PROTON RECOIL EFFECTS DUE TO VIRTUAL PHOTON EXCHANGE IN THE BINARY ENCOUNTER APPROXIMATION

BY

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I do solemnly declare that this dissertation represents my own work which has not been submitted for a degree at this or another university

Signature..

Dedicated to the memory of my Father

This dissertation of Vincent Habatwa Mweene is approved as fulfilling part of the requirements for the award of the Master of Science Degree in Physics by the University of Zambia

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ABSTRACT

The Binary Encounter Approximation cross-section for inner-shell ionization of atoms by protons is corrected for proton recoil, an effect due to the exchange of virtual photons in proton – electron scattering. The correction is found to be important only at very low projectile energies in high-Z targets.

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CONTENTS

INTRODUCTION

The Binary Encounter Approximation is one of three main approaches to the prediction of cross-sections for inner-shell ionization by charged particle impact. The other two are the Plane Wave Born Approximation[1,2], based on quantum mechanical scattering theory, and the Semiclassical Approximation[3], based on first-order time-dependent perturbation theory.

The first beginnings of the binary encounter approach date from the attempts of J. J. Thomson[4] in 1912 to calculate the energy lost by charged particles passing through matter. It was M. Gryzinski[5,6,7,8,9], however, who comprehensively developed the method and applied it to the prediction of several types of cross-sections. Important additions were later made by others, notably Stabler[10], Vriens[11] and Gerjuoy[12].

In the Binary Encounter Approximation (BEA), the complex ionization process is simplified by the assumption that it is dominated by a direct energy exchange from the projectile to the electron. In the derivation of expressions for the cross-sections, the other components of the target - the nucleus and the other electrons - are therefore ignored. Despite such a seemingly crude assumption, the BEA has been justified by its satisfactory agreement with experiment[13,14,15,16]. But even better agreement can be obtained if the BEA is corrected for the more important features of the ionization process which its basic assumption disregards. The best investigated have been:

(i) The Binding Effect - Before a slow projectile can dislodge an electron from its orbit, it has to penetrate into the shell to which the electron belongs[I7] and its presence there modifies, by its charge, the binding energies in the atom. This effect has been studied by Basbas et. al.,[I7] and Anholt et. al.[I8]

(ii) The Coulomb Retardation Effect[I5] - Contrary to the BEA assumption that the nuceus of the target atom is passive during the ionization process, it actually modifies the trajectory and the energy of a positive projectile by curving the one and reducing the other. For a negatively-charged projectile, the curve is reversed and the energy is increased. Thomas et. al.,[I5] Garcia[I4], Basbas et. al.,[I7] Bang et. al.,[3] Caruso et. al.,[I9] and Kocbach[20] have investigated this effect.

(iii) The Relativistic Effect - The classical formulation of the BEA is inadequate to deal with ionization of atoms in which the target electrons travel at relativistic velocities. Corrections for this effect have been studied by Amundsen et. al.,[2I] Anholt[22], Hansen[23], Avaldi et. al.,[24,25] and Sheth[I6].

(iv) Spin Effects - If the spins of the projectile and the electron are taken into account when the two particles interact, the energy transferred from one to the other is different from the case when the particles are assumed to be spinless[23].

Sheth[16] has included the effects of spin in the BEA.

This dissertation in an attempt to correct the BEA ionization cross-section for proton recoil effects in ionization of atoms by proton impact. The exchange of photons between the particles in proton - electron scattering is a consequence of the circumstance that virtual photons transmit the Coulomb force. The proton suffers a finite recoil as a result of the exchange of these photons. When this recoil is included, the differential scattering cross-section for proton - electron scattering is modified. The use of the new cross- section in the BEA leads to a different expression for the ionization cross-section.

The outline of the BEA method of obtaining the ionization cross-section is given in Section I of the dissertation. In Section II, the differential cross-section formula which incorporates proton recoil is derived. In Sections II, IV, V and VI, the ionization cross-section is derived by the steps outlined in Section I. The results of applying this cross-section to various cases of K-shell ionization by proton-impact are presented in Section VII. The discussion, in Section VIII, is followed by the conclusion, which closes the dissertation.

SECTION I - THE OUTLINE OF THE BEA METHOD

This outline summarises the method used by Gerjuoy[I2] to obtain the ionization cross-section in the BEA. This method is the most exact of the several available.

(i) The cross-section for the exchange of a fixed quantity of energy ΔE, when a proton and an electron of fixed initial velocities in the laboratory system of coordinates collide is found by relating it to the centre - of - mass differential scattering cross - section proper to the (Coulomb) interaction between them. This cross-section is denoted $\sigma_{\Delta E}(\bar{v}_I, \bar{v}_2)$, where $\bar{v}_I$ and $\bar{v}_2$ are the proton and electron velocities respectively when observed from the laboratory system.

(ii) The effective cross - section for the exchange of energy ΔE is obtained from $\sigma_{\Delta E}(\bar{v}_I, \bar{v}_2)$ by averaging it over all directions of the velocities $\bar{v}_I$ and $\bar{v}_2$. It is denoted $\sigma^{eff}_{\Delta E}(\bar{v}_I, \bar{v}_2)$.

(iii) The ionization cross - section, $\sigma(v_2)$, for an electron initially travelling with speed v_2 is obtained by integrating $\sigma^{eff}_{\Delta E}(\bar{v}_I, \bar{v}_2)$ over all vaues of ΔE resulting in ionization.

(iv) Finally, the ionization cross-section per electron in a given atomic shell is obtained from $\sigma(v_2)$ by averaging this quantity over the velocity distribution function of the electron. This step is necessary because v_2 cannot actually be fixed arbitrarily, but is determined by the velocity distribution function.

SECTION II – THE RECOIL DIFFERENTIAL SCATTERING CROSS – SECTION

The differential scattering cross – section for proton – electron recoil scattering can be derived from the relation

$$\sigma(\bar{n} \to \bar{n}') = \frac{q'}{q} \left| \frac{T_{fi}^{cov}}{8\pi W} \right|^2 ,$$ (Scadron, 1979:190)[26]

where

$\sigma(\bar{n} \to \bar{n}')$ is the differential scattering cross – section for two particles interacting arbitrarily, and seen from the centre – of – momentum (c–o–m) system, $\bar{n}$ is the direction of their relative velocity before scattering, seen from the laboratory system, and $\bar{n}'$ is the direction of the same vector after scattering.

q is the magnitude of the momentum of either particle viewed from the c–o–m system before scattering.

q' is the magnitude of the momentum of either particle viewed from the c–o–m system after scattering.

W is the total energy of the two particles seen from the c–o–m system.

T_{fi}^{cov} is the co–variant T–matrix element determined by the interaction between the two particles comprising the scattering system.

For elastic scattering, which obtains here, $q = q'$.

Therefore,

$$\sigma(\bar{n} \to \bar{n}') = \left| \frac{T_{fi}^{cov}}{8\pi W} \right|^2$$

For spin-$\frac{1}{2}$ recoil scattering,

$$\left| T_{fi}^{cov} \right|^2 = \frac{4e^4}{t^2} \left[(s - m_1^2c^4 - m_2^2c^4)^2 + st + \tfrac{1}{2}t^2 \right] \quad (1)$$

(Scadron, 1979:207)[26]

where

e is the charge of the electron.

s and t are Mandelstam invariants (Scadron, 1979:185)[26] which characterise the scattering system.

m_1 and m_2 are the rest-masses of, in this case, the proton and the electron respectively.

c is the speed of light in vacuum.

In the c-o-m system, $s = W^2$ and $t = -4q^2c^2W^2\sin^2\frac{\chi}{2}$ with χ as the scattering angle in that frame. When these definitions are used in expression (1), the result is

$$\left|T_{fi}^{cov}\right|^2 = \frac{e^4}{4q^4c^4\sin^4\frac{\chi}{2}}\left[(W^2-m_1^2c^4-m_2^2c^4)^2-4q^2c^2W^2\sin^2\frac{\chi}{2} + 8q^4c^4\sin^4\frac{\chi}{2}\right],$$

so that

$$\sigma(\bar{n}\rightarrow\bar{n}') = \frac{\alpha^2}{4q^4c^4\sin^4\frac{\chi}{2}}\left[\frac{(W^2-m_1^2c^4-m_2^2c^4)^2}{4W^2}-q^2c^2\sin^2\frac{\chi}{2} + \frac{2q^4c^4}{W^2}\sin^4\frac{\chi}{2}\right] \qquad (2)$$

where $\alpha = \frac{e^2}{4\pi}$.

Expression (2) is relativistic; to incorporate proton recoil effects into the BEA, it is enough to employ the low-energy limit of the expression. Observing that[27]

$$W^2 = (m_1\gamma_1 + m_2\gamma_2)^2 - (\bar{p}_1 + \bar{p}_2)^2c^2$$

and $$q^2c^2 = \frac{(W^2-(m_1+m_2)^2c^4)(W^2-(m_1-m_2)^2c^4)}{4W^2},$$

this limit is easily derived. Here,

$$\gamma_1 = \frac{1}{(1-v_1^2/c^2)^{\frac{1}{2}}}, \qquad \gamma_2 = \frac{1}{(1-v_2^2/c^2)^{\frac{1}{2}}},$$

$$\bar{p}_1 = m_1\gamma_1\bar{v}_1 \qquad \text{and} \qquad \bar{p}_2 = m_2\gamma_2\bar{v}_2.$$

Thus,

$$W^2 = m_1^2\gamma_1^2c^4 + m_2^2\gamma_2^2c^4 + 2m_1m_2\gamma_1\gamma_2c^4 - m_1^2\gamma_1^2v_1^2c^2$$

$$- m_2^2\gamma_2^2v_2^2c^2 - 2m_1m_2\gamma_1\gamma_2c^2\bar{v}_1\cdot\bar{v}_2$$

$$= m_1^2\gamma_1^2c^4\,(1 - v_1^2/c^2) + m_2^2\gamma_2^2c^4\,(1 - v_2^2/c^2) + 2m_1m_2\gamma_1\gamma_2c^4\left(1 - \frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right)$$

$$= m_1^2c^4 + m_2^2c^4 + 2m_1m_2\gamma_1\gamma_2c^4\left(1 - \frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right)$$

$$\cong m_1^2c^4 + m_2^2c^4 + 2m_1m_2c^4$$

$$= (m_1 + m_2)^2c^4 \doteq M^2c^4; \qquad M = m_1 + m_2\,.$$

Since $W^2 = m_1^2c^4 + m_2^2c^4 + 2m_1m_2\gamma_1\gamma_2c^4\left(1 - \frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right)$,

it follows that

$$W^2 - (m_1 + m_2)^2c^4 = 2m_1m_2\gamma_1\gamma_2c^4\left(1 - \frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right) - 2m_1m_2c^4$$

$$= 2m_1m_2c^4\left(\gamma_1\gamma_2 - \gamma_1\gamma_2\frac{\bar{v}_1\cdot\bar{v}_2}{c^2} - 1\right)$$

and $W^2 - (m_1 - m_2)^2c^4 = 2m_1m_2c^4\left(\gamma_1\gamma_2 - \gamma_1\gamma_2\frac{\bar{v}_1\cdot\bar{v}_2}{c^2} + 1\right).$

Thus $(W^2 - (m_1 + m_2)^2c^4)(W^2 - (m_1 - m_2)^2c^4) =$

$$4m_1^2m_2^2c^4\left(\gamma_1^2\gamma_2^2\left(1 - \frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right)^2 - 1\right)$$

$$= \quad 4m_1^2m_2^2c^4\left(\gamma_1^2\gamma_2^2 - 1 + \gamma_1^2\gamma_2^2\frac{(\bar{v}_1\cdot\bar{v}_2)^2}{c^4} - 2\gamma_1^2\gamma_2^2\frac{\bar{v}_1\cdot\bar{v}_2}{c^2}\right).$$

It is easy to verify that

$$\bar{v}_1\cdot\bar{v}_2 = \frac{v_1^2 + v_2^2 - v^2}{2}$$

where $\quad v = \left|\bar{v}_1 - \bar{v}_2\right|$

and $\gamma_1^2\gamma_2^2 - 1 = \frac{\gamma_1^2\gamma_2^2}{c^2}\left(v_1^2 + v_2^2 - \frac{v_1^2v_2^2}{c^2}\right).$

Hence, $(W^2 - (m_1 + m_2)^2c^4)(W^2 - (m_1 - m_2)^2c^4) =$

$$4m_1^2m_2^2\gamma_1^2\gamma_2^2c^4\left(\frac{v_1^2}{c^2} + \frac{v_2^2}{c^2} - \frac{v_1^2v_2^2}{c^4} + \frac{(v_1^2 + v_2^2 - v^2)^2}{4c^4} - \frac{(v_1^2 + v_2^2 - v^2)}{c^2}\right).$$

Rejecting terms of order v_1^4/c^4 , v_2^4/c^4 and v^4/c^4 gives

$$(W^2 - (m_1 + m_2)^2c^4)(W^2 - (m_1 - m_2)^2c^4) = 4m_1^2m_2^2\gamma_1^2\gamma_2^2v^2c^2 .$$

As a result,

$$q^2c^2 = 4m_1^2m_2^2\gamma_1^2\gamma_2^2v^2c^2 = \mu^2\gamma_1^2\gamma_2^2\,v^2c^2 ,$$

where $\quad \mu = \frac{m_1m_2}{M}$.

The other quantity of interest is

$$\frac{(W^2 - m_1^2c^4 - m_2^2c^4)}{4W^2} = \frac{(2m_1m_2\gamma_1\gamma_2c^2(c^2 - \bar{v}_1\cdot\bar{v}_2))^2}{4W^2}$$

$$= \mu^2\gamma_1^2\gamma_2^2(c^2 - \bar{v}_1\cdot\bar{v}_2)^2$$

$$= \mu^2\gamma_1^2\gamma_2^2c^4\left(1 - \frac{2\bar{v}_1\cdot\bar{v}_2}{c^2} + \frac{(\bar{v}_1\cdot\bar{v}_2)^2}{c^2}\right)$$

$$\simeq \mu^2\gamma_1^2\gamma_2^2c^4\left(1 + \frac{v^2}{c^2} - \frac{v_1^2}{c^2} - \frac{v_2^2}{c^2}\right) .$$

When all these low-energy limits are used in expression (2), the cross-section expression becomes

$$\sigma(\bar{n} \to \bar{n}') = \frac{\alpha^2}{4\mu^2v^4\gamma_1^2\gamma_2^2\sin^4\frac{\chi}{2}}\left(1 - \frac{v_1^2}{c^2} - \frac{v_2^2}{c^2} + \frac{v^2}{c^2} - \frac{v^2\sin^2\frac{\chi}{2}}{c^2} + \frac{2\mu^2v^4\sin^4\frac{\chi}{2}}{M^2c^4}\right) . \qquad (3)$$

Scadron uses a system of units such that the potential between an electron and a proton separated by a distance r is $-\frac{\alpha}{r}$; equation (3) is multiplied by $16\pi^2$ to convert it to electrostatic cgs units. The result is

$$\sigma(\bar{n} \to \bar{n}') = \frac{e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{4\mu^2v^4\sin^4\frac{\chi}{2}}\left(1 - \frac{v^2\sin^2\frac{\chi}{2}}{c^2} + \frac{(v^2 - v_1^2 - v_2^2)}{c^2} + \frac{2\mu^2v^4\sin^4\frac{\chi}{2}}{M^2c^4}\right) .$$

Since $(\mu/M)^2 \sim (1/2000)^2$ and in addition $(v/c)^4 \ll 1$, the last term of the expression contained in the outer parentheses is dropped:

$$\sigma(\bar{n} \to \bar{n}') = \frac{e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{4\mu^2v^4\sin^4\frac{\chi}{2}}\left(1 - \frac{v^2\sin^2\frac{\chi}{2}}{c^2} - \frac{(v_1^2 + v_2^2 - v^2)}{c^2}\right) . \qquad (4)$$

The term $-(v_1^2 + v_2^2 - v^2)/c^2$ is identified as representing recoil effects, since $-(v/c)^2\sin^2\frac{\chi}{2}$ is caused by spin effects.

The use of expression (4) at stage (i) of the steps outlined in the previous section incorporates the proton reocoil effect into the BEA.

SECTION III – THE DERIVATION OF $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$

(i) The Implicit Relation Between $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$ and $\sigma(\bar{n}\to\bar{n}')$

Let a proton, mass m_1, and fixed velocity $\bar{v}_1$ collide with an electron, mass m_2 and fixed velocity $\bar{v}_2$ in the laboratory (lab) system of coordinates. Let $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$ be the cross-section for the exchange of a fixed quantity of energy ΔE in the collision. Since every collision results in the exchange of some energy, the quantity

$$\sigma(\bar{v}_1,\bar{v}_2) = \int_{\text{all values of } \Delta E} \sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)\, d\Delta E$$

measures the total cross-section for interaction between the two particles.

On the other hand, each collision can be viewed as a scattering process characterised by a differential cross-section $\sigma(\bar{n}\to\bar{n}')$ in the centre - of - mass system; here, $\bar{n}$ is the direction, before scattering, of the relative velocity vector of the two particles, while $\bar{n}'$ is the unit vector giving the direction of the same vector after scattering. The total cross-section $\iint_{\text{all solid angles } \Omega'} \sigma(\bar{n}\to\bar{n}')\, d\Omega'$ measures the cross-section for interaction between the two particles, because every encounter between them results in a change of the direction of the relative velocity vector. In the double integral Ω' is the solid angle into which the relative velocity vector points after scattering. The two integrals, the one over ΔE and the other over Ω', measure the same quantity. Hence,

$$\int_{\text{all values of } \Delta E} \sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)\, d\Delta E = \iint_{\text{all solid angles } \Omega'} \sigma(\bar{n}\to\bar{n}')\, d\Omega' \quad . \tag{5}$$

The explicit form of relation (5) requires the expression connecting ΔE and Ω'

(ii) The Relation Between ΔE and Ω'

In the lab system, the proton and the electron have velocities after collision $\bar{v}_1'$ and $\bar{v}_2'$ respectively. When the collision is viewed from the c-m system, the particles have velocities, before collision

$$\bar{w}_1 = \bar{v}_1 - \bar{V}$$

and $\bar{w}_2 = \bar{v}_2 - \bar{V}$.

After collision, the c-m velocities are

$$\bar{w}_1' = \bar{v}_1' - \bar{V}$$

and $\bar{w}_2' = \bar{v}_2' - \bar{V}$.

In the expressions above, $\bar{V} = \dfrac{\bar{p}_1 + \bar{p}_2}{m_1 + m_2}$, and is the velocity of translation of the c-m system relative to the lab system. $\bar{p}_1$ and $\bar{p}_2$ are the proton and electron momenta, respectively, seen from the lab system.

The c-m velocities can also be expressed as

$$\bar{w}_1 = \bar{v}_1 - \left(\frac{m_1\bar{v}_1 + m_2\bar{v}_2}{m_1 + m_2}\right) = \frac{m_2}{M}(\bar{v}_1 - \bar{v}_2) = \frac{m_2\bar{v}}{M} ,$$

$$\bar{w}_2 = -\frac{m_1\bar{v}}{M} ,$$

$$\bar{w}_1' = \frac{m_2\bar{v}'}{M} \quad \text{and}$$

$$\bar{w}_2' = -\frac{m_1\bar{v}'}{M} .$$

Here $\bar{v}$ and $\bar{v}'$ are respectively defined as $\bar{v}_1 - \bar{v}_2$ and $\bar{v}_1' - \bar{v}_2'$ and are the relative velocities.

The definition of ΔE is

$$\Delta E = \tfrac{1}{2}m_1 v_1^2 - \tfrac{1}{2}m_1 v_1'^2 = \tfrac{1}{2}m_2 v_2'^2 - \tfrac{1}{2}m_2 v_2^2 .$$

Since $\bar{v}_1 = \bar{w}_1 + \bar{V}$ and $\bar{v}_1' = \bar{w}_1' + \bar{V}$,

$$\Delta E = \tfrac{1}{2}m_1(w_1^2 + 2\bar{w}_1 . \bar{V} + V^2 - 2\bar{w}_1' . \bar{V} - V^2 - w_1'^2) .$$

The fact that in elastic collisions the c-m magnitude of the momentum of a particle does not change[28] means that $w_1 = w_1'$. As a result,

$$\Delta E = m_1 wV(\cos\theta - \cos\theta') ,$$

where θ is the angle between $\bar{w}_1$ and $\bar{V}$,

θ' is the angle between $\bar{w}_1'$ and $\bar{V}$.

Using the relation connecting w and v yields

$$\Delta E = \frac{m_1 m_2 vV(\cos\theta - \cos\theta')}{M} . \tag{6}$$

Since all initial quantities are fixed, the only variable on the right-hand side of expression (6) is $\cos\theta'$. Therefore,

$$d\Delta E = \mu vV \sin\theta' d\theta' .$$

The c-m coordinate system has been chosen to have its z-direction pareallel with $\bar{V}$. The angular coordinates of $\bar{n}$ and $\bar{n}'$, which are the angular coordinates of $\bar{v}$ and $\bar{v}'$ respectively, are (θ, ϕ) and (θ', ϕ') ;

$$d\Omega' = \sin\theta' d\theta' d\phi' .$$

Finally,

$$\int_{\text{all values of }\Delta E} \sigma_{\Delta E}(\bar{v}_1, \bar{v}_2) d\Delta E = \int_0^{\pi}\int_0^{2\pi} \sigma(\bar{n} \to \bar{n}') d\phi' \sin\theta' d\theta' ,$$

so that

$$\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2) = \frac{1}{\mu v V}\int_0^{2\pi}\sigma(\bar{n}\to\bar{n}')d\phi' \qquad (7)$$

(iii) The Integral $\int_0^{2\pi}\sigma(\bar{n}\to\bar{n}')d\phi'$

Inserting expression (4) in equation (6) and integrating over ϕ' gives the explicit form of $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$. First, however, it is necessary to express the scattering angle χ in terms of θ, ϕ, θ' and ϕ'. χ is the angle between the vectors $\bar{n}$ and $\bar{n}'$. With fig. 1 to illustrate angles and vectors involved, the dependence of χ on the other angles is easily obtained. From the figure, it is clear that

$$\bar{n}.\bar{n}' = \cos\chi = (\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta).(\sin\theta'\cos\phi',\sin\theta'\sin\phi',\cos\theta')$$

On simplification, this becomes

$$\cos\chi = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi-\phi') .$$

With the aid of this expression, the integral is more easily performed; this task is made easier if equation (4) is written term by term, thus:

$$\sigma(\bar{n}\to\bar{n}') = \frac{e^4}{4\mu^2v^4\sin^4\frac{\chi}{2}}(1-v_1^2/c^2)(1-v_2^2/c^2)$$

$$- \frac{e^4}{4\mu^2v^2c^2\sin^2\frac{\chi}{2}}(1-v_1^2/c^2)(1-v_2^2/c^2)$$

$$- \frac{e^4}{4\mu^2v^4\sin^4\frac{\chi}{2}}(1-v_1^2/c^2)(1-v_2^2/c^2)\left(\frac{v_1^2+v_2^2-v^2}{c^2}\right) .$$

These integrals over ϕ' are essentially

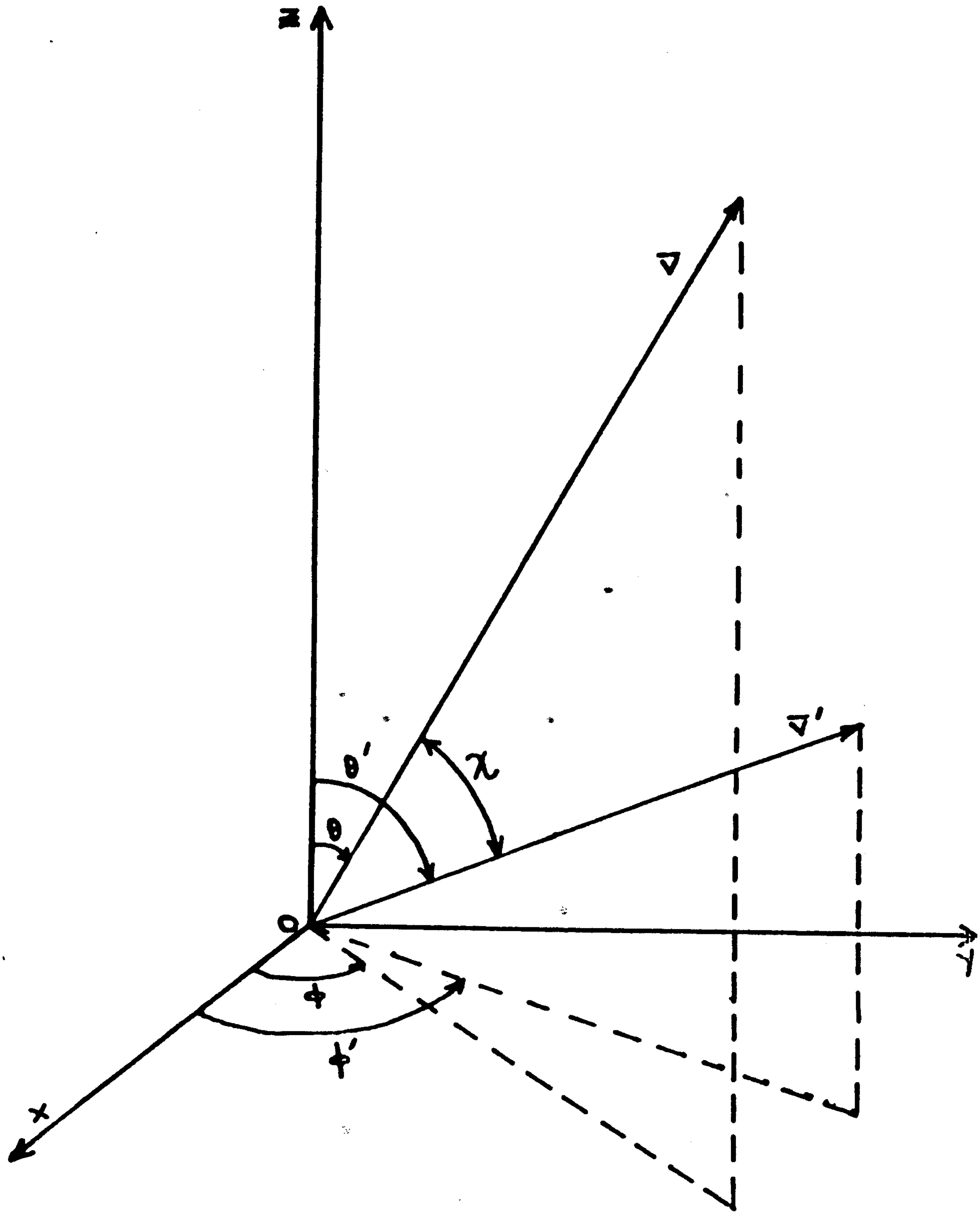

Fig. 1

$$\int_0^{2\pi} \frac{d\phi'}{\sin^2 \frac{\chi}{2}} \qquad \text{and} \qquad \int_0^{2\pi} \frac{d\phi'}{\sin^4 \frac{\chi}{2}} \ .$$

The substitution $x = \phi' - \phi$ leads to

$$\int_0^{2\pi-\phi} f(x)dx$$

where $f(x) = \dfrac{1}{\sin^2 \frac{\chi(x)}{2}}$

or $f(x) = \dfrac{1}{\sin^4 \frac{\chi(x)}{2}}$.

Observing that

$$\int_0^{2\pi-\phi} f(x)dx = \int_{-\phi}^{0} f(x)dx + \int_0^{2\pi-\phi} f(x)dx + \int_{2\pi-\phi}^{2\pi} f(x)dx - \int_{2\pi-\phi}^{2\pi} f(x)dx$$

$$= \int_0^{2\pi} f(x)dx + \int_{-\phi}^{0} f(x)dx - \int_{2\pi-\phi}^{2\pi} f(x)dx$$

$$= \int_0^{2\pi} f(x)dx \ ,$$

because the values of $f(x)$ are identical in the intervals $-\phi < x < 0$ and $2\pi - \phi < x < 2\pi$, the two integrals become

$$\int_0^{2\pi} \frac{dx}{\sin^2 \frac{\chi(x)}{2}} \qquad \text{and} \qquad \int_0^{2\pi} \frac{dx}{\sin^4 \frac{\chi(x)}{2}} \ .$$

Both are easily evaluated by the theorem of residues[29].

Thus $$\int_0^{2\pi} \frac{dx}{\sin^2 \frac{\chi}{2}} = \frac{8\pi}{|\cos\theta' - \cos\theta|}$$

and $$\int_0^{2\pi} \frac{dx}{\sin^4 \frac{\chi}{2}} = \frac{8\pi(1 - \cos\theta\cos\theta')}{|\cos\theta - \cos\theta'|^3} \ .$$

In consequence,

$$\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2) = \frac{8\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{4\mu^3 v^5 V\,|\cos\theta - \cos\theta'|^3}\left(1 + \frac{(v^2 - v_1^2 - v_2^2)}{c^2}\right) \times$$

$$(1 - \cos\theta\cos\theta') - \frac{8\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{4\mu^3 v^3 c^2 V\,|\cos\theta - \cos\theta'|} .$$

From equation (6),

$$\cos\theta - \cos\theta' = \frac{\Delta E}{\mu v V} ; \quad \text{and} \quad \cos\theta' = \cos\theta - \frac{\Delta E}{\mu v V} .$$

Hence,

$$\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2) = \frac{2\pi e^4 V^2(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{v^2|\Delta E|^3}\left(1 + \frac{(v^2 - v_1^2 - v_2^2)}{c^2}\right) \times$$

$$\left(1 - \cos^2\theta + \frac{\Delta E\cos\theta}{\mu v V}\right) - \frac{2\pi e^2(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{\mu^2 v^2 c^2|\Delta E|} . \qquad (8)$$

SECTION IV - THE CALCULATION OF $\sigma^{eff}_{\Delta E}(\bar{v}_1,\bar{v}_2)$

(i) The Definition Of $\sigma^{eff}_{\Delta E}(\bar{v}_1,\bar{v}_2)$

In the previous section, the cross-section, $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$, for the exchange of a quantity of energy ΔE from one particle to the other when an electron of fixed velocity $\bar{v}_2$ collides with a proton of fixed velocity $\bar{v}_1$ has been found. This quantity, depending as it does on fixed vectors, is not of direct use in the calculation of ionization cross-sections. Its average, denoted $\sigma^{eff}_{\Delta E}$, over all directions of the two velocities $\bar{v}_1$ and $\bar{v}_2$ is more useful, because it is a function of scalars only. The definition of $\sigma^{eff}_{\Delta E}$ is

$$\sigma^{eff}_{\Delta E}(v_1,v_2) = \frac{1}{4\pi v_1} \iint\limits_{\text{all directions } \bar{n}_2} \left|\bar{v}_1 - v_2\bar{n}_2\right| \sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)\,d\bar{n}_2 \qquad (9)$$

where $\bar{n}_2$ defines the direction of $\bar{v}_2$.

This definition holds only if the velocity distribution of the target electron is isotropic. This condition is satisfied in ionization experiments because the target electrons are in random motion.

(ii) The Calculation Of $\sigma^{eff}_{\Delta E}(v_1,v_2)$

It is necessary to transform the integral in the definition of $\sigma^{eff}_{\Delta E}$ to the variables $\bar{V}$ and $\bar{v}$ in order to perform it. The method whereby to do this is due to Gerjuoy[12].

The integral on the right-hand side of definition (9) is over the variable $\bar{n}_2$ and is therefore independent of $\bar{n}_1$, the unit vector $\bar{v}_1/v_1$. This allows the definition to be written as

$$\sigma^{eff}_{\Delta E}(\bar v_1,\bar v_2) = \frac{1}{4\pi v_1}\iint_{\bar n_2} |\bar v_1 - \bar v_2|\,\sigma_{\Delta E}(\bar v_1,\bar v_2)d\bar n_2\ \frac{1}{4\pi}\iint_{\bar n_1} d\bar n_1$$

$$= \frac{1}{16\pi^2 v_1}\iiiint v\,\sigma_{\Delta E}(\bar v_1,\bar v_2)d\bar n_1 d\bar n_2\ .$$

The variables of integration are independent of the magnitudes v_1 and v_2. Therefore,

$$\sigma^{eff}_{\Delta E} = \frac{1}{16\pi^2 v_1^3 v_2^2}\iiiint_{\bar n_1,\bar n_2} v\,\sigma_{\Delta E}(\bar v_1,\bar v_2)v_1^2 v_2^2 d\bar n_1 d\bar n_2\ . \tag{10}$$

Equation (10) can be transformed by the relation[30]

$$\iint F(\vartheta_1,\vartheta_2)\,\delta(\vartheta_1 - v_1)\,\delta(\vartheta_2 - v_2)d\vartheta_1 d\vartheta_2 = F(v_1,v_2).$$

Thus,

$$\sigma^{eff}_{\Delta E} = \frac{1}{16\pi^2 v_1^3 v_2^2}\iiiint\!\!\iint v\,\sigma_{\Delta E}(\vartheta_1,\vartheta_2,\bar n_1,\bar n_2)\,\delta(\vartheta_1 - v_1)\,\delta(\vartheta_2 - v_2)\ \times$$

$$\vartheta_1^2\vartheta_2^2 d\bar n_1 d\bar n_2 d\vartheta_1 d\vartheta_2\ . \tag{11}$$

Wherever v_1 and v_2 appeared under the integral sign, they have been replaced by ϑ_1 and ϑ_2. With

$$F(\bar\vartheta_1,\bar\vartheta_2) = \frac{v\,\sigma_{\Delta E}(\vartheta_1,\vartheta_2,\bar n_1,\bar n_2)}{16\pi^2 v_1^3 v_2^2}$$

for convenience, the integral in equation (11) is easily performed. In equation (11), $\vartheta_1^2 d\vartheta_1 d\bar n_1$ and $\vartheta_2^2 d\vartheta_2 d\bar n_2$ define volume elements in $\overline{\vartheta_1}$ and $\overline{\vartheta_2}$ spaces respectively: ϑ_1 is a vector with the direction of $\bar n_1$ but the magnitude ϑ_1, and $\overline{\vartheta_2}$ has the direction of $\bar n_2$ and the magnitude ϑ_2. Since in terms of $\bar v$ and $\bar V$

$$\bar v_1 = \bar V + \bar w_1 = \bar V + \frac{m\bar v}{M}$$

and $\bar{v}_2 = \bar{V} - \frac{m_1\bar{v}}{M}$,

the definitions of $\bar{\vartheta}_1$ and $\bar{\vartheta}_2$ are

$$\bar{\vartheta}_1 = \bar{V} + \frac{m_2\bar{v}}{M}$$
$$\bar{\vartheta}_2 = \bar{V} - \frac{m_1\bar{v}}{M} \quad . \tag{12}$$

Equation (11) is now slightly written :

$$\sigma^{eff}_{\Delta E} = \iiiint\!\!\iint F(\bar{\vartheta}_1,\bar{\vartheta}_2)\,\delta(\vartheta_1 - v_1)\,\delta(\vartheta_2 - v_2)\,d\bar{\vartheta}_1 d\bar{\vartheta}_2 \, .$$

The transformation of the variables from $\bar{\vartheta}_1, \bar{\vartheta}_2$ to $\bar{v}, \bar{V}$ is via the Jacobian determinant

$$\left| \begin{vmatrix} \dfrac{\partial\bar{\vartheta}_2}{\partial\bar{V}} & \dfrac{\partial\bar{\vartheta}_1}{\partial\bar{V}} \\ \dfrac{\partial\bar{\vartheta}_2}{\partial\bar{v}} & \dfrac{\partial\bar{\vartheta}_1}{\partial\bar{v}} \end{vmatrix} \right| = \left| \begin{vmatrix} 1 & 1 \\ \dfrac{m_2}{M} & -\dfrac{m_1}{M} \end{vmatrix} \right| = 1 \, .$$

Hence

$$\sigma^{eff}_{\Delta E} = \iiiint\!\!\iint F(\bar{v},\bar{V})\,\delta(\vartheta_1 - v_1)\,\delta(\vartheta_2 - v_2)\,d\bar{v}d\bar{V} \tag{13}$$

Equations (12) give

$$\bar{\vartheta}_1 = \left(V^2 + \frac{2m_2 vV\cos\theta}{M} + \frac{m_2^2 v_2^2}{M^2}\right)^{\frac{1}{2}}$$
$$\bar{\vartheta}_2 = \left(V^2 - \frac{2m_1 vV\cos\theta}{M} + \frac{m_1^2 v^2}{M^2}\right)^{\frac{1}{2}} \, . \tag{14}$$

Because $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$ is a function of v, θ and V only, the integrations over the variables ϕ, θ_v and ϕ_v can be performed at once. (θ,ϕ) are the angular coordinates in $\bar{V}$ - space; while (θ_v, ϕ_v) are the angular coordinates in

$\bar{v}$ - space. Thus

$$\sigma_{\Delta E}^{eff} = 8\pi^2 \iiint F(v,V,x)\,\delta(\vartheta_1 - v_1)\,\delta(\vartheta_2 - v_2)\,v^2 V^2\,dv\,dV\,dx$$

where $x = \cos\theta$. The negative sign arising from $d(\cos\theta) = -\sin\theta\,d\theta$ has been absorbed by interchanging the limits of integration. The relation[30]

$$\int f(y)\,\delta(g(y))\,dy = \sum_i \left\{ \left| \left(\frac{dg}{dy}\right)^{-1} \right| f(y) \right\}_{y=y_i} \tag{15}$$

facilitates the integrations over x and V. In the relation, y_i are the roots of $g(y) = 0$. For the integral over the variable $x = \cos\theta$, the function g is chosen to be $\vartheta_1 - v_1$. Therefore:

$$\frac{dg}{dx} = \left(V^2 + \frac{2m_2 vVx}{M} + \frac{m_2^2 v^2}{M^2}\right)^{-\frac{1}{2}} \frac{m_2 vV}{M} = \frac{m_2 vV}{M(g(x) + v_1)}\,.$$

The root is

$$x_i = \frac{M}{2m_2 vV}\left(v_1^2 - V^2 - \frac{m_2^2 v^2}{M}\right).$$

At the root, the reciprocal of the derivative is $\frac{Mv_1}{m_2 vV}$.

The identification

$$f(y) = \iint 8\pi^2 F(v,V,x)\,\delta(\vartheta_2 - v_2)\,v^2 V^2\,dv\,dV$$

is made, and with the understanding that all values of x now change to x_i,

$$\sigma_{\Delta E}^{eff} = 8\pi^2 \frac{Mv_1}{m_2} \iint F(v,V,x)\,vV\,\delta(\vartheta_2(x_i) - v_2)\,dv\,dV\,.$$

Relation (15) is used again, this time in conjunction with V and the other δ-function.

$$g(V) = \mathcal{V}_2(x_i) - v_2$$
$$= \left(\frac{MV^2}{m_2} + \frac{m_1v^2}{M} - \frac{m_1v_1^2}{m_2}\right)^{\frac{1}{2}} - v_2 \ .$$

$$\frac{dg}{dV} = \frac{MV}{m_2}\,\frac{1}{g(V) + v_2} \ .$$

The one root of $g(V) = 0$ is

$$V_i = \left(\left(m_1v_1^2 + m_2v_2^2 - \frac{m_1m_2v^2}{M}\right)/M\right)^{\frac{1}{2}} .$$

With the understanding that V_i now replaces V wherever this variable appears in the integrand,

$$\sigma^{eff}_{\Delta E} = 8\pi^2 v_1 v_2 \int_{v_L}^{v_U} vF(v)dv.$$

v_U and v_L are th upper and the lower limits respectively of the integration. Thus

$$\sigma^{eff}_{\Delta E} = \frac{1}{2v_1^2v_2}\int_{v_L}^{v_U} v^2\sigma_{\Delta E}(v)dv.$$

With $\sigma_{\Delta E}(\bar{v}_1,\bar{v}_2)$ written as the sum of three terms, equation (9) can also be evaluated as three separate terms. These terms are conveniently identified as the 'Rutherford term' (corresponding to the first term of equation (4)), the 'spin term' (the second one in equation (4)) and the 'recoil term' (corresponding to the last term in equation (4)). Thus

$$\sigma^{eff}_{\Delta E} = A_1\int_{v_L}^{v_U} V_i^2\left(1 - \cos^2\theta_i + \frac{\Delta E\cos\theta_i}{\mu vV}\right) dv$$
$$+ A_2\int_{v_L}^{v_U} dv \; + A_3\left[\frac{v_1^2 + v_2^2}{c^2}\int_{v_L}^{v_U} V_i^2\left(1 - \cos^2\theta_i + \frac{\Delta E\cos\theta_i}{\mu vV_i}\right)dv\right.$$
$$\left. - \frac{1}{c^2}\int_{v_L}^{v_U} v^2V_i^2\left(1 - \cos^2\theta_i + \frac{\Delta E\cos\theta_i}{\mu vV_i}\right) dv \right] ,$$

where $A_1 = \dfrac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{v_1^2 v_2 |\Delta E|^3}$,

$$A_2 = \frac{-\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{v_1^2 v_2 \mu^2 c^2 |\Delta E|}$$

and $A_3 = \dfrac{-\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{v_1^2 v_2 |\Delta E|^3}$.

The Rutherford contribution to $\sigma^{\mathrm{eff}}_{\Delta E}$ is[12]

$$\frac{A_1}{4}\Big[(v_1^2 - v_2^2)(v_2'^2 - v_1'^2)\Big(\frac{1}{v_L} - \frac{1}{v_U}\Big) + (v_1^2 + v_2^2 + v_1'^2 + v_2'^2)(v_U - v_L) - \frac{1}{3}(v_U^3 - v_L^3)\Big] ,$$

where $v_1' = \Big(v_1^2 - \dfrac{2\Delta E}{m_1}\Big)^{\frac{1}{2}}$

and $v_2' = \Big(v_2^2 + \dfrac{2\Delta E}{m_2}\Big)^{\frac{1}{2}}$.

The spin contribution is

$A_2(v_U - v_L)$.

The first term of the recoil contribution is

$$\frac{A_3}{4}\frac{(v_1^2 + v_2^2)}{c^2}\Big[(v_1^2 - v_2^2)(v_2'^2 - v_1'^2)\Big(\frac{1}{v_L} - \frac{1}{v_U}\Big) + (v_1^2 + v_2^2 + v_1'^2 + v_2'^2)(v_U - v_L) - \frac{1}{3}(v_U^3 - v_L^3)\Big]$$

because the factor under the integral sign is essentially the same one as in the Rutherford contribution. The second term of the recoil contribution is essentially

$$\int V_i^2 v^2\Big(1 - \cos^2\theta_i + \frac{\Delta E \cos\theta_i}{\mu v V_i}\Big)\, dv .$$

Here, $V_i = \left(\frac{m_1 v_1^2 + m_2 v_2^2}{M} - \frac{\mu v^2}{M} \right)^{\frac{1}{2}}$

$= (a - bv^2)^{\frac{1}{2}}$,

where $a = \frac{m_1 v_1^2 + m_2 v_2^2}{M}$

$b = \frac{\mu}{M}$

and $\cos\theta_i = \frac{M}{2m_2 vV_i} \left(v_1^2 - V_i^2 - \frac{m_2^2 v_2^2}{M} \right)$

$= \frac{1}{2vV_i} \left(v_1^2 - v_2^2 + \left(\frac{m_1 - m_2}{M} \right) v^2 \right)$,

by using the expression for V_i.

Writing $\cos\theta_i = \frac{1}{2vV_i} (d + gv^2)$, with $d = v_1^2 - v_2^2$ and

$g = \frac{m_1 - m_2}{M}$, the integral becomes

$$\int v^2 V_i^2 \left(1 - \frac{1}{4v^2 V_i^2} (d^2 + 2gv^2 d + g^2 v^4) + \frac{\Delta E}{\mu vV_i} \frac{1}{2vV_i} (d + gv^2) \right) dv$$

$$= \frac{1}{4} \int \left(\left(\frac{2\Delta Eg}{\mu} + 4a^2 - 2gd \right) v^2 - (g^2 + b) v^4 + \left(\frac{2\Delta Ed}{\mu} - d^2 \right) \right) dv.$$

Using $\Delta E = \frac{1}{2} m_1 v_1^2 - \frac{1}{2} m_1 v_1'^2$, the simplifications

$4a^2 - 2gd + \frac{2\Delta Eg}{\mu} = v_1^2 + v_2^2 + v_1'^2 + v_2'^2$,

$g^2 + b = 1$,

and $\frac{2\Delta Ed}{\mu} - d^2 = (v_1^2 - v_2^2)(v_2'^2 - v_1'^2)$

are easily obtained. The integration is then

$$\frac{1}{4} \Big[(v_1^2 + v_2^2 + v_1'^2 + v_2'^2) \frac{(v_U^3 - v_L^3)}{3} - \frac{1}{5} (v_U^5 - v_L^5)$$

$$- (v_2^2 - v_1^2)(v_1'^2 - v_2'^2)(v_U - v_L) \Big] .$$

As a result, the second part of the recoil contribution is

$$-\frac{A_3}{4c^2}\Big[(v_1^2 + v_2^2 + v_1'^2 + v_2'^2)\frac{(v_U^3 - v_L^3)}{3} - \frac{(v_U^5 - v_L^5)}{5}$$
$$- (v_1^2 - v_2^2)(v_2'^2 - v_1'^2)(v_U - v_L)\Big].$$

$\sigma_{\Delta E}^{eff}$ is the sum of the four terms which have just been obtained. It is completely defined when the limits v_U and v_L are specified.

(iii) The Derivation Of The Limits

The inequality $-1 \leq \cos\theta' \leq 1$ must hold for the polar angle θ' of $\bar{n}'$. From equation (6),

$$-1 \leq \cos\theta - \frac{\Delta E}{\mu v V} \leq 1.$$

Herefrom, interest is confined to the case $\Delta E \geq 0$; whence

$$-1 + \frac{\Delta E}{\mu v V} \leq \cos\theta \leq 1.$$

The integration over $x = \cos\theta$ transforms the inequalities to

$$-1 + \frac{\Delta E}{\mu v V} \leq \cos\theta_i$$

and $\cos\theta_i \leq 1.$

With the value of $\cos\theta_i$, the first inequality is

$$-1 + \frac{\Delta E}{\mu v V} \leq \left(v_1^2 - V^2 - \frac{m_2^2 v^2}{M^2}\right)\frac{M}{2m_2 vV}.$$

On simplification, this yields

$$\left(V - \frac{m_2 v}{M}\right)^2 \leq v_1'^2 ,$$

while the second inequality gives

$$(V + \frac{m_2 v}{M})^2 \geq v_1'^2 .$$

These two inequalities define a region in the v,V plane over which the remaining two integrations are performed. The relation that completes the definition of this region is

$$M V^2 + \mu v^2 = m_1 v_1^2 + m_2 v_2^2 .$$

It comes from energy conservation between the lab and c-m systems or from the condition for the nonvanishing of $\delta(\vartheta_2(x_i) - v_2)$.

The two inequalities resolve into

$$V \leq \frac{m_2 v}{M} + v_1' \quad ,$$

$$V \geq \frac{m_2 v}{M} - v_1' \quad ,$$

$$V \geq - \frac{m_2 v}{M} + v_1 \qquad \text{and}$$

$$V \leq - \frac{m_2 v}{M} - v_1 .$$

Since v and V are coordinates in spherical systems, only the first quadrant of the v,V plane is of interest. The line

$$V = - \frac{m_2 v}{M} - v_1$$

never passes into this region, and the last inequality is therefore discarded. The region defined by the ellipse and the first three inequalities is illustrated in fig.2. The points v_α, v_β, v_γ, v_δ, v_{ac} and v_{bc} are the intersections of the curves with each other. The limits v_U and v_L are always the intersections of the ellipse with the boundaries of the hatched region. They depend on the particular shape of the ellipse and the intercepts and slopes of the

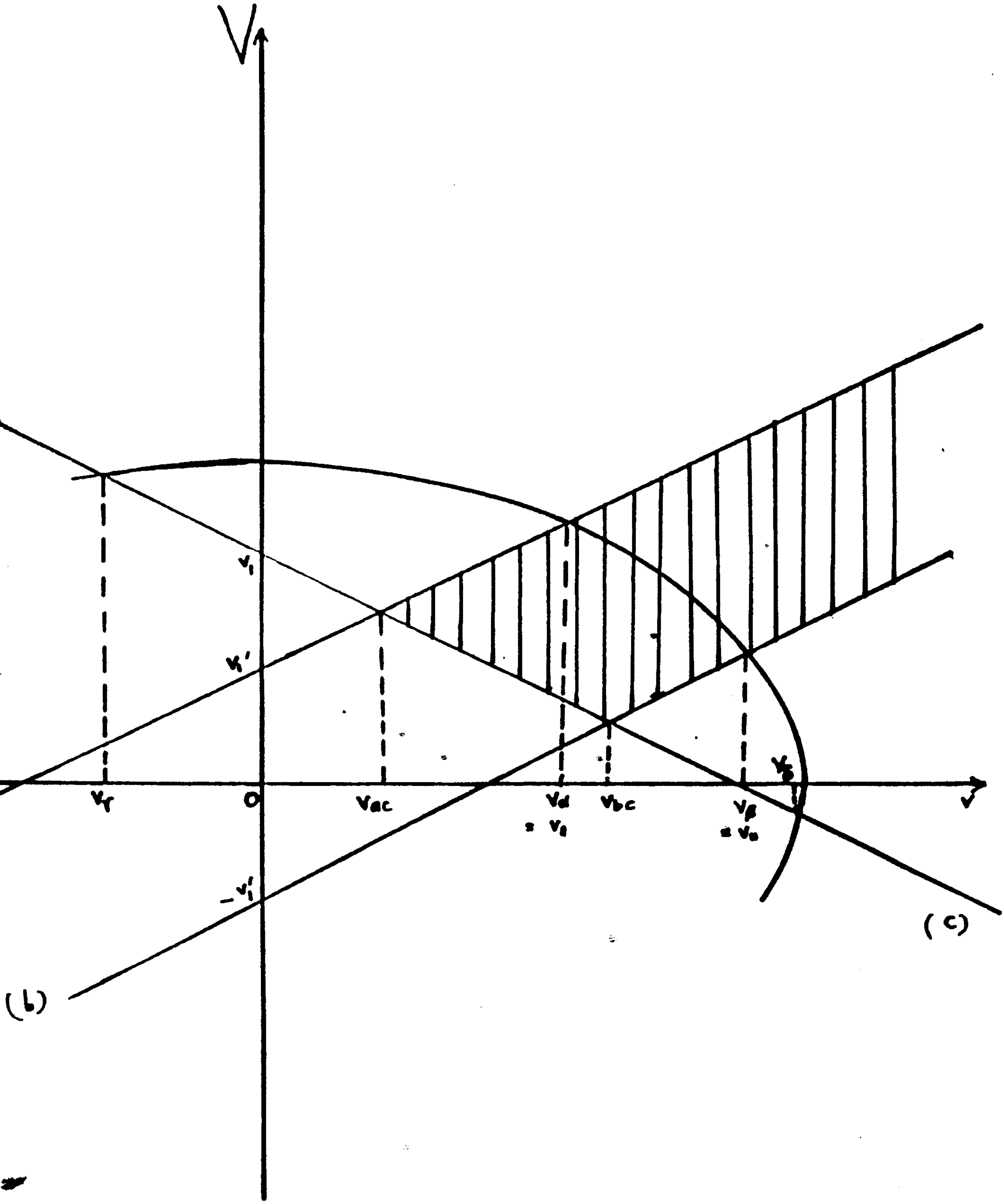

Fig. 2

Case 1

lines. Altogether, there are five different sets of limits. They are:

Case (1): This is the one illustrated in fig. 2. Then

$v_L = v_\alpha$ and $v_U = v_\beta$.

Solving the simultaneous system

$$MV^2 + \mu v^2 = m_1 v_1^2 + m_2 v_2^2 = 2E = m_1 v_1'^2 + m_2 v_2'^2$$

$$V - \frac{m_2}{M} v = v_1'$$

gives the solutions $- v_1' + v_2'$ and $- v_1' - v_2'$.

Therefore $v_\alpha = v_L = v_2' - v_1'$.

The solution of the system

$$MV^2 + \mu v^2 = m_1 v_1'^2 + m_2 v_2'^2$$

$$V - \frac{m_2}{M} v = - v_1'$$

gives $v_\beta = v_U = v_1' + v_2'$.

The conditions for this pair of limits to occur are, from the diagram, $v_{ac} \geq v_\alpha$, $v_\beta \geq v_{bc}$ or equivalently, $v_\gamma \leq v_{ac}$, $v_{bc} \leq v_\delta$.

Case (2): This is illustrated in fig. 3. It is evident that $v_L = v_\alpha = v_2' - v_1'$. Solving the system

$$MV^2 + \mu v^2 = m_1 v_1^2 + m_2 v_2^2$$

$$V + \frac{m_2}{M} v = v_1$$

gives $v_\delta = v_U = v_1 + v_2$. These limits are conditional on $v_{ac} \leq v_\alpha$,

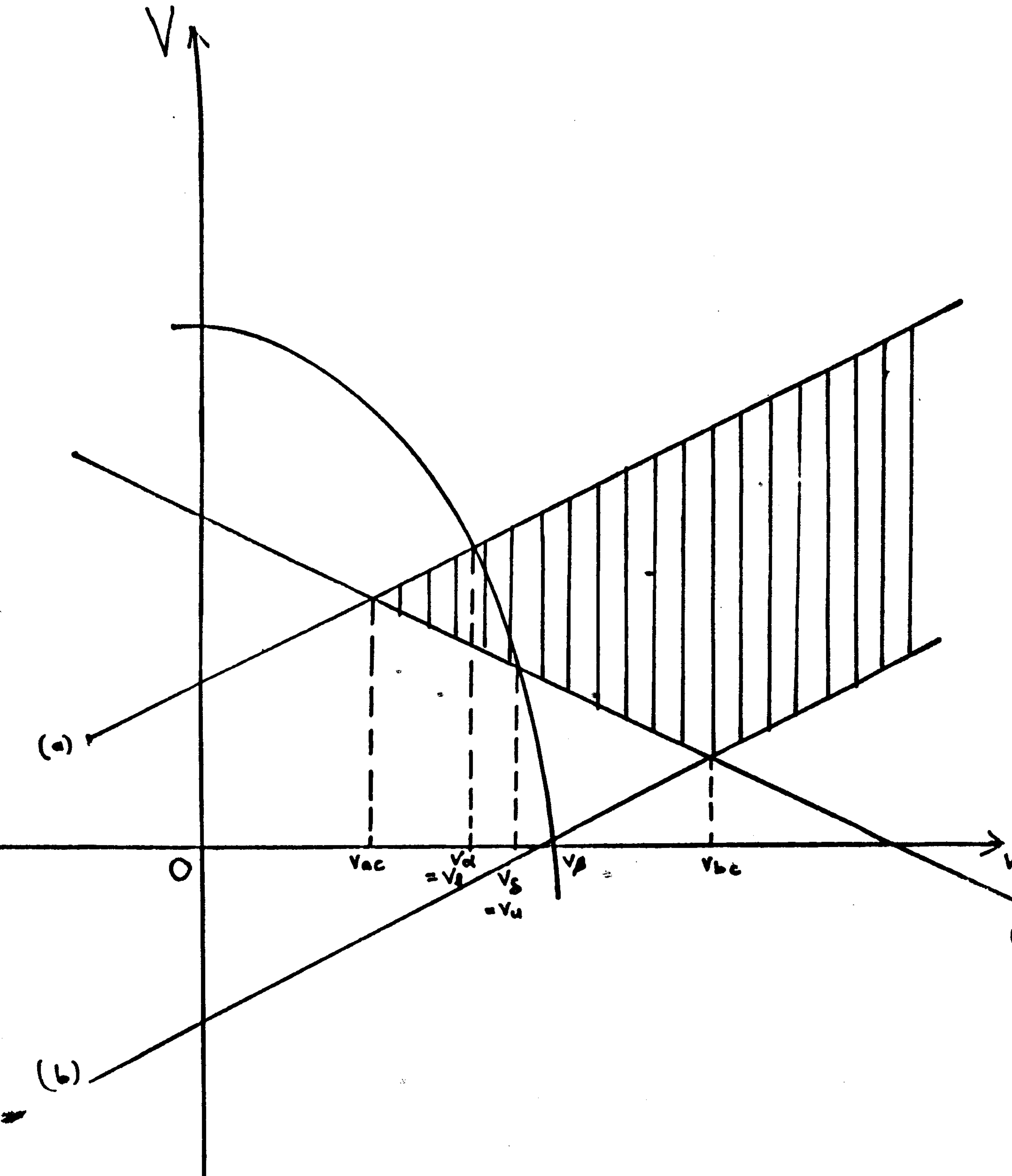

Fig. 3

Case 2

$v_\delta \leq v_{bc}$; which conditions are equivalent to $v_{ac} \leq v_\gamma$, $v_\delta \leq v_{bc}$.

Case (3): Fig. 4 illustrates this case. $v_U = v_\delta$, but $v_L = v_\gamma$. v_γ is obtained from solving the simultaneous equations

$$MV^2 + \mu v^2 = m_1 v_1^2 + m_2 v_2^2$$

$$V + \frac{m_2 v}{M} = v_1.$$

Thus $v_L = v_1 - v_2$. The two limits occur if $v_{ac} \leq v_\gamma$, $v_{bc} \leq v_\beta$; equivalently, $v_{ac} \leq v_\gamma$, $v_\delta \leq v_{bc}$.

Case (4): The limits, as fig. 5 shows, are now $v_L = v_\gamma = v_1 - v_2$ and $v_\beta = v_U = v_1' + v_2'$, and apply only when $v_{ac} \leq v_\gamma$, $v_{bc} \leq v_\beta$; equivalently, the conditions are $v_{ac} \leq v_\gamma$ and $v_\delta \geq v_{bc}$.

Case (5): This case occurs if the ellipse does not intersect the hatched region; then $\sigma^{eff}_{\Delta E} = 0$.

The intersections v_{ac} and v_{bc} are

$$v_{ac} = \frac{M}{2m_2}(v_1 - v_1'),$$

$$v_{bc} = \frac{M}{2m_2}(v_1 + v_1').$$

The four sets of conditions which determine the four sets of limits can be transformed to equivalent conditions on ΔE. For case (1), the condition $v_\gamma \leq v_{ac}$ is

$$v_1 - v_2 \leq \frac{M}{2m_2}(v_1 - v_1')$$

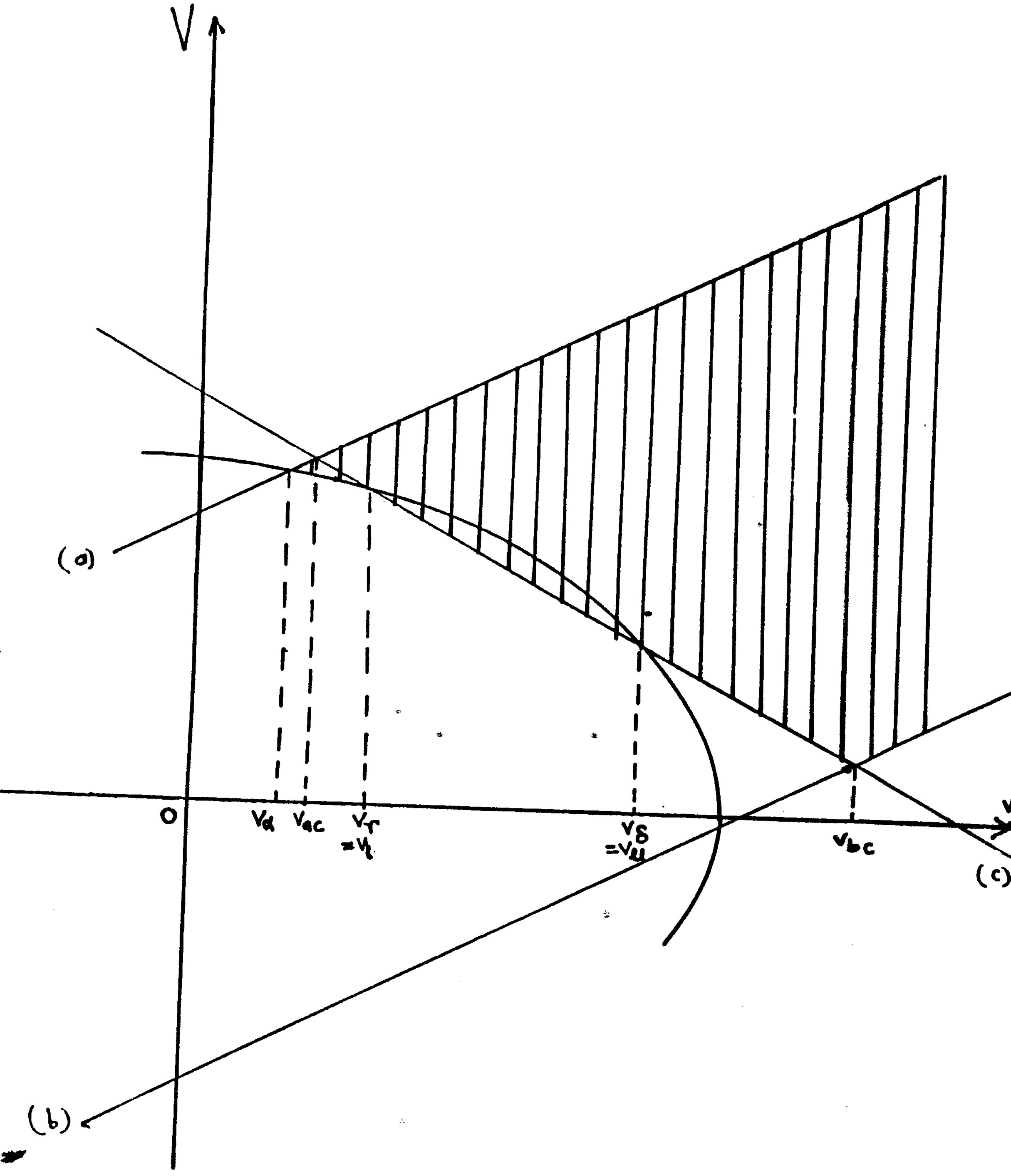

Fig. 4

Case 3

$$\Rightarrow 2m_2(v_1 - v_2) - Mv_1 \leq - v_1'$$

$$\Rightarrow v_1' \leq (m_1 - m_2)v_1 + 2m_2v_2 .$$

Squaring:

$$v_1'^2 \leq v_1^2(m_1^2 + m_2^2 - 2m_1m_2) + 4m_2^2v_2^2 + 4m_2(m_1 - m_2)v_1v_2 ,$$

provided that $(m_1 - m_2)v_1 + 2m_2v_2 \geq 0$.

Therefore, with $v_1'^2 = v_1^2 - \frac{2\Delta E}{m_1}$,

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(\frac{m_1v_1^2}{2} - \frac{m_2v_2^2}{2} + (m_1 - m_2)\frac{v_1v_2}{2}\right) ,$$

provided that $2m_2v_2 \geq (m_1 - m_2)v_1$.

The condition $v_{bc} \leq v_\delta$ gives

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(\frac{m_1v_1^2}{2} - \frac{m_2v_2^2}{2} - (m_1 - m_2)\frac{v_1v_2}{2}\right) ,$$

provided that $2m_2v_2 \geq (m_2 - m_1)v_1$.

Since the two conditions hold simultaneously, they can be combined into

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(\frac{m_1v_1^2}{2} - \frac{m_2v_2^2}{2} + |m_1 - m_2|\frac{v_1v_2}{2}\right) ,$$

as long as $2m_2v_2 \geq |m_1 - m_2| v_1$.

The proton - electron case ensures that $m_1 > m_2$. In consequence, the condition is

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_1 - m_2)\frac{v_1v_2}{2}\right) ,$$

provided that $2m_2v_2 \geq (m_1 - m_2)v_1$.

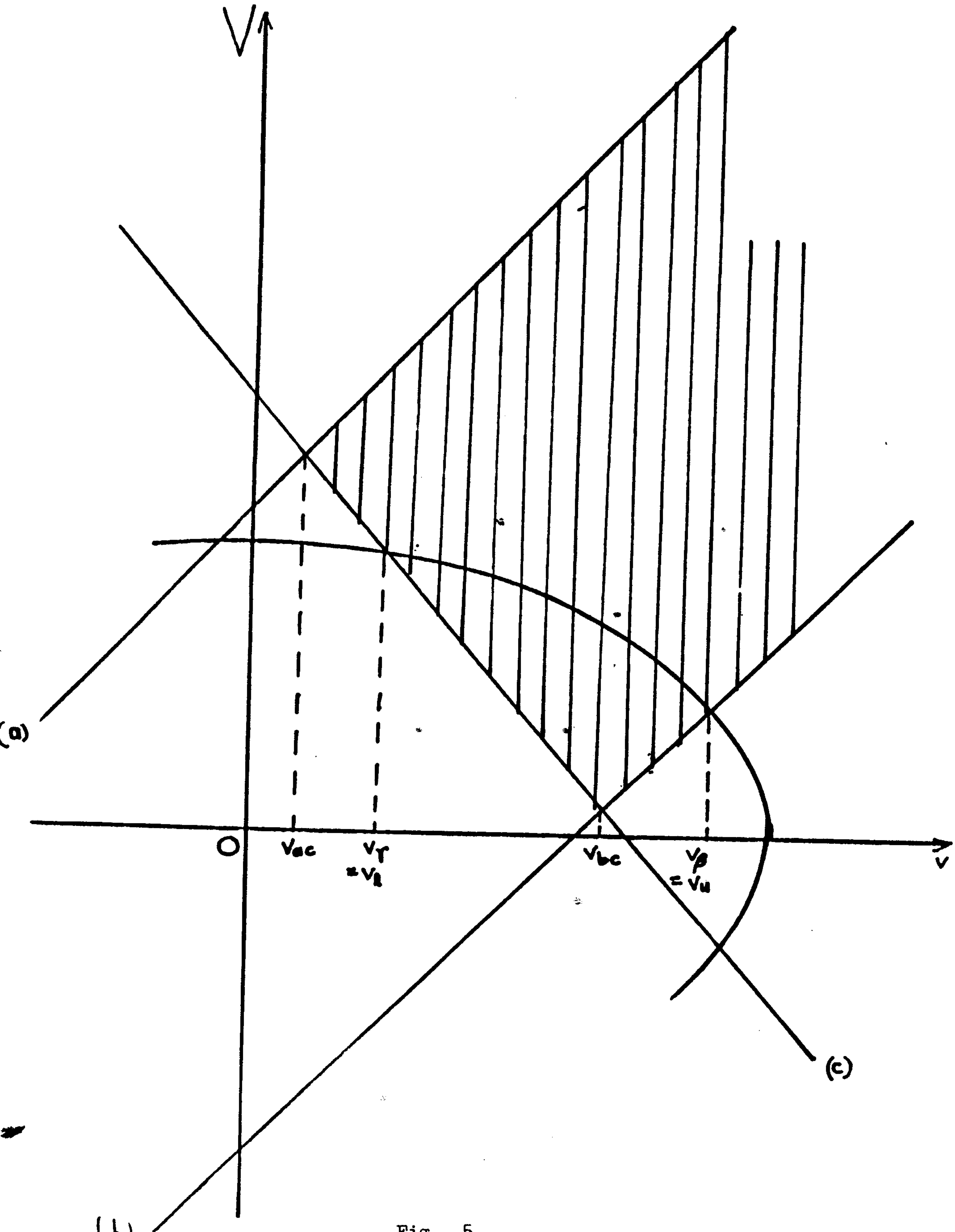

Fig. 5

Case 4

The conditions for case (2), namely $v_\gamma \leq v_{ac}$ and $v_\delta \leq v_{bc}$ give

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_2 - m_1)\frac{v_1v_2}{2}\right),$$

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_1 - m_2)\frac{v_1v_2}{2}\right)$$

respectively. It is clear that cases with $m_1 < m_2$ are excluded; they would result in

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_2 - m_1)\frac{v_1v_2}{2}\right) \quad \text{and}$$

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_2 - m_1)\frac{v_1v_2}{2}\right),$$

which is not a closed region. The circumstance $m_1 > m_2$ makes it superfluous to mention the condition $2m_2v_2 + (m_1 - m_2)v_1 \geq 0$ as it is automatically satisfied.

For case (3), the conditions $v_{ac} \leq v_\gamma$ and $v_\delta \leq v_{bc}$ give

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_1 - m_2)\frac{v_1v_2}{2}\right)$$

and $\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_2 - m_1)\frac{v_1v_2}{2}\right)$.

These conditions hold at the same time, so that

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - |m_1 - m_2|\frac{v_1v_2}{2}\right).$$

Since $m_1 > m_2$, this condition is

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_1 - m_2)\frac{v_1v_2}{2}\right).$$

The conditions for case (4), $v_{ac} \leq v_\gamma$ and $v_{bc} \leq v_\delta$ transform to

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_2 - m_1)\frac{v_1v_2}{2}\right) \quad \text{and}$$

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_2 - m_1)\frac{v_1v_2}{2}\right).$$

If $m_1 > m_2$, it is impossible to reconcile these two conditions; this case is of no interest for proton - electron scattering.

When all the results are collected:

(1) $v_L = v_2' - v_1'$, $v_U = v_1' + v_2'$ when

$$\Delta E \geq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_1 - m_2)\frac{v_1v_2}{2}\right),$$

as long as $2m_2v_2 \geq (m_1 - m_2)v_1$.

(2) $v_L = v_2' - v_1'$, $v_U = v_1 + v_2$ when

$$\frac{4m_1m_2}{M^2}\left(E_1 - E_2 + (m_1 - m_2)\frac{v_1v_2}{2}\right) \leq \Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_1 - m_2)\frac{v_1v_2}{2}\right).$$

(3) $v_L = v_1 - v_2$, $v_U = v_1 + v_2$ when

$$\Delta E \leq \frac{4m_1m_2}{M^2}\left(E_1 - E_2 - (m_1 - m_2)\frac{v_1v_2}{2}\right).$$

SECTION V - THE CALCULATION OF $\int \sigma^{eff}_{\Delta E}(v_1, v_2)\, d\Delta E$

The integral $\sigma(v_2) = \int \sigma^{eff}_{\Delta E}(v_1, v_2) d\Delta E$ is the cross - section for the ejection of an electron of speed v_2 from its shell, by the impact of a proton of speed v_1, if the limits are chosen appropriately. The lower limit has to be the binding energy of the electron, while the upper limit has to be the kinetic energy of the proton. This integral introduces the effect of the target atom's other components into the cross-section, since the binding energy of the electron is determined by the whole atom. Since v_L and v_U, of which $\sigma^{eff}_{\Delta E}$ is a function, are themselves functions of ΔE, the expression for $\sigma(v_2)$ depends on which one of the regions (1) to (3) of Section IV is being dealt with. The expressions for $\sigma(v_2)$ are:

Case (1): Inserting the appropriate expressions for v_L and v_U in $\sigma^{eff}_{\Delta E}$ and integrating over ΔE gives for the Rutherford term the expression[14]

$$\frac{\pi}{3} \frac{e^4}{v_1^2 v_2} (1 - v_1^2/c^2)(1 - v_2^2/c^2)\left(- \frac{2v_1'^3}{\Delta E^2}\right).$$

The spin term is

$$A \int \frac{(v_2' + v_1' - v_2' + v_1')}{\Delta E}\, d\Delta E ,$$

where $A = - \dfrac{\pi e^4}{v_1^2 v_2 \mu^2 c^2} (1 - v_1^2/c^2)(1 - v_2^2/c^2).$

Here, $\displaystyle\int \frac{v_1'}{\Delta E} d\Delta E = 2v_1' + v_1 \ln\left|\frac{v_1 - v_1'}{v_1 + v_1'}\right|$ and the spin term is

$$2A\left(2v_1' + v_1 \ln\left|\frac{v_1 - v_2'}{v_1 + v_2'}\right|\right).$$

The first part of the recoil term is

$$-\frac{\pi}{3}\frac{e^4}{v_1^2 v_2}(1 - v_1^2/c^2)(1 - v_2^2/c^2)\frac{(v_1^2 + v_2^2)}{c^2}\left(\frac{-2v_1'^3}{\Delta E^2}\right).$$

The second part is, with $B = \dfrac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{4v_1^2 v_2 c^2}$,

$$B\int\left[\frac{(v_1^2 - v_2^2)(v_2'^2 - v_1'^2)(v_U - v_L)}{\Delta E^3} + \frac{(v_1^2 + v_2^2 + v_1'^2 + v_2'^2)(v_U^3 - v_L^3)}{3\Delta E^3} - \frac{1}{5}\frac{(v_U^5 - v_L^5)}{\Delta E^3}\right]d\Delta E.$$

$$\int\frac{(v_1^2 - v_2^2)(v_2'^2 - v_1'^2)(v_U - v_L)}{\Delta E^3}\,d\Delta E = 2(v_1^2 - v_2^2)\left[-\frac{(v_2^2 - v_1^2)}{2}\times\left(\frac{v_1'^3}{v_1^2\Delta E^2} + \frac{v_1'}{m_1 v_1^2\Delta E} + \frac{1}{m_1^2 v_1^3}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) - \frac{2}{\mu}\left(\frac{v_1'}{\Delta E} + \frac{1}{m_1 v_1}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right)\right].$$

$$\int\frac{(v_1^2 + v_2^2 + v_1'^2 + v_2'^2)(v_U^3 - v_L^3)}{3\Delta E^3}\,d\Delta E = \frac{4}{3}\left\{-\frac{(v_1^2 + 3v_2^2)(v_1^2 + v_2^2)}{2}\times\left(\frac{v_1'}{v_1^2\Delta E^2} + \frac{v_1'}{m_1 v_1^2\Delta E} + \frac{1}{m_1^2 v_1^3}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) - \left[\frac{(m_1 - m_2)(v_1^2 + 3v_2^2)}{m_1 m_2} + \frac{2(v_1^2 + v_2^2)(3m_1 - m_2)}{m_1 m_2}\right]\left(\frac{v_1'}{\Delta E} + \frac{1}{m_1 v_1}\ln\left|\frac{v_1' - v_1}{v_1' - v_1}\right|\right) + 2\frac{(3m_1 - m_2)}{m_1 m_2}\times\frac{(m_1 - m_2)}{m_1 m_2}\left(2v_1' + v_1\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right)\right\}.$$

$$-\frac{1}{5}\int\frac{(v_U^5 - v_L^5)}{\Delta E^3}\,d\Delta E = -\frac{2}{5}\left\{-\frac{(5v_2^4 + 10v_1^2 v_2^2 + v_1^4)}{2}\left(\frac{v_1'^3}{v_1^2\Delta E^2} + \frac{v_1'}{m_1 v_1^2\Delta E} + \frac{1}{m_1^2 v_2^3}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) + 4\left(\frac{5}{m_2^2} - \frac{10}{m_1 m_2} + \frac{1}{m_1^2}\right)\left(2v_1' + v_1\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) - 4\left(\frac{5v_2^2}{m_2} + 5\left(\frac{v_1^2}{m_2} - \frac{v_2^2}{m_1}\right) - \frac{v_1^2}{m_1}\right)\left(\frac{v_1'}{\Delta E} + \frac{1}{m_1 v_1}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right)\right\}.$$

Adding the various contributions gives for the second part of the recoil term

$$\frac{2\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{3v_1^2v_2c^2}\Bigg[\Big(\frac{v_1^4}{5}-v_1^2v_2^2\Big)\Big(\frac{v_1'^3}{v_1^2\Delta E^2}+\frac{v_1'}{m_1v_1^2\Delta E}$$

$$+\frac{1}{m_1^2v_1^3}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)+\frac{1}{m_1m_2}\Big(\frac{v_1'}{\Delta E}+\frac{1}{m_1v_1}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)\Big(-2m_1v_1^2$$

$$-\frac{3m_2v_1^2}{5}+m_2v_2^2\Big)+\frac{2}{m_1^2m_2^2}\Big(2v_1'+v_1\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)\Big(\frac{m_2^2}{5}+m_1m_2\Big)\Bigg].$$

Thus, for this case, $\sigma(v_2)$ is

$$\frac{\pi e^4}{3v_1^2v_2}(1-v_1^2/c^2)(1-v_2^2/c^2)\frac{(-2v_1'^3)}{\Delta E^2}-\frac{2\pi e^4}{v_1^2v_2\mu^2c^2}(1-v_1^2/c^2)(1-v_2^2/c^2)\times$$

$$\Big(2v_1'+v_1\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)+\frac{2\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{3v_1^2v_2c^2}\Bigg[\Big(\frac{v_1^4}{5}-v_1^2v_2^2\Big)\times$$

$$\Big(\frac{v_1'^3}{v_1^2\Delta E^2}+\frac{v_1'}{m_1v_1^2\Delta E}+\frac{1}{m_1^2v_1^3}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)+\frac{1}{m_1m_2}\Big(\frac{v_1'}{\Delta E}+\frac{1}{m_1v_1}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)\times$$

$$\Big(-2m_1v_1^2-\frac{3m_2v_1^2}{5}+m_2v_2^2\Big)+\frac{2}{m_1^2m_2^2}\Big(2v_1'+v_1\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\Big)\Big(\frac{m_2^2}{5}+m_1m_2\Big)\Bigg]$$

$$-\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)(v_1^2+v_2^2)(-2v_1'^3)/(3v_1^2v_2c^2\Delta E^2).$$

Case (2): The Rutherford contribution is[14]

$$\frac{\pi e^4}{3v_1^2v_2}\Big(\frac{3}{\Delta E}\Big(\frac{v_1}{m_1}-\frac{v_2}{m_2}\Big)+\frac{1}{\Delta E^2}(v_2'^3-v_2^3-v_1^3-v_1'^3)\Big)(1-v_1^2/c^2)(1-v_2^2/c^2).$$

The spin term is

$$A\int\frac{(v_1+v_2-(v_2'-v_1'))}{\Delta E}d\Delta E=A\Big((v_1+v_2)\ln\Delta E+2v_1'$$

$$+v_1\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|-2v_2'-v_2\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\Big).$$

The first part of the recoil term is

$$-\frac{\pi e^4(v_1^2+v_2^2)}{3v_1^2v_2c^2}\left(\frac{3}{\Delta E}\left(\frac{v_1}{m_1}-\frac{v_2}{m_2}\right)+\frac{1}{\Delta E}(v_2'^3-v_2^3-v_1^3-v_1'^3)\right)(1-v_1^2/c^2)(1-v_2^2/c^2)$$

The second part is

$$B\int\frac{(v_1^2-v_2^2)(v_2'^2-v_1'^2)(v_1+v_2-(v_2'-v_1'))}{\Delta E^3}\,d\Delta E$$

$$+B\int\frac{(v_1^2+v_2^2+v_1'^2+v_2'^2)((v_1+v_2)^3-(v_2'-v_1')^3)}{3\Delta E^3}\,d\Delta E$$

$$-\frac{B}{5}\int\frac{((v_1+v_2)^5-(v_2'-v_1')^5)}{\Delta E^3}\,d\Delta E.$$

$$\int\frac{(v_1^2+v_2^2+v_1'^2+v_2'^2)((v_1+v_2)^3-(v_2'-v_1')^3)}{3\Delta E^3}\,d\Delta E$$

$$=\frac{2}{3}\Bigg\{-\frac{(v_1^2+v_2^2)(v_1+v_2)^3}{2\Delta E^2}-\frac{(m_1-m_2)}{m_1m_2}\frac{(v_1+v_2)^3}{\Delta E}-(v_1^2+v_2^2)\times$$

$$\left[-\frac{(v_2^2+3v_1^2)}{2}\left(\frac{v_2'^3}{v_2^2\Delta E^2}-\frac{v_2'}{m_2v_2^2\Delta E}+\frac{1}{m_2^2v_2^3}\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)+\left(\frac{2}{m_2}-\frac{6}{m_1}\right)\times\right.$$

$$\left(-\frac{v_2'}{\Delta E}+\frac{1}{m_2v_2}\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)+\frac{(v_1^2+3v_2^2)}{2}\left(\frac{v_1'^3}{v_1^2\Delta E^2}+\frac{v_1'}{m_1v_1^2\Delta E}+\frac{1}{m_1^2v_1^3}\times\right.$$

$$\left.\left.\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\right)+\left(\frac{6}{m_2}-\frac{2}{m_1}\right)\left(\frac{v_1'}{\Delta E}+\frac{1}{m_1v_1}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\right)\right]-\frac{(m_1-m_2)}{m_1m_2}\times$$

$$\left[(v_2^2+3v_1^2)\left(-\frac{v_2'}{\Delta E}+\frac{1}{m_2v_2}\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)+\left(\frac{2}{m_2}-\frac{6}{m_1}\right)\left(2v_2'+v_2\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)\right.$$

$$\left.+(v_1^2+3v_2^2)\left(\frac{v_1'}{\Delta E}+\frac{1}{m_1v_1}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\right)-\left(\frac{6}{m_2}-\frac{2}{m_1}\right)\left(2v_1'+v_1\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\right)\right]\Bigg\}.$$

$$-\frac{1}{5}\int\left[\frac{(v_1+v_2)^5-(v_2'-v_1')^5}{\Delta E^3}\right]d\Delta E=\frac{1}{10}\frac{(v_1+v_2)^5}{\Delta E^2}$$

$$+\frac{1}{5}\left\{-\frac{(v_2^4 + 10v_1^2v_2^2 + 5v_1^4)}{2}\left(\frac{v_2'^3}{v_2^2\Delta E^2} - \frac{v_2'}{m_2v_2^2\Delta E} + \frac{1}{m_2^2v_2^3}\ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\right)\right.$$

$$+\left(\frac{4v_2^2}{m_2^2} + \frac{20(m_1v_1^2 - m_2v_2^2)}{m_1m_2} - \frac{20v_1^2}{m_1}\right)\left(-\frac{v_2'}{\Delta E} + \frac{1}{m_2v_2}\ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\right) + \left(\frac{4}{m_2^2}\right.$$

$$\left.\left. - \frac{40}{m_1m_2} + \frac{20}{m_1^2}\right)\left(2v_2' + v_2\ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\right)\right\} - \frac{1}{5}\left\{-\frac{(v_1^4 + 5v_2^4 + 10v_1^2v_2^2)}{2}\left(\frac{v_1'^3}{v_1^2\Delta E^2}\right.\right.$$

$$+\left.\frac{v_1'}{m_1v_1^2\Delta E} + \frac{1}{m_1^2v_1^3}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) + \left(\frac{20(m_1v_1^2 - m_2v_2^2)}{m_1m_2} + \frac{20v_2^2}{m_2} - \frac{4v_1^2}{m_1}\right)\times$$

$$\left.\left(-\frac{v_1'}{\Delta E} - \frac{1}{m_1v_1}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) + \left(\frac{4}{m_1^2} + \frac{20}{m_2^2} + \frac{40}{m_1m_2}\right)\left(2v_1' + v_1\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right)\right\}\cdot$$

$$(v_1^2 - v_2^2)\int\frac{(v_2'^2 - v_1'^2)(v_1 + v_2 - (v_2' - v_1'))\,d\Delta E}{\Delta E^3} =$$

$$-\frac{(v_1^2 - v_2^2)(v_2^2 - v_1^2)(v_1 + v_2)}{2\Delta E^2} - \frac{2}{\mu}\frac{(v_1^2 - v_2^2)(v_1 + v_2)}{\Delta E} + (v_1^2 - v_2^2)\times$$

$$(v_2^2 - v_1^2)\left\{-\frac{1}{2}\left(\frac{v_1'^3}{v_1^2\Delta E^2} + \frac{v_1'}{m_1v_1^2\Delta E} + \frac{1}{m_1^2v_1^3}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right) + \frac{1}{2}\left(\frac{v_2'^3}{v_2^2\Delta E^2}\right.\right.$$

$$\left.\left. - \frac{v_2'}{m_2v_2^2\Delta E} + \frac{1}{m_2^2v_2^3}\ln\left|\frac{v_2' + v_2}{v_2' + v_2}\right|\right)\right\} + \frac{2(v_1^2 - v_2^2)}{\mu}\left\{-\frac{v_1'}{\Delta E} - \frac{1}{m_1v_1}\ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\right.$$

$$\left. + \frac{v_2'}{\Delta E} - \frac{1}{m_2v_2}\ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\right\}\cdot$$

Combining all these terms gives the second part of the recoil term as

$$\frac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{\mu^2v_1^2v_2^2c^2}\left\{\frac{1}{3\Delta E^2}\left(\frac{1}{5}(v_1^5 + v_2^5) - (v_1^2v_2^3 + v_1^3v_2^2)\right)\right.$$

$$-\frac{1}{m_1m_2\Delta E}\left(\frac{2}{3}(m_1v_1^3 - m_2v_2^3) + \frac{1}{3}(m_2v_1^3 - m_1v_2^3) + (m_1v_1 - m_2v_2)v_1v_2\right)$$

$$+ \frac{1}{3}\Big(\frac{v_2'^3}{v_2^2\Delta E^2} - \frac{v_2'}{m_2 v_2^2 \Delta E} + \frac{1}{m_2^2 v_2^3} \ln\left|\frac{v_2' + v_2}{v_2' + v_2}\right|\Big)(v_1^2 v_2^2 - \frac{v_2^4}{5}) + \frac{1}{3}\Big(\frac{v_1'^3}{v_1^2 \Delta E^2}$$

$$+ \frac{v_1'}{m_1 v_1^2 \Delta E} + \frac{1}{m_1^2 v_1^3} \ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\Big)(\frac{v_1^4}{5} - v_1^2 v_2^2) + \frac{1}{m_1 m_2}\Big(-\frac{v_2'}{\Delta E} + \frac{1}{m_2 v_2} \times$$

$$\ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\Big)(-\frac{m_1 v_1^2}{3} + 2\,\frac{m_2 v_2^2}{3} + \frac{m_1 v_2^2}{5}) + \frac{1}{m_1 m_2}\Big(\frac{v_1'}{\Delta E} + \frac{1}{m_1 v_1} \ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\Big) \times$$

$$(-\frac{2m_1 v_1^2}{3} + \frac{m_2 v_2^2}{3} - \frac{m_2 v_1^2}{5}) + \frac{1}{m_1^2 m_2^2}\Big(2v_2' + v_2 \ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\Big)(-\frac{2m_1^2}{15} - \frac{10 m_1 m_2}{3})$$

$$+ \frac{1}{m_1^2 m_2^2}\Big(2v_1 + v_1 \ln\left|\frac{v_1' - v_1}{v_1' + v_1}\right|\Big)(\frac{2m_2^2}{15} - \frac{10 m_1 m_2}{3})\Big\} .$$

The expression for $\sigma(v_2)$ is therefore

$$\pi e^4\Big(\frac{3}{\Delta E}\big(\frac{v_1}{m_1} - \frac{v_2}{m_2}\big) + \frac{1}{\Delta E^2}(v_2'^3 - v_2^3 - v_1^3 - v_1'^3)\Big)\frac{(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{3v_1^2 v}$$

$$- \frac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{\mu^2 v_1^2 v_2 c^2}\Big((v_1 + v_2)\ln \Delta E + 2(v_1' - v_2')$$

$$+ v_1 \ln\left|\frac{v_1' + v_1}{v_1' + v_1}\right| - v_2 \ln\left|\frac{v_2' - v_2}{v_2' + v_2}\right|\Big) - \frac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{3v_1^2 v_2 c^2} \times$$

$$(v_1^2 + v_2^2)\Big(\frac{3}{\Delta E}\big(\frac{v_1}{m_1} - \frac{v_2}{m_2}\big) + \frac{1}{\Delta E^2}(v_2'^3 - v_2^3 - v_1^3 - v_1'^3)\Big)$$

$$+ \frac{\pi e^4(1 - v_1^2/c^2)(1 - v_2^2/c^2)}{\mu^2 v_1^2 v_2 c^2}\Big\{\frac{1}{3\Delta E^2}\Big(\frac{1}{5}(v_1^5 + v_2^5) - (v_1^2 v_2^3 + v_1^3 v_2^2)\Big)$$

$$- \frac{1}{m_1 m_2 \Delta E}\Big(\frac{2}{3}(m_1 v_1^3 - m_2 v_2^3) + \frac{1}{3}(m_2 v_1^3 - m_1 v_2^3) + (m_1 v_1 - m_2 v_2) v_1 v_2\Big)$$

$$+ \frac{1}{3}\Big(\frac{v_2'^3}{v_2^2 \Delta E^2} - \frac{v_2'}{m_2 v_2^2 \Delta E} + \frac{1}{m_2^2 v_2^3} \ln\left|\frac{v_2' + v_2}{v_2' + v_2}\right|\Big)(v_1 v_2 - \frac{v_2^4}{5})$$

$$+\frac{1}{3}\left(\frac{v_1'^3}{v_1^2\Delta E^2}+\frac{v_1'}{m_1v_1^2\Delta E}+\frac{1}{m_1^2v_1^3}\ln\left|\frac{v_1'+v_1}{v_1'+v_1}\right|\right)\left(\frac{v_1^4}{5}-v_1^2v_2^2\right)$$

$$+\frac{1}{m_1m_2}\left(-\frac{v_2'}{\Delta E}+\frac{1}{m_2v_2}\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)\left(-\frac{m_1v_1^2}{3}+\frac{2m_2v_2^2}{3}+\frac{m_1v_2^2}{5}\right)+\frac{1}{m_1m_2}\left(\frac{v_1'}{\Delta E}\right.$$

$$\left.+\frac{1}{m_1V_2}\ln\left|\frac{v_1'-v_1}{v_1'+v_1}\right|\right)\left(-\frac{2m_1v_1^2}{3}+\frac{m_2v_2^2}{3}-\frac{m_1v_2^2}{5}\right)+\frac{1}{m_1^2m_2^2}\left(2v_2'+v_2\ln\left|\frac{v_2'-v_2}{v_2'+v_2}\right|\right)\times$$

$$\left(\frac{-2m_1^2}{15}-\frac{10m_1m_2}{3}\right)+\frac{1}{m_1^2m_2^2}\left(2v_1'+v_1\ln\left|\frac{v_1'+v_1}{v_1'+v_1}\right|\right)\left(\frac{2m_2^2}{15}-\frac{10m_1m_2}{3}\right)\Bigg\}\ . \qquad (17)$$

Case (3) : The Rutherford term is now[14]

$$\frac{\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{3v_1^2v_2}\left(\frac{-2v_2^3}{\Delta E^2}-\frac{6v_2}{m_2\Delta E}\right)\ .$$

The spin term is $2Av_2\ln\Delta E$.

The recoil term is

$$-\frac{\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)(v_1^2+v_2^2)}{3v_1^2v_2c^2}\left(\frac{2v_2^3}{\Delta E^2}-\frac{6v_2}{m_2\Delta E}\right)+\frac{\pi e^4(1-v_1^2/c^2)}{3v_1^2v_2c^2}\times$$

$$(1-v_2^2/c^2)\left\{2(v_1^2-v_2^2)v_2\left(\frac{-2}{\mu\Delta E}-\frac{(v_2^2-v_1^2)}{2\Delta E^2}\right)+\frac{2}{3}(v_2^3+3v_1^2v_2)\times\right.$$

$$\left.\left(-\frac{(v_1^2+v_2^2)}{\Delta E}-\frac{(2m_1-m_2)}{m_1m_2\Delta E}\right)+\frac{1}{10\Delta E^2}(10v_1^4v_2+20v_1^2v_2^3+2v_2^5)\right\}\ .$$

Thus $\sigma(v_2)$ is

$$\frac{\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{3v_1^2v_2}\left(\frac{-2v_2^3}{\Delta E^2}-\frac{6v_2}{m_2\Delta E}\right)-\frac{2\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{v_1^2v_2\mu^2c^2}\times$$

$$v_2\ln\Delta E\quad+\frac{\pi e^4(1-v_1^2/c^2)(1-v_2^2/c^2)}{3v_1^2v_2c^2}\left\{\left(\frac{6v_2}{m_2\Delta E}-\frac{2v_2^3}{\Delta E^2}\right)(v_1^2+v_2^2)\right.$$

$$+ 2v_2(v_1^2 - v_2^2)\left(-\frac{2}{\mu \Delta E} - \frac{(v_2^2 - v_1^2)}{2\Delta E^2} \right) + \frac{2}{3}(v_2^3 + 3v_1^2 v_2)\left(-\frac{(v_1^2 + v_2^2)}{E}\right.$$

$$\left. - \frac{(2m_1 - m_2)}{m_1 m_2 \Delta E}\right) + \frac{1}{10\Delta E^2}(10v_1^4 v_2 + 20v_1^2 v_2^3 + 2v_2^5) \Bigg\} \; . \qquad (18)$$

SECTION VI – THE AVERAGE OF $\sigma(v_2)$ OVER THE ELECTRON VELOCITY DISTRIBUTION FUNCTION

The cross – section $\sigma(v_2)$ has to be averaged over the velocity distribution function of the target electron in order to get the ionization cross – section. This is because in practice v_2 is not arbitrarily fixed, but is determined by the velocity distribution function of the target electron. Thus[31,32]

$$\sigma_I = \int_0^\infty \sigma(v_2) f(v_2)\, 4\pi v_2^2\, dv_2$$

$$= \int_0^\infty \sigma(v_2)\, \rho(v_2)\, dv_2 \quad . \tag{19}$$

where $\rho(v_2) = 4\pi v_2^2 f(v_2)$ and $f(v_2)$ is the electron velocity distribution function. The function $f(v_2)$ is $\Phi^*(v_2)\Phi(v_2)$, where $\Phi(v_2)$ is the solution, for the particular shell, of the Schroedinger equation in momentum space[33]. Hartree–Fock wave-functions[34,35] are the most accurate solutions, but more usually, hydrogenic functions are used. These lead to[13,14,36]

$$\rho(v_2) = \frac{32}{\pi} \frac{v_2^7}{(v_0^2 + v_2^2)^4} , \tag{20}$$

with $v_0 = \left(\frac{2E_0}{m_2}\right)^{\frac{1}{2}}$. E_0 is the binding energy of the electron.

It is evident that averaging $\sigma(v_2)$ over $f(v_2)$ is the second way in which the nucleus of the target atom exerts an influence on the BEA ionization cross – section. With $\rho(v_2)$ as in equation (20), integral (19) is best performed numerically.

SECTION VII - RESULTS

In each of the formulas (16) - (18), the first term is the uncorrected BEA cross - section, differing from that in ref. 14 only by the presence here of the relativistic mass correction factors $1 - v_1^2/c^2$ and $1 - v_2^2/c^2$; the second term represents corrections due to spin effects;[16,26] and the third term arises from recoil effects. To gauge the contribution of the recoil term to the cross - section, two computer programmes were written. The first one computed the uncorrected cross - section; that is, with the recoil term left out; and the second one computed the corrected cross - section. The ratio $R = \dfrac{\text{corrected cross-section}}{\text{uncorrected cross-section}}$ conveniently quantifies the recoil contribution to the cross - section.

The numerical regime adopted for the computation was 15 - point Gauss - Laguerre quadrature.[37] A mesure of the error involved in the integrations was obtained from comparing the numerically - calculated and the exact values of various integrals over the range $(0,\infty)$. The highest error recorded was 14%. In view of the general accuracy of Gaussian quadrature methods, this value was taken to be a reasonable indicator of the error. The programmes were confirmed to contain no logical errors when the appropriate one successfully reproduced the K - shell ionization values for Mg given in ref. 14.

The elements Ti, Cu and Ag were chosen as test cases. The recoil effect should be significant in all cases because of the relatively high Z - values - 22, 29 and 47 respectively. Moreover, the Z - value spread should reveal the way in which this effect varies with this parameter. For each one of these test elements, the cross - sections were computed for a wide energy range in order to bring out the dependence of the effect on proton energy.

The cross - sections are given in the tables which follow. Though they are given to only three signifacant figures in these tables, the value of R is calculated from the original values which were to 9 decimal places.

As well as the theoretical values, the experimental values of the cross - sections are tabulated, whenever these are available from the literature.

proton energy (keV)	uncorrected cross-section (barns)	corrected cross-section (barns)	experimental cross-section (barns)	R
90	0.141	0.141		1.00078
100	0.194	0.195		1.00073
110	0.287	0.287		1.00065
120	0.408	0.408		1.00058
130	0.548	0.548		1.00052
140	0.699	0.699		1.00048
150	0.858	0.859		1.00045
200	2.17	2.17		1.00039
300	7.94	7.94		1.00032
400	19.8	19.8		1.00030
500	39.6	39.6		1.00027
600	61.4	61.5		1.00027
700	93.4	93.4		1.00026
800	138	138		1.00024
900	189	189		1.00024
1000	242	242		1.00023

TABLE 1

K – SHELL IONIZATION CROSS – SECTIONS FOR Ti (Z = 22)

proton energy (keV)	uncorrected cross-section (barns)	corrected cross-section (barns)	experimental cross-section (barns)	R
90	0.00509	0.00511		1.00395
100	0.00739	0.00741		1.00313
200	0.0887	0.0888		1.00117
300	0.338	0.338		1.00078
500	1.82	1.82	1.75	1.00059
625	3.89	3.89	3.38	1.00054
750	6.87	6.88	6.18	1.00052
875	10.2	10.2	9.88	1.00050
1000	15.0	15.0	15.0	1.00049
1250	29.1	29.1	29.8	1.00043
1500	45.4	45.4	48.3	1.00044
1750	66.6	66.6	73.0	1.00043
2000	92.7	92.7	98.8	1.00041
2250	121	121	137	1.00039
2500	150	150	171	1.00036
2750	183	183	210	1.00036
3000	218	218	242	1.00034
3940	353	353	363	1.00028
6070	640	640	615	1.00017
9130	919	919	875	1.00012
12210	1070	1070		1.00024
18290	1114	1115		1.00088
23980	1066	1069		1.00293
30130	970	974		1.00453
35610	899	905		1.00636
39560	845	853		1.00940

TABLE 2

K - SHELL IONIZATION CROSS - SECTIONS FOR Cu (Z = 29)

The experimental values are from ref. 40

proton energy (keV)	uncorrected cross-section (barns)	corrected cross-section (barns)	experimental cross-section (barns)	R
100	0.00000401	0.00000447		1.11407
200	0.000185	0.000188		1.01974
300	0.000983	0.000992		1.00871
400	0.00290	0.00291		1.00550
500	0.00647	0.00650		1.00378
600	0.0126	0.0127	0.0080	1.00315
800	0.0332	0.0332	0.032	1.00235
1000	0.0745	0.0747	0.077	1.00200
1200	0.130	0.131	0.16	1.00181
1400	0.219	0.219	0.26	1.00170
1600	0.343	0.343	0.40	1.00161
1800	0.484	0.485	0.57	1.00156
2000	0.652	0.653	0.80	1.00152
4000	4.81	4.82		1.00129
8000	23.7	23.7		1.00101
12000	48.5	48.5		1.00076
16000	72.2	72.3		1.00053
20000	92.0	92.1		1.00039
24000	108	108		1.00046
28000	119	119		1.00058
32000	127	127		1.00079
36000	133	133		1.00194
40000	136	136		1.00267

TABLE 3

K - SHELL IONIZATION CROSS - SECTIONS FOR Ag (Z = 47)

The experimental values are from ref. 41

SECTION VII – DISCUSSION

Tables (1) – (3) in Section VII show how the recoil effect depends on the projectile energy on the one hand and on the Z – value of the target species on the other. At low projectile energies, the effect is relatively large, but it decreases with increasing projectile energy. Beyond a certain point, the decreasing trend is reversed, and the recoil effect begins to increase with projectile energy. This behaviour is well exhibited in the cross – sections for the elements Cu and Ag. In the examination of Ti, energies beyond 1 MeV were not considered, but presumably, the recoil effect reverses its decrease with increasing proton energy beyond this value.

The recoil effect is relatively large at low energies of the projectle because the electrons which the proton collides with have the largest momentum and so relativistic effects are enhanced. This can be seen from the cross – section curve which has essentially the shape of the velocity distribution function of the electron. Thus, this curve has its maximum where the distribution function peaks. This implies that low proton speeds correspond to high electron speeds, and at the lowest projectile speeds, the collisions which make the most important contribution to the cross – section are those in which the electrons have speeds comparable to c. These are the collisions in which relativistic effects, like recoil, are important.

As the projectile energy increases, the electrons that are important in the ionization collisions are the ones with smaller and smaller energy. The recoil correction progressively decreases. But the projectile momentum is increasing and therefore, after a certain point, the recoil effect begins to increase again.

Tables (1) – (3) reveal that for a given projectile energy, the recoil effect increases with Z of the target atom. Thus, at 500 keV, R is 1.00027 for Ti, 1.00059 for Cu and 1.00378 for Ag. This dependence on Z is even more marked at low proton energies. At 100 keV, R is 1.00073 for Ti, 1.00313 for Cu and 1.01974 for Ag. The Z - value of the target does not explicitly appear in the cross - section formulas developed, but the dependence of the results on this parameter is contained in the electron binding energy - which appers as a limit in the integral $\sigma(v_2)$ and in the velocity distribution function - which is itself a function of Z.

The recoil effect increases with Z because this parameter indicates how tightly bound K - shell electrons are: the distribution function has higher and higher values at high electron speeds as Z increases. Thus the contribution of high energy electrons to the ionization cross - section is more important.

For the elements and the energies investigated, the recoil correction has a highest value of 11%, for Ag at 100 keV. But at 200 keV, it has diminished to 2%, and its lowest value in that element in only 0.04%. For Cu, its highest value is 0.9%, at 39.56 MeV. The lowest value is 0.012% at 9.13 MeV. For Ti, the highest and lowest values are 0.078% (at 90 keV) and 0.023% (at 1 MeV) respectively. Thus, apart from at very low projectile energies in high-Z elements, the recoil effect is very small. Just how small becomes apparent when its extent at a given energy in one element is compared to the value, at the same energy, of one of the corrections mentioned in the Introduction.

One method of correcting the Binary Encounter Method for electron relativistic motion is to use in place of expression (20) for the velocity distribution function a different one derived from Dirac wavefunctions. The Dirac functions result in a distribution denser at close distances to the nucleus than expression (20), and ionization cross - sections are increased. The ratio of the BEA cross - section obtained with a Dirac distribution function to that obtained with a hydrogenic distribution function measures the correction due to these wavefunctions. In Cu at 500 keV, this correction[16] is 8%, but the recoil correction is only 0.06%.

It is evident from the tables that the recoil correction would be significant at energies lower than those investigated here. However, the Binary Encounter Model is doubtful at these energies, and meaningful interpretation would be difficult. It would however be interesting to extend the investigation to higher - Z elements.

CONCLUSION

The recoil effect has been investigated. In the three elements examined, it has been evident at all energies; however, its scale is small except at low energies in high - Z elements. Since experimental cross - sections are available to about 10% accuracy, the recoil effect usefully modifies cross - sections only at very low energies in high - Z elements.

APPENDIX

COMPUTER PROGRAMMES

PROGRAMME TO COMPUTE UNCORRECTED CROSS - SECTIONS

```
      implicit double precision (a-h,o-z)
c     xa is the array containing the nodes for the 15-point Gauss-
c     Laguerre numerical algorithm used to perform the average of tl
c     energy exchange cross-section over the velocity distribution
c     function of the electron. The array wa contains the weights.
      dimension xa(15),wa(15)
      common/b1/rmp/b2/rme/b3/vp/b4/pi/b7/ebg/b5/cee/b6/rmu/b8/ap/b9
c     rmp=proton mass,rme=electron mass,vp=proton speed,cee is the s
c     of light in vacuum,rmu is the reduced mass of the electron-pr
c     system,cm is the total mass of the electron and proton and ap
c     constant introduced for convenience.
      rme=1.
      rmp=1838.66
      pi=3.14159
      cee=137.
c     writing the heading.
      write(3,18)
 18   format(4x,11henergy(kev),14x,22hcross-section(10-24m2))
c     reading the nodes and weights from an external data file
      read(1,6)(xa(i),i=1,15)
      read(1,6)(wa(i),i=1,15)
      read(1,12)ebg
c     ebg is the electron binding energy and is in kev.
 6    format(4f15.12)
 12   format(f15.7)
      fg=1000.
c     fg is the unit of energy
      cm=rme+rmp
      rmu=rme*rmp/cm
      ebg=ebg*1000./fg
 14   read(1,12)ep
c     ep is the incident electron energy in kev
      if(ep.eq.0.) go to 40
c     the above condition terminates the programme; the last value
c     proton energy in the data file should therefore be 0.
      tep=ep
c     tep stores the electron energy in its original units.
      ep=ep*1000./fg
      vp=dsqrt(2.*ep/rmp)
      sum=0.
c     this do loop performs the integration by the gauss-laguerre m
      do 20 k=1,15
      ve=xa(k)
c     ve is electron speed
      ee=rme*ve*ve/2.
c     ee is electron kinetic energy
      ap=dsqrt((rme*ve*ve+rmp*vp*vp)/rmu)
      a=4.*rmp*rme*(ep-ee+ve*vp*(rmp-rme)/2.)/(rmp+rme)**2
      b=4.*rmp*rme*(ep-ee-ve*vp*(rmp-rme)/2.)/(rmp+rme)**2
c     a and b are energy points necessary in the determination of w
```

```
c       of the three expressions for the un-averaged ionization cross-
c       cross-section should be used for the various parameters now
c       obtaining.
        call dist(ve,res)
c       dist is a subroutine that works out values of the velocity
c       distribution function for given values of ve, denoted res.
c       the next series of statements determines which of the three c
c       section expressions should be used.
        if(ep.lt.a) go to 24
        if(ebg.lt.a) go to 26
        call fun3(ve,ebg,ep,f3)
        rr=f3
c       rr is the ionization cross-section for a fixed electron energ
        go to 28
 26     if(ebg.lt.b) go to 30
        call fun3(ve,a,ep,f3)
        call fun2(ve,ebg,a,f2)
        rr=f3+f2
        go to 28
 30     call fun3(ve,a,ep,f3)
        call fun2(ve,b,a,f2)
        call fun1(ve,b,f1b)
        call fun1(ve,ebg,f1ebg)
        rr=f3+f2+f1b-f1ebg
        go to 28
 24     if(ep.lt.b) go to 32
        if(ebg.lt.b) go to 34
        call fun2(ve,ebg,ep,f2)
        rr=f2
        go to 28
 34     call fun2(ve,b,ep,f2)
        call fun1(ve,b,f1b)
        call fun1(ve,ebg,f1ebg)
        rr=f2+f1b-f1ebg
        go to 28
 32     call fun1(ve,ep,f1ep)
        call fun1(ve,ebg,f1ebg)
        rr=f1ep-f1ebg
 28     sum=sum+res*rr*wa(k)*(1.-(ve/cee)**2)
 20     continue
        gg= 4.8**4*1.0d-16/(1.6*1000.)**2
        sum=(sum*gg)*(1.-(vp/cee)**2)
c       printing in the output file the proton energy and the ionizat
c       cross-section at this energy.
        write(3,38)tep,sum
 38     format(e20.10,10x,e20.10)
        go to 14
 40     stop
        end
c       the velocity distribution function subroutine
```

```
      subroutine dist(x,y)
      implicit double precision (a-h,o-z)
      common/b4/pi/b7/ebg/b2/rme
      v0=dsqrt(2.*ebg/rme)
c     v0 is the speed of an electron whose energy is the binding en
      y=((32./pi)*v0**5*x*x)/(v0*v0+x*x)**4
      return
      end
c     the expression for the cross-section for case (3) (see thesis
      subroutine fun1(x,y,z)
      implicit double precision (a-h,o-z)
      common/b2/rme/b3/vp/b4/pi/b1/rmp/b5/cee/b6/rmu/b9/cm
      z=(pi/3.)*(-2.*x**3/(y*y)-6.*x/(rme*y))/(vp*vp*x)
     1-pi*dlog(y)/((vp*rmu*cee)**2)
      return
      end
      subroutine fun2(x,y1,y2,z)
      implicit double precision (a-h,o-z)
      call fff2(x,y1,t1)
      call fff2(x,y2,t2)
      z=t2-t1
      return
      end
      subroutine fun3(x,y1,y2,z)
      implicit double precision (a-h,o-z)
      common/b1/rmp/b2/rme/b3/vp/b4/pi
      bb=(rmp-rme)*vp
      aa=2.*rme*x
      if(aa.lt.bb) go to 10
      call fff3(x,y1,t1)
      call fff3(x,y2,t2)
      z=t2-t1
      go to 12
 10   z=0.
 12   return
      end
c     the cross section expression for case (2)
      subroutine fff2(x,y,z)
      implicit double precision (a-h,o-z)
      common/b1/rmp/b2/rme/b3/vp/b4/pi/b5/cee/b6/rmu/b8/cm
c     vpp and vep are proton and electron speeds after collision
c     respectively.
      vpp=dsqrt(vp*vp-2.*y/rmp)
      vep=dsqrt(x*x+2.*y/rme)
      z=(pi/3.)*(3.*(vp/rmp-x/rme)/y+(vep**3-x**3-vp**3-vpp**3)
     1/(y*y))/(vp**2*x)
     2-pi*((vp+x)*dlog(y)+2.*(vpp-vep)+vp*dlog((vp-vpp)/(vpp+vp))
     3-x*dlog((vep-x)/(vep+x)))/((vp*rmu*cee)**2*x)
      return
      end
```

```
c       the cross-section expression for case (1)
        subroutine fff3(x,y,z)
        implicit double precision (a-h,o-z)
        common/b1/rmp/b2/rme/b3/vp/b4/pi/b5/cee/b6/rmu
        vpp=dsqrt(vp**2-2.*y/rmp)
        vep=dsqrt(x**2+2.*y/rme)
        z=-(pi/3.)*((2.*vpp**3)/(y*y))/(vp*vp*x)
       1-(2.*pi/((vp*cee*rmu)**2*x))*(2.*vpp+dlog((vp-vpp)/(vp+vpp)))
        return
        end
```

PROGRAMME TO COMPUTE CORRECTED CROSS - SECTIONS

```
      implicit double precision (a-h,o-z)
c     xa is the array containing the nodes for the 15-point Gauss-
c     Laguerre numerical algorithm used to perform the average of the
c     energy exchange cross-section over the velocity distribution
c     function of the electron. The array wa contains the weights.
      dimension xa(15),wa(15)
      common/b1/rmp/b2/rme/b3/vp/b4/pi/b7/ebg/b5/cee/b6/rmu/b8/ap/b9/
c     rmp=proton mass,rme=electron mass,vp=proton speed,cee is the sp
c     of light in vacuum,rmu is the reduced mass of the electron-prot
c     system,cm is the total mass of the electron and proton and ap i
c     constant introduced for convenience.
      rme=1.
      rmp=1838.66
      pi=3.14159
      cee=137.
c     writing the heading.
      write(3,18)
 18   format(4x,11henergy(kev),14x,22hcross-section(10-24m2))
c     reading the nodes and weights from an external data file
      read(1,6)(xa(i),i=1,15)
      read(1,6)(wa(i),i=1,15)
      read(1,12)ebg
c     ebg is the electron binding energy and is in kev.
 6    format(4f15.12)
 12   format(f15.7)
      fg=1000.
c     fg is the unit of energy
      cm=rme+rmp
      rmu=rme*rmp/cm
      ebg=ebg*1000./fg
 14   read(1,12)ep
c     ep is the incident electron energy in kev
      if(ep.eq.0.) go to 40
c     the above condition terminates the programme; the last value of
c     proton energy in the data file should therefore be 0.
      tep=ep
c     tep stores the electron energy in its original units.
      ep=ep*1000./fg
      vp=dsqrt(2.*ep/rmp)
      sum=0.
c     this do loop performs the integration by the gauss-laguerre met
      do 20 k=1,15
      ve=xa(k)
c     ve is electron speed
      ee=rme*ve*ve/2.
c     ee is electron kinetic energy
      ap=dsqrt((rme*ve*ve+rmp*vp*vp)/rmu)
      a=4.*rmp*rme*(ep-ee+ve*vp*(rmp-rme)/2.)/(rmp+rme)**2
      b=4.*rmp*rme*(ep-ee-ve*vp*(rmp-rme)/2.)/(rmp+rme)**2
c     a and b are energy points necessary in the determination of whi
```

```
c     of the three expressions for the un-averaged ionization cross-
c     cross-section should be used for the various parameters now
c     obtaining.
      call dist(ve,res)
c     dist is a subroutine that works out values of the velocity
c     distribution function for given values of ve, denoted res.
c     the next series of statements determines which of the three cr
c     section expressions should be used.
      if(ep.lt.a) go to 24
      if(ebg.lt.a) go to 26
      call fun3(ve,ebg,ep,f3)
      rr=f3
c     rr is the ionization cross-section for a fixed electron energy
      go to 28
 26   if(ebg.lt.b) go to 30
      call fun3(ve,a,ep,f3)
      call fun2(ve,ebg,a,f2)
      rr=f3+f2
      go to 28
 30   call fun3(ve,a,ep,f3)
      call fun2(ve,b,a,f2)
      call fun1(ve,b,f1b)
      call fun1(ve,ebg,f1ebg)
      rr=f3+f2+f1b-f1ebg
      go to 28
 24   if(ep.lt.b) go to 32
      if(ebg.lt.b) go to 34
      call fun2(ve,ebg,ep,f2)
      rr=f2
      go to 28
 34   call fun2(ve,b,ep,f2)
      call fun1(ve,b,f1b)
      call fun1(ve,ebg,f1ebg)
      rr=f2+f1b-f1ebg
      go to 28
 32   call fun1(ve,ep,f1ep)
      call fun1(ve,ebg,f1ebg)
      rr=f1ep-f1ebg
 28   sum=sum+res*rr*wa(k)*(1.-(ve/cee)**2)
 20   continue
      gg= 4.8**4*1.0d-16/(1.6*1000.)**2
      sum=(sum*gg)*(1.-(vp/cee)**2)
c     printing in the output file the proton energy and the ionizati
c     cross-section at this energy.
      write(3,38)tep,sum
 38   format(e20.10,10x,e20.10)
      go to 14
 40   stop
      end
c     the velocity distribution function subroutine
```

```
      subroutine dist(x,y)
      implicit double precision (a-h,o-z)
      common/b4/pi/b7/ebg/b2/rme
      v0=dsqrt(2.*ebg/rme)
c     v0 is the speed of an electron whose energy is the binding ener
      y=((32./pi)*v0**5*x*x)/(v0*v0+x*x)**4
      return
      end
c     the expression for the cross-section for case (3) (see thesis)
      subroutine fun1(x,y,z)
      implicit double precision (a-h,o-z)
      common/b2/rme/b3/vp/b4/pi/b1/rmp/b5/cee/b6/rmu/b9/cm
      z=(pi/3.)*(-2.*x**3/(y*y)-6.*x/(rme*y))/(vp*vp*x)
     1-pi*dlog(y)/((vp*rmu*cee)**2)+
     2(pi/(3.*(vp*cee)**2*x))*
     3(((vp**2+x**2)/cee**2)*(2.*x**3/(y*y)+6.*x/(rme*y))-2.*x*
     4(vp**2-x**2)*((x**2-vp**2)/(2.*y**2)+2./(rmu*y))-2.*(x**3/3.+
     5vp**2*x)*((x**2+vp**2)/(y*y)+(2.*rmp-rme)/(rmp*rme*y))+(vp**4*
     6+2.*vp**2*x**3+x**5/5.)/(y*y))
      return
      end
      subroutine fun2(x,y1,y2,z)
      implicit double precision (a-h,o-z)
      call fff2(x,y1,t1)
      call fff2(x,y2,t2)
      z=t2-t1
      return
      end
      subroutine fun3(x,y1,y2,z)
      implicit double precision (a-h,o-z)
      common/b1/rmp/b2/rme/b3/vp/b4/pi
      bb=(rmp-rme)*vp
      aa=2.*rme*x
      if(aa.lt.bb) go to 10
      call fff3(x,y1,t1)
      call fff3(x,y2,t2)
      z=t2-t1
      go to 12
 10   z=0.
 12   return
      end
c     the cross section expression for case (2)
      subroutine fff2(x,y,z)
      implicit double precision (a-h,o-z)
      common/b1/rmp/b2/rme/b3/vp/b4/pi/b5/cee/b6/rmu/b8/cm
c     vpp and vep are proton and electron speeds after collision
c     respectively.
      vpp=dsqrt(vp*vp-2.*y/rmp)
      vep=dsqrt(x*x+2.*y/rme)
      rz1=(pi/3.)*(3.*(vp/rmp-x/rme)/y+(vep**3-x**3-vp**3-vpp**3)
     1/(y*y))/(vp**2*x)
     2-pi*((vp+x)*dlog(y)+2.*(vpp-vep)+vp*dlog((vp-vpp)/(vpp+vp))
     3-x*dlog((vep-x)/(vep+x)))/((vp*rmu*cee)**2*x)
     4-(pi/3.)*(3.*(vp/rmp-x/rme)/y+(vep**3-x**3-vp**3-vpp**3)
     5/(y*y))*(x**2+vp**2)/((vp*cee)**2*x)
      bj=pi/((rmu*cee*vp)**2*x)
      rz2=((vp**5+x**5)/5.-(vp**2*x**3+vp**3*x**2))/(3.*y*y)
```

```
 rz3=-(2.*(rmp*vp**3-rme*x**3)/3.+(rme*vp**3-rmp*x**3)/3.+vp*x*
1*vp-rme*x))/(rmp*rme*y)
 rz4=(vep**3/(x*y)**2-vep/(rme*y*x**2)+dlog((vep-x)/(vep+x))/(r
1**2*x**3))*((vp*x)**2-x**4/5.)/3.
 rz5=(vpp**3/(vp*y)**2+vpp/(rmp*y*vp**2)+dlog((vp-vpp)/(vp+vpp)
1(rmp**2*vp**3))*(vp**4-(vp*x)**2)/3.
 rz6=(-vep/y+dlog((vep-x)/(vep+x))/(rme*x))*(-rmp*vp**2/3.+2.*r
1**2/3.+rmp*x**2/5.)/(rme*rmp)
 rz7=(vpp/y+dlog((vp-vpp)/(vp+vpp))/(rmp*vp))*(-2.*rmp*vp**2/3.
1rme*x**2/3.-rme*vp**2/5.)/(rme*rmp)
 rz8=(2.*vep+x*dlog((vep-x)/(vep+x)))*(-2.*rmp**2/15.-10.*rme*
1*rmp/3.)/(rme*rmp)**2
 rz9=(2.*vpp+vp*dlog((vpp-vp)/(vpp+vp)))*(2.*rme**2/15.-10*rme
1*rmp/3.)/(rme*rmp)**2
 z=rz1+(rz2+rz3+rz4+rz5+rz6+rz7+rz8+rz9)*bj
 return
 end
c      the cross-section expression for case (1)
 subroutine fff3(x,y,z)
 implicit double precision (a-h,o-z)
 common/b1/rmp/b2/rme/b3/vp/b4/pi/b5/cee/b6/rmu
 vpp=dsqrt(vp**2-2.*y/rmp)
 vep=dsqrt(x**2+2.*y/rme)
 rz1=-(pi/3.)*((2.*vpp**3)/(y*y))/(vp*vp*x)
1-(2.*pi/((vp*cee*rmu)**2*x))*(2.*vpp+dlog((vp-vpp)/(vp+vpp)))
1+(pi/3.)*((2.*vpp**3)/(y*y))*(x**2+vp**2)/((vp*cee)**2*x)
 bj=2.*pi/(3.*(vp*cee)**2*x)
 rz2=(vp**4/5.-(vp*x)**2)*(vpp**3/(vp*y)**2+vpp/(rmp*vp**2*y)+
1dlog((vp-vpp)/(vp+vpp))/(rmp**2*vp**3))
 rz3=(vpp/y+dlog((vp-vpp)/(vp+vpp))/(rmp*vp))*(-2.*rmp*vp**2-3
1rme*vp**2/5.+rme*x**2)/(rme*rmp)
 rz4=2.*(2.*vpp+vp*dlog((vp-vpp)/(vp+vpp)))*(rme**2/5.+rme*rmp
1(rme*rmp)**2
 z=rz1+bj*(rz2+rz3+rz4)
 return
 end
```

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