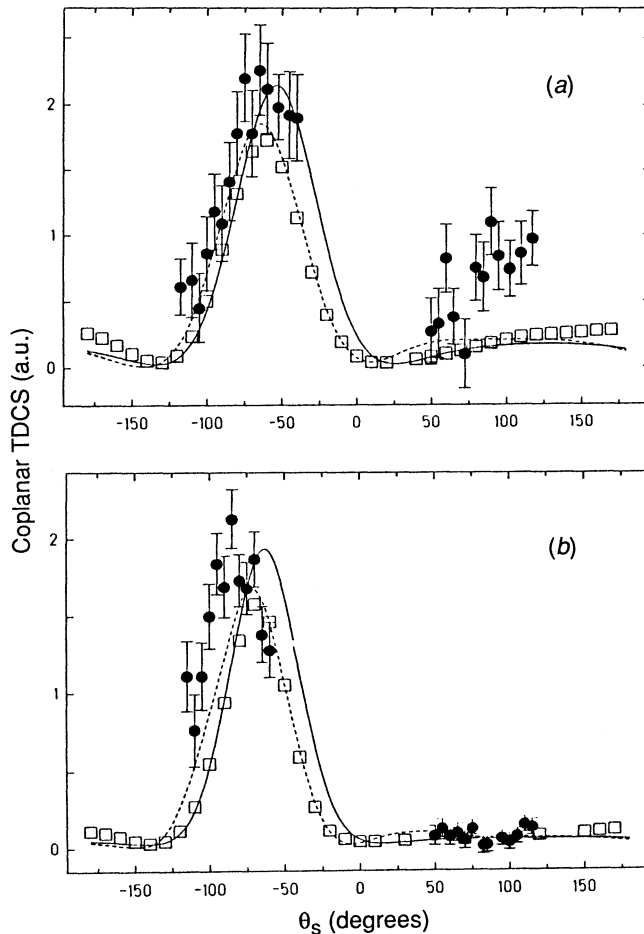
**Fig. 3.** As for Fig. 1 but with $E_0 = 250$ eV, $E_s = 14$ eV: (a) $\theta_f = 5°$ and (b) $\theta_f = 8°$.

coordinates $r = (r, \theta)$, the slow and fast electron angles $\theta_s, \theta_f$ being measured with respect to the incident direction (i.e. $\theta_0 = 0$). We follow the convention that

$$-\pi < \theta \leq \pi.$$

Negative angles correspond to clockwise, positive to anti-clockwise rotation of the $\theta = 0$ axis. Each experiment was a series of measurements of the TDCS, as $\theta_s$ varied with all other parameters $(E_s, E_0, \theta_f)$ fixed.

Ehrhardt and his collaborators (Ehrhardt *et al.* 1986, 1989) have made absolute measurements of the TDCS for $E_0 = 250$ eV, $E_s = 5$ eV, $\theta_f = 3°, 8°$ and for $E_0 = 150$ eV, $E_s = 3, 5, 10$ eV, $\theta_f = 4°, 10°, 16°$. Lohmann *et al.* (1984) have made relative measurements for $E_0 = 250$ eV, $E_s = 5, 10, 14$ eV, $\theta_f = 3°, 5°, 8°$. In Table 1 of their paper Lohmann *et al.* (1984) quoted absolute cross sections obtained
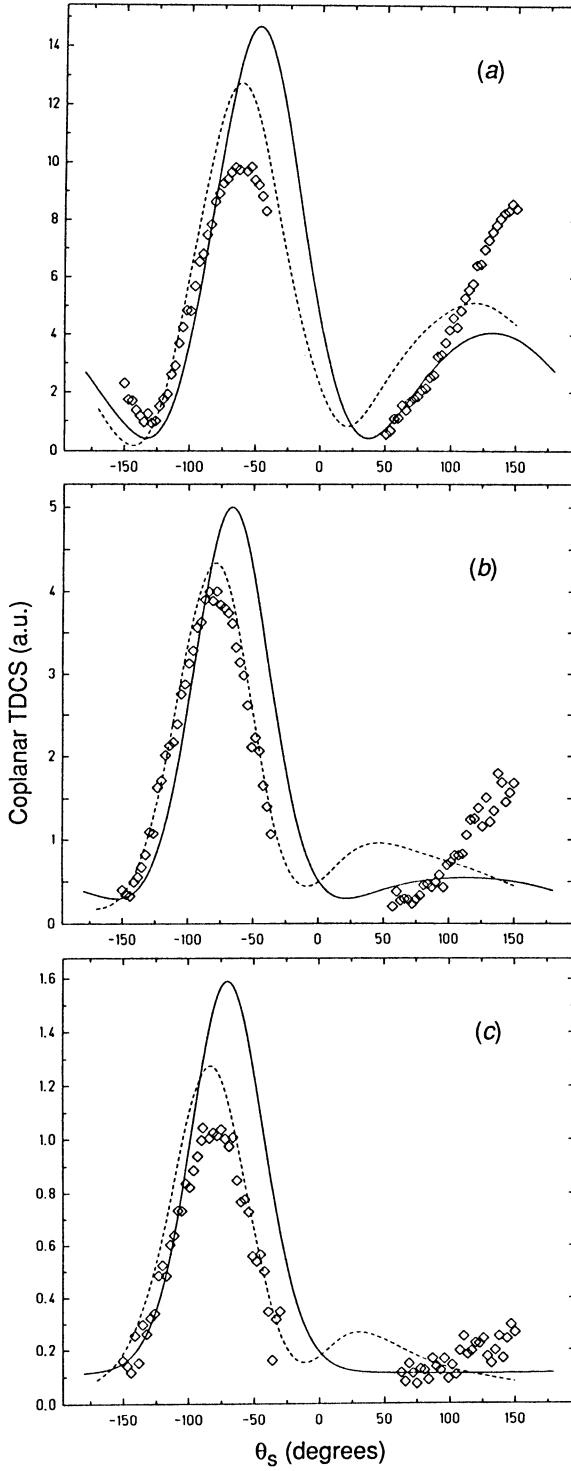
**Fig. 4.** As for Fig. 1 but with $E_0 = 150$ eV, $E_s = 3$ eV: (a) $\theta_f = 4°$, (b) $\theta_f = 10°$, (c) $\theta_f = 16°$.
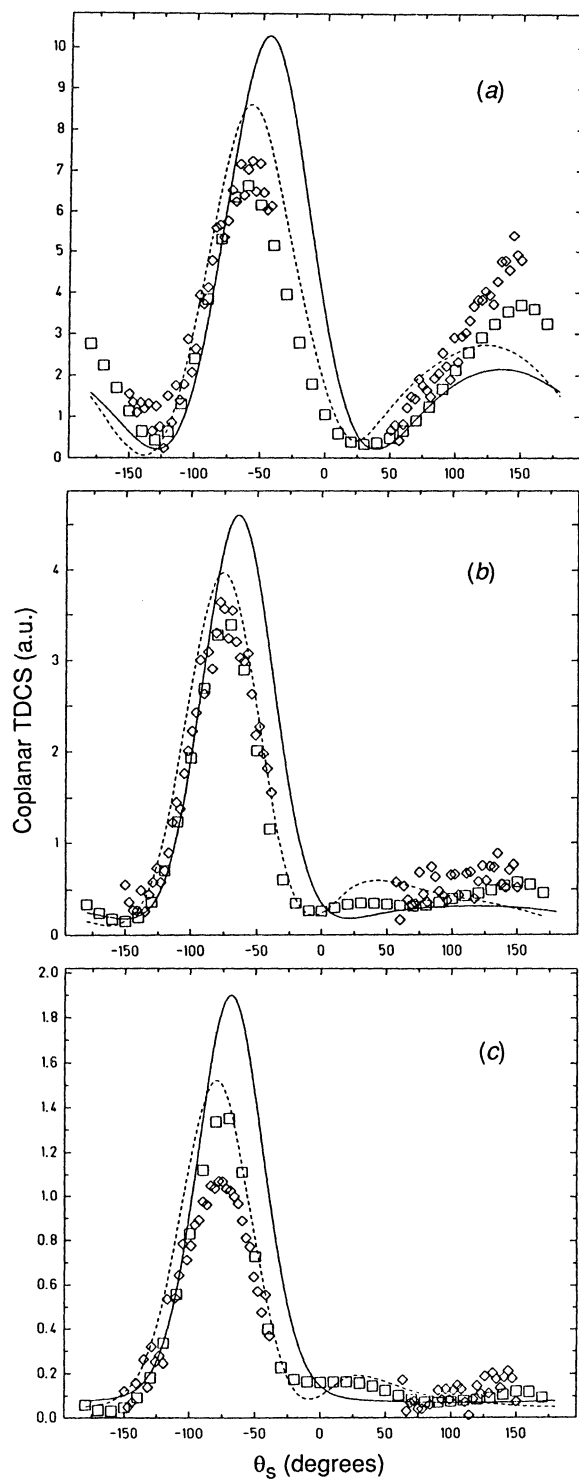
**Fig. 5.** As for Fig. 1 but with $E_0 = 150$ eV, $E_s = 5$ eV: (a) $\theta_f = 4°$, (b) $\theta_f = 10°$, (c) $\theta_f = 16°$.
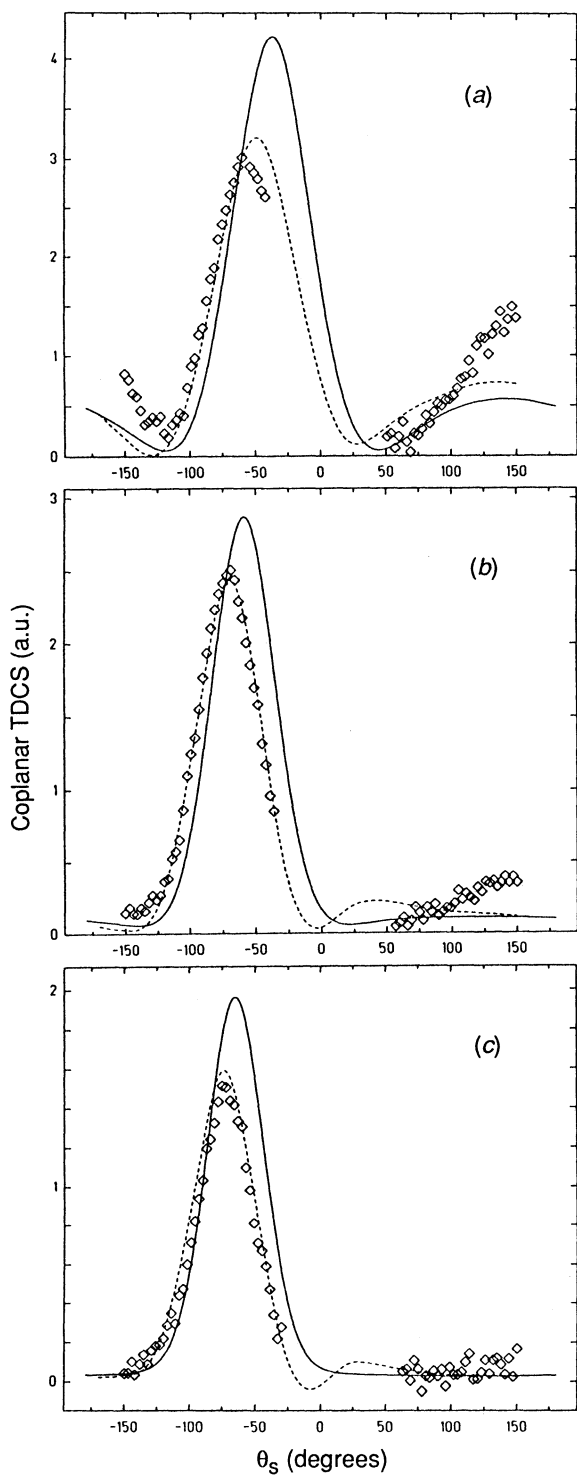
**Fig. 6.** As for Fig. 1 but with $E_0 = 150$ eV, $E_s = 10$ eV: (a) $\theta_f = 4°$, (b) $\theta_f = 10°$, (c) $\theta_f = 16°$.

by normalisation of their relative data to the second Born calculations of Byron *et al.* (1983) at $E_0 = 250$ eV, $E_s = 10$ eV, $\theta_f = 5°$ and $\theta_s = -70°$. We use the normalised data in our figures; for present purposes we did not consider it worth while to change the normalisation.

Also shown in our figures are theoretical results calculated in the first Born (B1) and the eikonal-Born series (EBS) approximation of Byron *et al.* (1983, 1985), and in the coupled pseudo-state model of Curran and Walters (1987). We consider the latter two approximations to be amongst the best quantum calculations presently available, against which it is useful to judge the present work. Comparison with B1 is crucial, since it is improvement upon B1 which shows whether our approximations are good or bad. The defects in B1 for asymmetric geometry, which one hopes to correct with a better theory, are now documented (see e.g. Curran and Walters 1987): the binary peak is generally too large and needs to be moved to more negative $\theta_s$; the recoil peak is too small and needs to be shifted to larger positive $\theta_s$. This is made clear by comparison with the experimental data in Figs 1–6.

Our effective charges approximations (i), (ii) and (iii) are exhibited in Fig. 1 for $E_0 = 250$ eV. It is clear that these choices do not work—the results differ little from B1. This is illustrative of our more general experience that effective charges chosen to satisfy (21) and (22), particularly (22), give poor results. A sharp contrast to this is provided by the CPBX approximation which in the binary region gives a substantial improvement over B1 (Figs 1–3, 5) and generally moderately good agreement with experiment (Figs 1–6). The failure of the effective charge approximations (i)–(iii) is consistent with the earlier results of Rudge and Schwartz (1966) and Schulz (1973).

**Table 1. Comparison of the momentum transfer direction $\theta_K$ and the angular position of the binary peak as given by experiment and theory for $E_0 = 250$ eV**

| $E_s$ | $\theta_f$ | $\theta_K$ | Expt[A] | DWIA-I | DWIA-II | DWIA-III | B1[B] | CPBX | B2[C] |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 3 | 52 | 63±5 | 63 | 53 | 84 | 52 | 63 | 63 |
| 5 | 5 | 64 | 69±2 | 70 | 63 | 83 | 64 | 74 | 71 |
| 5 | 8 | 71 | 78±2 | 73 | 71 | 82 | 71 | 79 | 77 |
| 10 | 5 | 58 | 70±2 | 65 | 58 | 80 | 58 | 68 | 66 |
| 10 | 8 | 67 | 81±2 | 70 | 69 | 78 | 67 | 75 | — |
| 14 | 5 | 54 | 70±3 | 64 | 57 | 78 | 54 | 64 | — |
| 14 | 8 | 63 | 84±2 | 68 | 64 | 79 | 63 | 72 | — |

[A] Lohmann *et al.* (1984).
[B] Byron *et al.* (1983).
[C] Byron *et al.* (1985).

A careful comparison of CPBX with the data of Ehrhardt *et al.* (1986, 1989) suggests that there is a tendency for CPBX to slightly overestimate the binary peak height, although this is not always the case (see Fig. 6*b*); it should be remembered that Ehrhardt *et al.* did not give extensive experimental error estimates for their data and that we are comparing with the scatter of experimental points which they have kindly supplied. Also they estimated a normalisation error of 15% in the generation of their absolute data. However, the comparison between the pseudo-state calculation of Curran and Walters (1987) and CPBX would tend to support the view that CPBX may be slightly

too large in the binary region. The CPBX generally yields a good estimate of the position of the binary peak (see Table 1).

Of particular interest is the comparison with the new experimental data of Ehrhardt *et al.* (1989) at $E_0 = 150$ eV, $E_s = 3, 10$ eV. At $E_s = 3$ eV (Fig. 4) the CPBX exceeds the experimental maximum by approximately 28%, 8% and 23% (again it is important to remember that there is a 15% normalisation error and no error bars given for the experimental data) at the angles $\theta_f = 4°, 10°, 16°$ respectively. In comparison with the older data at $E_0 = 150$ eV, $E_s = 5$ eV (Fig. 5), the corresponding excesses are 20%, 10%, 44%. The difference of 44% at $\theta_f = 16°$ seems rather large. Here (Fig. 5c) even the coupled pseudo-state approximation of Curran and Walters (1987) is larger than the experimental data by a significant amount; CPBX is a mere 13% above the pseudo-state numbers at the maximum.

The situation at $E_0 = 150$ eV, $E_s = 10$ eV (Fig. 6) presents a somewhat different picture to Figs 4 and 5. Here for $\theta_f = 10°$ and $16°$ there is very good accord between CPBX and experiment, especially at $\theta_f = 10°$ (Fig. 6b); for $\theta_f = 4°$ (Fig. 6a) the experimental and CPBX peak heights are again in quite good agreement, but the experimental peak looks significantly sharper. However, a lack of experimental data around the peak and absence of error bars makes it difficult to come to any specific conclusions.

Generally speaking, the CPBX is much less successful in the recoil direction; occasionally, however, the pseudo-state TDCS exhibits some interesting structure in the recoil direction. In particular, when the cross section is small, it can have two maxima, with the position of the first of these in rough accord with the single maximum of CPBX (see e.g. Fig. 5c). However, the TDCS is very small in these cases and it would be unwise to draw any general conclusions. Finally, it is interesting to note that the large recoil peaks were observed in cases when the momentum transfer and hence the $\boldsymbol{k}_{\mathrm{recoil}}$ of (4) was small, and if $\|\boldsymbol{k}_{\mathrm{recoil}}\|$ becomes greater than 1 the recoil peak dies away. For example contrast Fig. 1a where $\|\boldsymbol{K}\| = 0 \cdot 27$ a.u., i.e. $\|\boldsymbol{k}_{\mathrm{recoil}}\|_{\mathrm{max}} = 0 \cdot 64$ a.u. and Fig. 2b where $\|\boldsymbol{K}\| = 0 \cdot 62$ a.u., i.e. $\|\boldsymbol{k}_{\mathrm{recoil}}\|_{\mathrm{max}} = 1 \cdot 4$ a.u.

## 6. Conclusions

We have compared various effective charge approximations, within the context of a first order perturbative model, with the latest good quality experimental data and recent calculations for high energy asymmetric geometry. We have explored a number of prescriptions where in the limit of zero ejection energy the slow electron sees the full nuclear charge, while the scattered electron is totally screened from the nucleus. These have returned only poor results. We are of the opinion that these prescriptions have nothing to offer. We were able to achieve reasonable but not perfect agreement with experiment in the important binary peak region by assuming that the nucleus was totally unscreened for both the outgoing electrons, i.e. the CPBX approximation. These results are consistent with earlier more complex calculations which employ effective charges. For example, Smith *et al.* (1979) considered a different asymmetric geometry from ours in a number of distorted wave approximations, getting their best results with an approximation where the scattered and ejected electron move in pure Coulomb fields of unit charge, i.e. essentially the same

choice of $z$ values as in the CPBX. However, this approximation failed at large scattering angles paralleling the failure of the CPBX in the recoil direction. Weigold *et al.* (1979) employed various effective charge models within the framework of the distorted wave impulse approximation and found only poor results when they imposed the Peterkop condition. They found their best results for the forward peak when $z_s = z_f = 1$ (as did Lohmann *et al.* 1984).

These results and ours suggest that there is a need to further investigate the role of the interaction between the fast electron and the nucleus. If nothing else the CPBX approximation presents a formula for generating a significantly better TDCS than the first Born approximation in the important binary peak region. Also once programmed, it is not so time consuming as the other high quality methods presently in use. These two observations recommend the CPBX as a suitable vehicle for calculating reasonable integrated ionisation cross sections, i.e. double, single differential and total.

Finally, we remark that there has recently appeared an alternative approach to this problem (Brauner *et al.* 1989) where a correlated three body continuum wavefunction is used to describe the final state. We will present a more detailed discussion of this work elsewhere (Curran *et al.* 1990).

Also we should mention the treatment of Popov and Benayoun (1981) (see also Avaldi *et al.* 1986; Klar and Franz 1986) who produced an interesting semiclassical approach to ionisation where the triple differential cross sections, calculated in for example the first Born or impulse approximation, are modified by taking into account classically, the changes in the asymptotic paths of the two electrons due to post collisional interactions.

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### References

Abramowitz, M., and Stegun, I. A. (1972). 'Handbook of Mathematical Functions' (Dover: New York).
Avaldi, R., Camilloni, R., Popov, Yu. V., and Stefani, G. (1986). *Phys. Rev.* A **33**, 851.
Bethe, H. A., and Salpeter, E. E. (1957). 'Quantum Mechanics of One and Two Electron Atoms' (Springer: Berlin).
Brauner, M., Briggs, J. S., and Klar, H. (1989). *J. Phys.* B **22**, 2265.
Byron, Jr, F. W., Joachain, C. J., and Piraux, B. (1983). *Phy. Lett.* A **99**, 427.
Byron, Jr, F. W., Joachain, C. J., and Piraux, B. (1985). *J. Phys.* B **18**, 3203.
Coleman, J. P. (1969). 'Case Studies in Atomic Collision Physics', Vol. 1 (Eds E. W. McDaniel and M. R. C. McDowell) (North Holland: Amsterdam).

Curran, E. P. (1986). Ph.D. thesis, Queen's University of Belfast.
Curran, E. P., and Walters, H. R. J. (1987). *J. Phys.* B **20**, 337.
Curran, E. P., Whelan, C. T., and Walters, H. R. J. (1990). *J. Phys.* B (in press).
Ehrhardt, H., Jung, K., Knoth, G., and Schlemmer, P. (1986). *Z. Phys.* D **1**, 3.
Ehrhardt, H., and Schlemmer, P. (1989). personal communication.
Geltman, S., and Hidalgo, M. B. (1974). *J. Phys.* B **7**, 831.
Goldberger, M. L., and Watson, K. M. (1964). 'Collision Theory' (Wiley: New York).
Klar, H., and Franz, A. (1986). *Phys. Rev.* A **33**, 2103.
Klar, H., Roy, A. C., Schlemmer, P., Jung, K., and Ehrhardt, H. (1987). *J. Phys.* B **20**, 821.
Lanczos, C. (1964). *Journal SIAM, Num. Anal.* **1**, 86.
Lohmann, B., McCarthy, I. E., Stelbovics, A. T., and Weigold, E. (1984). *Phys. Rev.* A **30**, 758.
Peterkop, R. K. (1960). *Proc. Phys. Soc. London* **77**, 1220.
Peterkop, R. K. (1962). *Optics Spectrosc.* **13**, 87.
Popov, Yu. V., and Benayoun, J. J. (1981). *J. Phys.* B **14**, 3513.
Roy, A., Roy, K., and Sil, N. C. (1980). *J. Phys.* B **13**, 3443.
Rudge, M. R. H. (1968). *Rev. Mod. Phys.* **40**, 564.
Rudge, M. R. H., and Schwartz, S. B. (1966). *Proc. Phys. Soc. London* **88**, 563.
Rudge, M. R. H., and Seaton, M. J. (1965). *Proc. R. Soc. London* A **283**, 262.
Schulz, M. (1971). *J. Phys.* B **4**, 1476.
Schulz, M. (1973). *J. Phys.* B **6**, 2580.
Schweitzer, C., and Klapish, M. (1987). Fourteenth ICPEAC Conf., Abstracts of Contributed Papers (Eds J. Geddes *et al.*), p. 380.
Sinha, C., and Sil, N. C. (1979). *J. Phys.* B **12**, 1711.
Smith, J. J., Winters, K. H., and Bransden, B. H. (1979). *J. Phys.* B **12**, 1723.
Weigold, E., Noble, C. J., Hood, S. T., and Fuss, I. (1979). *J. Phys.* B **12**, 291.
Whelan, C. T., Walters, H. R. J., Hanssen, J., and Dreizler, R. M. (1989). *Z. Phys.* D **14**, 85.
Whelan, C. T., Walters, H. R. J., and Dreizler, R. M. (1990). Rutherford Lab. Report RAL-90.

## Appendix A

We derive the result (10) from the scattering amplitude (7). The wavefunctions $\Psi^+$ and $\chi_j^-$ appearing in (10) satisfy

$$\Psi^+ = \Phi_i + (E - H + i\eta)^{-1} V_i \Phi_i, \tag{A1}$$

$$\chi_j^- = \Phi_j + (E - H_j - W_j - i\eta)^{-1} W_j \Phi_j, \tag{A2}$$

where $E$ is the total energy and the limit $\eta \to 0^+$ is to be understood, and

$$H_j = T_s + T_f, \tag{A3}$$

so that

$$H = H_j + V_j. \tag{A4}$$

Using (A1) the scattering amplitude (7) may be written as

$$f(\boldsymbol{k}_f, \boldsymbol{k}_s) = -\frac{1}{(2\pi)^{5/2}} \langle \Phi_j \mid V_j + V_j (E - H + i\eta)^{-1} V_i \mid \Phi_i \rangle. \tag{A5}$$

Consider now the following transformation of the operator in (A5):

$$V_j + V_j(E-H+i\eta)^{-1}V_i = V_j + (V_j - W_j)(E-H+i\eta)^{-1}V_i$$

$$+ W_j\{(E-H+i\eta)^{-1} - (E-H_j-W_j+i\eta)^{-1}\}V_i$$

$$+ W_j(E-H_j-W_j+i\eta)^{-1}V_i$$

$$= V_j + (V_j - W_j)(E-H+i\eta)^{-1}V_i$$

$$+ W_j(E-H_j-W_j+i\eta)^{-1}(V_j-W_j)(E-H+i\eta)^{-1}V_i$$

$$+ W_j(E-H_j-W_j+i\eta)^{-1}V_i$$

$$= \{1 + W_j(E-H_j-W_j+i\eta)^{-1}\}$$

$$\times \{V_i + (V_j-W_j)(E-H+i\eta)^{-1}V_i\} + (V_j-V_i). \qquad (A6)$$

Inserting (A6) into (A5) and using (A1) and (A2) we obtain

$$f(\mathbf{k}_f, \mathbf{k}_s) = -\frac{1}{(2\pi)^{5/2}}\{\langle \chi_j^- | V_j - W_j | \Psi^+\rangle$$

$$+ \langle \chi_j^- | V_i - V_j + W_j | \Phi_i\rangle + \langle \Phi_j | V_j - V_i | \Phi_i\rangle\}. \qquad (A7)$$

From (8), (6) and (11), the last term in (A7) has the form

$$\langle \Phi_j | (V_j - V_i) | \Phi_i\rangle = \langle \exp\{i(\mathbf{k}_s \cdot \mathbf{r}_s + \mathbf{k}_f \cdot \mathbf{r}_f)\} | V_s | \psi_0(r_s)\exp(i\mathbf{k}_0 \cdot \mathbf{r}_f)\rangle$$

$$= (2\pi)^3 \delta(\mathbf{k}_f - \mathbf{k}_0)\langle \exp(i\mathbf{k}_s \cdot \mathbf{r}_s) | V_s | \psi_0(r_s)\rangle$$

$$= 0, \qquad (A8)$$

since $\mathbf{k}_f \neq \mathbf{k}_0$, where $\epsilon_0 < 0$. With the last term zero, equation (A7) is the result (10).

## Appendix B

When $W_j$ has the form (12) the second term in (10) becomes, using (6), (11) and (12),

$$\langle \chi_j^- | V_i - V_j + W_j | \Phi_i\rangle = \langle \zeta_a^-(\mathbf{k}_f, \mathbf{r}_f) | \exp(i\mathbf{k}_0 \cdot \mathbf{r}_f)\rangle\langle \zeta_b^-(\mathbf{k}_s, \mathbf{r}_s) | -V_s(\mathbf{r}_s) + V_b(\mathbf{r}_s) | \psi_0(\mathbf{r}_s)\rangle$$

$$+ \langle \zeta_a^-(\mathbf{k}_f, \mathbf{r}_f) | V_a(\mathbf{r}_f) | \exp(i\mathbf{k}_0 \cdot \mathbf{r}_f)\rangle\langle \zeta_b^-(\mathbf{k}_s, \mathbf{r}_s) | \psi_0(\mathbf{r}_s)\rangle. \quad (A9)$$

From (14) and $(T_s + V_s)\psi_0(r_s) = \epsilon_0 \psi_0(r_s)$, it is easy to show that

$$\langle \zeta_b^-(\mathbf{k}_s, \mathbf{r}_s) | -V_s(\mathbf{r}_s) + V_b(\mathbf{r}_s) | \psi_0(\mathbf{r}_0)\rangle = \left(\frac{k_s^2}{2} - \epsilon_0\right)\langle \zeta_b^-(\mathbf{k}_s, \mathbf{r}_s) | \psi_0(\mathbf{r}_s)\rangle. \quad (A10)$$

Also writing (14) in the integral form

$$\zeta_a^-(\pmb{k}_f, \pmb{r}_f) = \exp(i\,\pmb{k}_f \cdot \pmb{r}_f) + \left(\frac{k_f^2}{2} - T_f - i\eta\right)^{-1} V_a(\pmb{r}_s)\,\zeta_a^-(\pmb{k}_f, \pmb{r}_f)$$

$$= \exp(i\,\pmb{k}_f \cdot \pmb{r}_f) + \frac{2}{(2\pi)^3} \int d\pmb{k}\; \frac{\exp(i\,\pmb{k} \cdot \pmb{r}_f)\langle \exp(i\,\pmb{k} \cdot \pmb{r}_f)\,|\, V_a(\pmb{r}_f)\,\zeta_a^-(\pmb{k}_f, \pmb{r}_f)\rangle}{k_f^2 - k^2 - i\eta},$$

$$\text{(A11)}$$

and remembering that $k_0 \neq k_1$, when $\epsilon_0 < 0$, it is again easy to demonstrate that

$$\langle \zeta_a^-(\pmb{k}_f, \pmb{r}_f)\,|\, \exp(i\,\pmb{k}_0 \cdot \pmb{r}_f)\rangle = \frac{2\langle \zeta_a^-(\pmb{k}_f, \pmb{r}_f)\,|\, V_a(\pmb{r}_f)\,|\, \exp(i\,\pmb{k}_0 \cdot \pmb{r}_f)\rangle}{k_f^2 - k_0^2}. \qquad \text{(A12)}$$

Note that when considering the overlap of two continuum functions it is necessary to proceed cautiously as in (A12) and (A9). Substituting (A10) and (A12) in (A9) and using the fact that

$$k_f^2 + k_s^2 = k_0^2 + 2\epsilon_0, \qquad \text{(A13)}$$

we see that (A9) is zero.