

# Electron Capture from Hydrogenic Systems by Positrons and Positive Muons

by

Umar Dujain Ubaid Al-Kaabi

A Thesis Presented to the

FACULTY OF THE COLLEGE OF GRADUATE STUDIES  
KING FAHD UNIVERSITY OF PETROLEUM & MINERALS  
DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the  
Requirements for the Degree of

**MASTER OF SCIENCE**

In

**PHYSICS**

June, 1997

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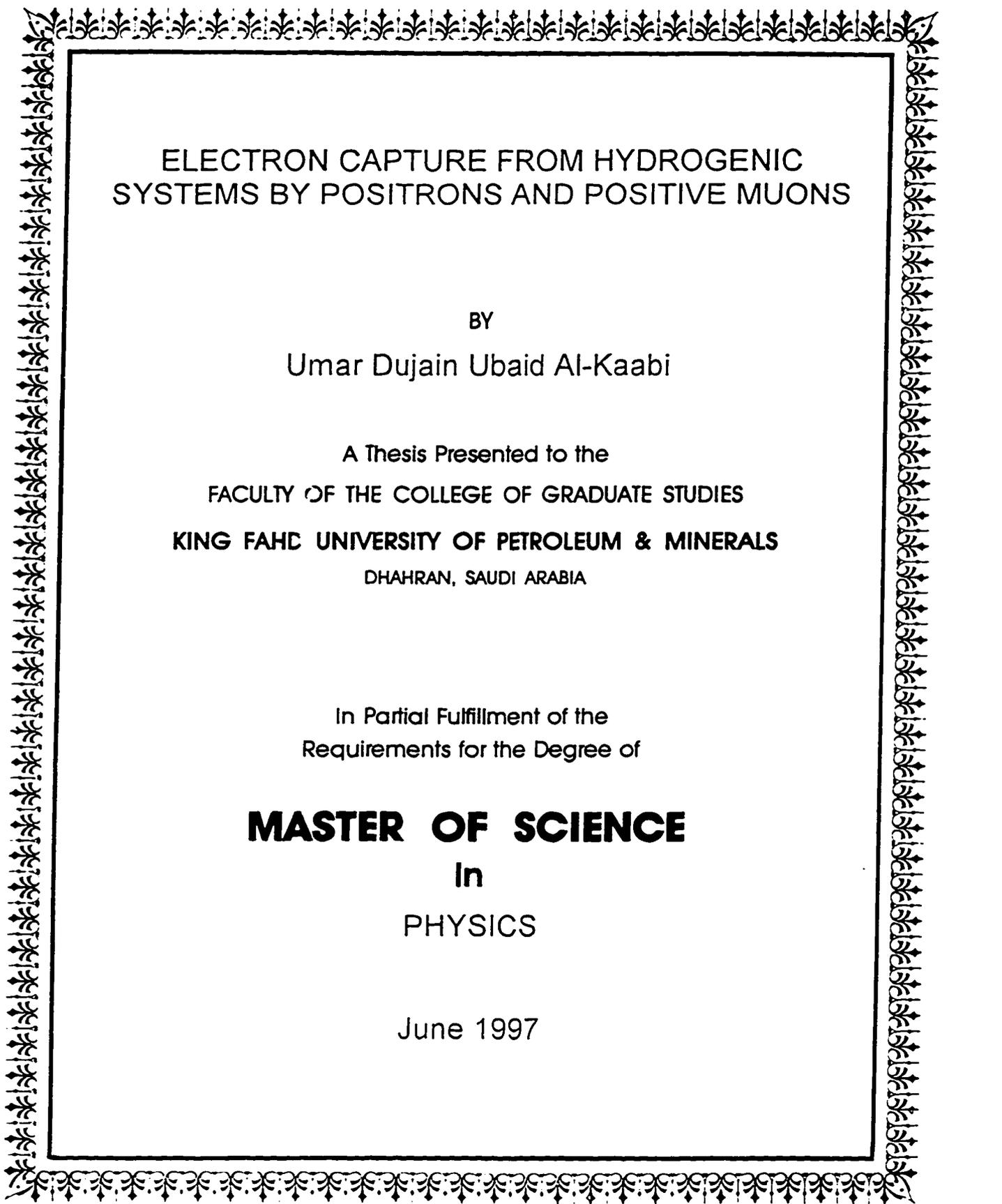
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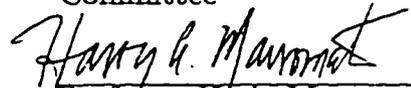
COLLEGE OF GRADUATE STUDIES

This thesis, written by Umar Dujain Ubaid Al-Kaabi under the direction of his Thesis Advisor and approved by his Thesis Committee, has been presented to and accepted by the Dean of the College of Graduate Studies, in partial fulfillment of the requirements for the degree of MASTER OF SCIENCE.

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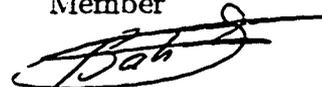
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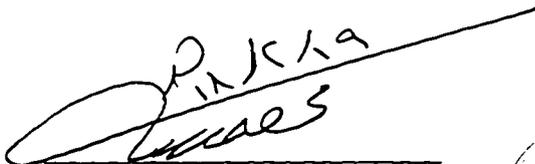
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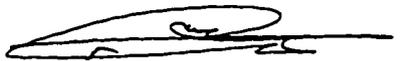
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# ABSTRACT

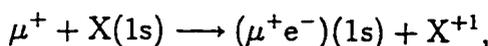
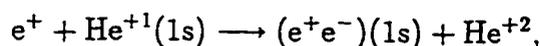
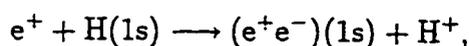
NAME: Umar Dujain Ubaid Al-Kaabi

TITLE: ELECTRON CAPTURE FROM HYDROGENIC SYSTEMS BY POSITRONS AND POSITIVE MUONS

MAJOR: PHYSICS

DATE: June, 1997.

In the present study the cross sections of the following reactions have been calculated in the frame work of the impulse approximation:



where X stands for H, He<sup>+1</sup>, Li<sup>+2</sup>, C<sup>+5</sup>, N<sup>+6</sup>, O<sup>+7</sup> and Fe<sup>+25</sup>. Though the impulse approximation was introduced as an improvement on the Born approximation, it was found to be systematically worse for scattering of electrons off atoms. However, for electron capture total cross sections from hydrogenic systems by positrons, in the energy range for which the impulse approximation is valid, the impulse approximation seems to be better. In this thesis the calculation shows features in the differential cross sections which indicate that even if the impulse approximation proves worse than the Born approximation for the total cross sections in these cases, the differential cross section may be better described by it.

MASTER OF SCIENCE DEGREE

KING FAHD UNIVERSITY OF PETROLEUM AND MINERALS

DHAHRAN, SAUDI ARABIA

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# ABSTRACT (Arabic)

## خلاصة الرسالة

الاسم : عمر دجين عبيد الكعبي

عنوان الدراسة : التقاط الإلكترونات من الذرات الهيدروجينية بواسطة

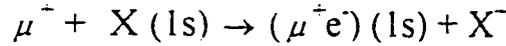
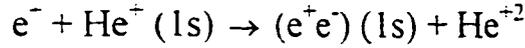
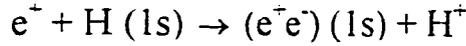
البوزيترون و الميون الموجب

التخصص : فيزياء

تاريخ الشهادة : يونيو ١٩٩٧

تتعلق هذه الأطروحة بدراسة و حساب المقاطع المستعرضة باستخدام التقريب الزخمي للتفاعلات

التالية :



حيث يقوم الرمز X مقام ذرات كل من  $H$  ،  $He^+$  ،  $Li^{+2}$  ،  $C^{+5}$  ،  $N^{+6}$  ،  $O^{+7}$  ،  $Fe^{+25}$ . بالرغم من أن التقريب الزخمي يعتبر تحسينا على تقريب بورن لحساب المقاطع المستعرضة، إلا أننا وجدناه يعطي نتائج أسوأ لتبعثر الإلكترونات بواسطة الذرات، ونتائج أفضل عند استخدامه لحساب المقاطع المستعرضة الكلية للتقاط الإلكترونات بواسطة البوزيترون في الذرات الهيدروجينية وذلك خلال مجال طاقة يقع ضمن المجال التجريبي. كما تبين هذه الأطروحة أن توصيف المقاطع المستعرضة باستخدام التقريب الزخمي يكون أفضل من توصيف تقريب بورن، رغم أن توصيف التقريب الزخمي أعطى نتائج أسوأ للمقاطع المستعرضة الكلية.

درجة الماجستير في العلوم

جامعة الملك فهد للبترول والمعادن

الظهران، المملكة العربية السعودية

يونيو ١٩٩٧

# Chapter 1

## Introduction

### 1.1 Introduction

Positronium ( $e^+e^-$ ) and muonium ( $\mu^+e^-$ ) have attracted a great deal of interest because they only contain leptons (i.e. particles which are not affected by the strong interactions) and hence are particularly suitable systems to verify the predictions of quantum electrodynamics.

Positronium is a bound hydrogenic system made of a positron  $e^+$  (the antiparticle of the electron, having the same mass as the electron, but the opposite electric charge) and an electron.

Muonium is a bound hydrogenic system made of a positive muon  $\mu^+$ , a particle which is very similar to the positron  $e^+$ , except that it has a mass of about 207 times the mass of an electron, the opposite charge and that it is unstable, with life time of 2.2 microseconds. Positronium was first observed in 1951 and muonium in 1960. Table 1.1 gives the values of the reduced mass, the radius and the ionization potential for positronium and muonium, compared with those of the hydrogen atom.

System	Reduced Mass	Radius	Ionization Potential
( $pe$ )	1	1	1
( $e^+e^-$ )	0.5	2	0.5
( $\mu^+e^-$ )	1	1	1

Table 1.1: Some properties of muonium and positronium atoms are compared with those of the hydrogen atom.

## 1.2 History and Background

The problem of electron transfer between atomic systems is inherently more complicated than that of excitation of one atomic system to another because it cannot be reduced to a two-body problem.

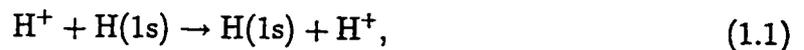
We consider the transfer of an electron from an atomic system to form a bound state with the incident particle. The method appropriate to an approximate solution of the relevant scattering problem depends largely on the relative magnitudes of the velocity of relative motion of the incident particle and the atomic system. If the magnitude of the relative velocity of the incident particle is much less than the orbital speed of the bound electron, then the process may be treated as semi-adiabatic, and the method of perturbed stationary states [9] or some modification thereof may be employed.

On the other hand, if the magnitude of the velocity of the incident particle is much greater than the speed of the bound electron methods allied to Born's approximation seem appropriate, and it is with this velocity range that we are concerned. The intermediate range has proved intractable by both methods.

Now considering the high velocity case and we denote the incident particle-atom interaction by  $V_{12}$ , and the incident particle's interaction with the transferred electron by  $V_{13}$ . The original attack on the problem by Oppenheimer [16] and Brinkman & Kramers [17] was based on the argument that the matrix element to be evaluated is  $\langle \psi_f | V_{13} | \psi_i \rangle$ , where  $\psi_i$  and  $\psi_f$  are the initial and final state wave functions involved in Born's approximation. No account was taken of the  $V_{12}$  interaction, since at suf-

ficiently high velocities of impact  $\psi_i$  and  $\psi_f$  are almost orthogonal and independent of coordinates involved in  $V_{12}$ . Further support was lent to this approach when Mott [18] pointed out that on physical grounds one would expect that the only effect of the  $V_{12}$  interaction would be to change slightly the direction of propagation of the incoming plane wave. When the calculations of Brinkman and Kramers for protons in atomic hydrogen (referred to as O.B.K. approximation) were compared with experiment performed in molecular hydrogen (on the assumption that chemical binding energies could be neglected compared with impact energies, when the latter exceed some tens of KeV), it was found the O.B.K. approximation gave too large results by about 50%, even without considering capture into excited states. To remedy this, Bates and Dalgarno argued that while the orthogonality mentioned held if  $\psi_i$  and  $\psi_f$  were exact, it did not do so for the approximate wave functions introduced into  $\langle \psi_f | V_{13} | \psi_i \rangle$  and might well be compensated for by those in  $\langle \psi_f | V_{12} | \psi_i \rangle$ . It seemed clear that the matrix element would be reduced by interference of waves from the two centres. The improvement in the calculated cross-sections was marked. This will be referred to as B.D.J.S. approximation.

Bassel & Gerjuoy [19] have taken into account the additional interaction provided by the static field of the target system. Their results of capture into the ground state exceed the B.D.J.S. results by about the same amount as does the contribution from capture into excited states. Pradhan [20] attempted to apply the impulse approximation to the symmetric resonant process



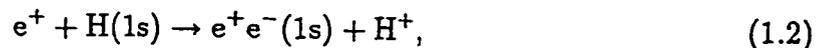
but to simplify the calculation he replaced  $\langle \psi_f | V_{23} | \omega_{13}^+ \psi_i \rangle$  by  $\langle \psi_f | V_{13} | \omega_{13}^+ \psi_i \rangle$  which can be evaluated in closed form. Despite the fact that these matrix elements describe completely different physical processes, Pradhan argued that they are equal to a fairly reasonable approximation at high energies. This claim was repeated by Pradhan and Tripathy [20] who corrected an error in Pradhan's numerical work; because of which it

turned out to be invalid.

McDowell [3] also carried out calculations for the symmetric resonant process. He used the correct form of the impulse approximation to the matrix element, but to reduce the complexity of the calculation he argued that since  $(1/a - b)$  is of order  $1/m_2$  the term  $(1/a - b)\mathbf{k}_i$  could be neglected in the argument of  $g_i$ . This amounts to replacing  $g_i(\mathbf{t}_1)$  by  $g_i(\mathbf{k})$ . The advantage is that when the initial state is an s-state it removes the angular dependence of  $g_i$ . However, it is evident from  $(1/a - b)\mathbf{k}_i = \mathbf{v}$ , McDowell's simplification is invalid, and the resulting error increases with increasing energy.

Cheshire [5] evaluated the impulse approximation without any further approximation other than those inherent in the numerical methods used. Cheshire's results are in close agreement with the results of calculations by Coleman and McDowell [1].

The impulse approximation cross sections for positronium formation in positron-hydrogen collision have been evaluated by Cheshire. However, experimental studies of positronium and muonium formation are not abundant and the agreement in the corresponding theoretical values is not satisfactory [6]. More accurate cross sections have been obtained for the process



by applying the impulse approximation [7]. Moreover, the first Born and Coulomb Born approximations have been applied to calculate positronium [10] and muonium formation cross sections [8] from various hydrogenic systems.

### 1.3 Objective

As far as our knowledge goes, no theoretical calculations have been made on positronium formation from hydrogenic target, by using the impulse approximation. The main objective of this study is to calculate the total cross sections for the formation

of positronium and muonium atoms in their ground states from various hydrogenic systems namely, H, He,  $\text{Li}^{2+}$ ,  $\text{C}^{5+}$ ,  $\text{N}^{6+}$ ,  $\text{O}^{7+}$  and  $\text{Fe}^{25+}$ , using the impulse approximation  $R_{if}^I$ . The impulse approximation for  $R_{if}$  is obtained by replacing the exact wave function  $\Psi_i^+$  in  $R_{if}$  by

$$\Psi_i^I = (\omega_{13}^+ + \omega_{12}^+ - 1)\psi_i, \quad (1.3)$$

such that the final form of  $R_{if}^I$  is

$$R_{if}^I = \langle \psi_f | V_{if} | (\omega_{13}^+ + \omega_{12}^+ - 1)\psi_i \rangle \quad (1.4)$$

For an incident particle of a mass much greater than that of the electron, it has been shown [9] that  $\omega_{12}^+$  can be replaced by unity, so that  $R_{if}$  becomes

$$R_{if}^I = \langle \psi_f | V_{if} | \omega_{13}^+\psi_i \rangle \quad (1.5)$$

We find that the impulse approximation does not give the expected improvement on the Born approximation for the total cross section for the process, in that the experimental data is closer to the Born results than the impulse results. However, there is no data on the differential cross sections, which we have also calculated here. The unexpectedly poor fit and the differential cross section significance is discussed in Chapter 4.

# Chapter 2

## Theory

### 2.1 Introduction

The process of electron transfer between atomic systems is referred to as *electron capture*, which is a special case of a more general process, the rearrangement collision, which will be discussed in the following paragraph. Then its results will be applied to our electron capture process.

In the rearrangement collision we consider a collision between a structureless projectile particle of mass  $m_1$  and charge  $z_1$ , and a target ionized atom consisting of a nucleus with mass  $m_2$  and charge  $z_2$ , and one electron. In this study we will use atomic units for all except two quantities, cross sections which will be expressed in units of  $\pi a_0^2$  ( $a_0^2 = 8.8 \times 10^{-17} \text{cm}^2$ ) and energies for which different units will be used depending on the problem under consideration.

The position vectors of the electron 3 with respect to the projectile 1, and the target nucleus 2 are denoted by  $\mathbf{x}$  and  $\mathbf{r}$  respectively and  $\mathbf{R}$  is the position vector of the projectile with respect to the target nucleus (see Figure 2-1). The position vector of 1 with respect to the centre of mass 2 and 3 is  $\boldsymbol{\sigma}$ , and  $\boldsymbol{\rho}$  is that of the centre of mass

of 1 and 2 with respect to 2. The relationships between the vectors are given by [4]

$$\mathbf{R} = \mathbf{r} - \mathbf{x}, \quad (2.1)$$

$$\boldsymbol{\sigma} = b\mathbf{r} - \mathbf{x}, \quad (2.2)$$

$$\boldsymbol{\rho} = \mathbf{r} - a\mathbf{x}, \quad (2.3)$$

where

$$a = \frac{m_1}{m_1 + 1}, \quad (2.4)$$

$$b = \frac{m_2}{m_2 + 1}. \quad (2.5)$$

In the centre of mass frame of reference the Hamiltonian of the system is

$$H = H_0 + V_{12} + V_{13} + V_{23}, \quad (2.6)$$

where  $V_{ij}$  is the interaction potential between the particles labelled  $i$  and  $j$ , and  $H_0$  is the kinetic energy operator,  $H_0$  takes its simplest form when expressed in terms of the relative coordinates of any two particles and the coordinates of the third particle with respect to the centre of mass of the other two [9]. Thus  $\mathbf{r}$  and  $\boldsymbol{\sigma}$ , and  $\mathbf{x}$  and  $\boldsymbol{\rho}$  are suitable sets of independent coordinates and

$$H_0 = -\frac{1}{2b}\nabla_{\mathbf{r}}^2 - \frac{1}{2\mu_i}\nabla_{\boldsymbol{\sigma}}^2 = -\frac{1}{2a}\nabla_{\mathbf{x}}^2 - \frac{1}{2\mu_f}\nabla_{\boldsymbol{\rho}}^2, \quad (2.7)$$

where

$$\mu_i = \frac{m_1(m_2 + 1)}{m_1 + m_2 + 1}, \quad (2.8)$$

$$\mu_f = \frac{m_2(m_1 + 1)}{m_1 + m_2 + 1}, \quad (2.9)$$

in the case of electron capture  $\mu_i$  and  $\mu_f$  are respectively the initial and final reduced

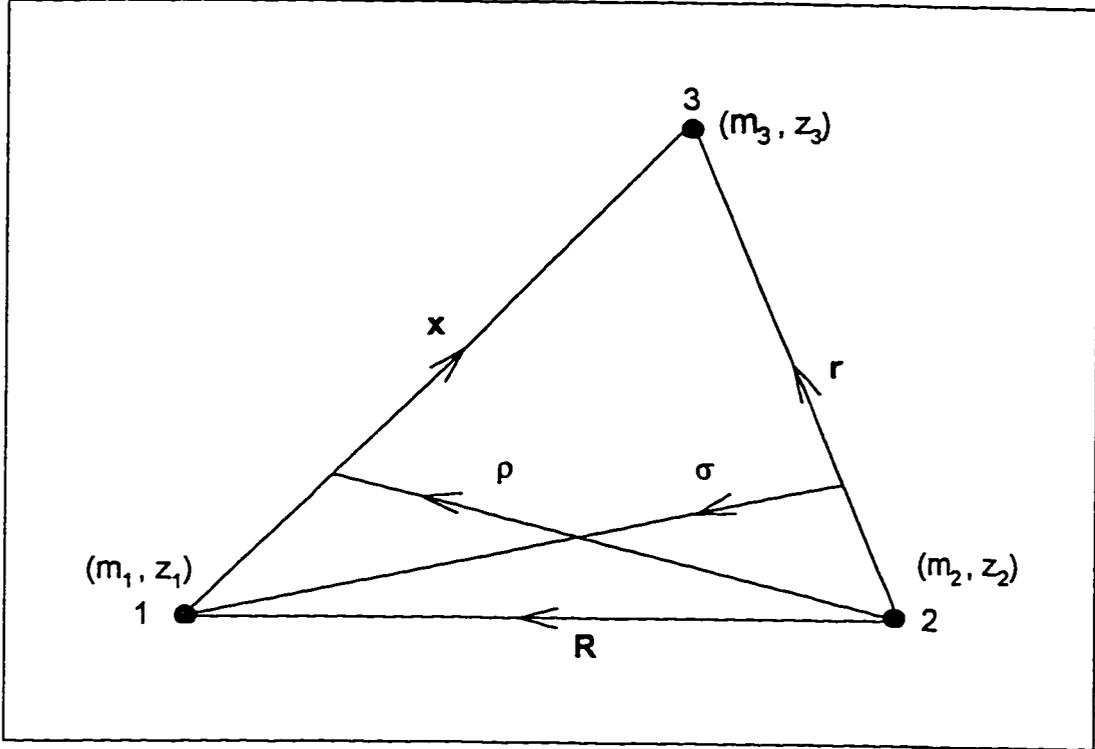


Figure 2-1: Definition of the coordinate system.

masses of the system.

It is occasionally necessary to express functions of  $r$  and  $\sigma$  in terms of  $x$  and  $\rho$  or vice versa. The required relationships are readily deduced from Eqs. (2.1), (2.2) and (2.3) and since

$$(1 - ab) = \frac{a}{\mu_i} = \frac{b}{\mu_f}, \quad (2.10)$$

they may be written in the form

$$x = br - \sigma, \quad (2.11)$$

$$\rho = a\left(\frac{1}{\mu_i}r + \sigma\right), \quad (2.12)$$

$$r = ax + \rho, \quad (2.13)$$

$$\sigma = b\left(\rho - \frac{1}{\mu_f}x\right). \quad (2.14)$$

The interaction potential between the projectile 1 and the target nucleus 2 goes to zero more rapidly than  $\frac{1}{\sigma}$  as  $\sigma \rightarrow \infty$ . Hence, at infinite separation of the target 2 and the projectile 1 before the collision the motion of the system is determined by the initial unperturbed Hamiltonian

$$H_i = H_0 + V_{23}, \quad (2.15)$$

the corresponding three particle wave function satisfies the Schrödinger equation

$$(H_i - E)\psi_i = 0, \quad (2.16)$$

which has a solution of the form

$$\psi_i = \exp(i\mathbf{k}_i \cdot \boldsymbol{\sigma}) \varphi_i(r), \quad (2.17)$$

where  $\varphi_i(r)$  is the target (1 and 2) eigenfunction,  $\mathbf{k}_i$  is the initial relative momentum of the projectile and target, and  $E$  is the total energy of the system in atomic units, and is given by

$$E = \frac{1}{2\mu_i} k_i^2 - E_b, \quad (2.18)$$

where  $E_b$  is the absolute value of the binding energy of the initial bound state (1 and 2). We have chosen the normalization factor of (2.17) so that  $\psi_i$  represents a projectile beam of unit density incident on the target.

The electron capture total cross section  $Q$  for the process of capture from the ground state of the target to the ground state of the projectile-electron system is given by [1]

$$Q = \frac{\mu_i \mu_f k_f}{4\pi^2 k_i} \int |R_{if}|^2 d\Omega, \quad (2.19)$$

where  $k_f$  is the final relative momentum of the free particles, the integration range is

over the solid angle  $\Omega$  from zero to  $4\pi$  and the transition matrix element  $R_{if}$  is

$$R_{if} = \langle \psi_f | V_f | \Psi_i^+ \rangle, \quad (2.20)$$

where  $\Psi_i^+$  satisfies

$$H\Psi_i^+ = E\Psi_i^+, \quad (2.21)$$

with appropriate boundary conditions. Also, we have the initial and final unperturbed Hamiltonians and the corresponding wavefunctions

$$H_i\psi_i = E\psi_i, \quad (2.22)$$

$$H_f\psi_f = E\psi_f, \quad (2.23)$$

with perturbations  $V_i$  and  $V_f$  defined by

$$H = H_i + V_i = H_f + V_f, \quad (2.24)$$

where

$$V_i = V_{12} + V_{13}, \quad (2.25)$$

$$V_f = V_{12} + V_{23}, \quad (2.26)$$

Choosing spherical polar coordinates  $(r, \theta, \varphi)$  with polar axis in the direction of the incident beam, Eq. (2.19) reduces to

$$Q = \frac{\mu_i\mu_f k_f}{4\pi^2 k_i} \int_{-1}^1 |R_{if}|^2 d(\cos\theta) \quad (\pi a_0^2), \quad (2.27)$$

where  $\theta$  is the angle between  $\mathbf{k}_i$  and  $\mathbf{k}_f$ , the initial and final relative momenta of the free particles, respectively.

In general the only significant contribution to the integral in Eq. (2.27) comes from a very narrow cone about the forward direction [9]. For this reason it is convenient

to replace the integral with respect to  $\cos \theta$  by an integral with respect to momentum transfer, in which the integrand is a more slowly varying function of the variables of integration. The relevant momentum transfer vectors  $\mathbf{p}$  and  $\mathbf{q}$  are defined as

$$\mathbf{p} = a\mathbf{k}_f - \mathbf{k}_i, \quad (2.28)$$

$$\mathbf{q} = b\mathbf{k}_i - \mathbf{k}_f. \quad (2.29)$$

Since  $\theta$  is the angle between  $\mathbf{k}_i$  and  $\mathbf{k}_f$ , Eq. (2.27) can be expressed as

$$Q = \frac{1}{2\pi^2 a v^2} \left( \frac{\mu_f}{\mu_i} \right) \int_{p_{\min}}^{p_{\max}} dp p |R_{if}|^2 (\pi a_0^2), \quad (2.30)$$

or

$$Q = \frac{1}{2\pi^2 b v^2} \left( \frac{\mu_f}{\mu_i} \right) \int_{q_{\min}}^{q_{\max}} dq q |R_{if}|^2 (\pi a_0^2), \quad (2.31)$$

with  $v = \frac{k_i}{\mu_i}$  and the integration limits are

$$p_{\min} = |a k_f - k_i|, \quad p_{\max} = a k_f + k_i, \quad (2.32)$$

$$q_{\min} = |b k_i - k_f|, \quad q_{\max} = b k_i + k_f. \quad (2.33)$$

In numerical calculations Eq. (2.30) will be used together with the equation

$$Q = \frac{1}{4\pi^2 a v^2} \left( \frac{\mu_f}{\mu_i} \right) \int_{p_{\min}^2}^{p_{\max}^2} |R_{if}|^2 dp^2 (\pi a_0^2). \quad (2.34)$$

Since the total energy in the centre of mass frame is conserved in the collision, it is evident that

$$\frac{k_i^2}{\mu_i} - \frac{k_f^2}{\mu_f} = \Delta E = E_f - E_i, \quad (2.35)$$

where  $E_i$  and  $E_f$  are the negative energies (in Rydbergs) of the initial and final bound states, respectively. Also, from Eqs. (2.28) and (2.29) together with Eq. (2.35), we

can derive an important relationship between  $\mathbf{p}$  and  $\mathbf{q}$ , that is

$$\frac{p^2}{a} - \frac{q^2}{b} = \Delta E. \quad (2.36)$$

This equation can be used to express  $\mathbf{q}$ , in term of  $\mathbf{p}$  and vice versa, this allows us to go from Eq. (2.30) to Eq. (2.31).

## 2.2 The Impulse Approximation

In classical dynamics an impulsive force is a force of very large magnitude which acts for an infinitesimal length of time. Clearly, when considering the effects of an impulsive force all finite forces can be neglected in the duration time of the impulsive force. A similar situation occurs in the scattering of a particle by a bound system in which the duration of the collision is short compared with some time characteristic of the target, for example the orbital period of a bound particle. In that case it may be assumed that the target binding forces do not play an important role in the collision . This assumption which will be termed the *impulse approximation*, forms the basis of the quantum mechanical impulse approximation, but in general the impulse approximation also involves some subsidiary assumption which enables one to reduce the cross sections formulae to a tractable form.

In comparison with the Born approximation for this problem, which involves the assumption that the interaction between the two particles is assumed to be weak, the impulse approximation retains the assumption that particle 3 can be regarded as free but for the two-particle matrix elements we will take the exact ones for the same process. Hence, the quantum mechanical impulse approximation represents an attempt to describe many-body scattering approximately in terms of known two-body scattering transition matrix elements.

The wave function for the three-particle system corresponding to an initial unper-

turbed state  $\psi_i$  and outgoing-wave boundary conditions are [9]

$$\Psi_i^+ = \Omega^+ \psi_i, \quad (2.37)$$

where

$$\Omega^+ = 1 + G^+ V_i, \quad (2.38)$$

and  $G^+$  is defined as

$$G^+ = \frac{1}{E - H + i\epsilon}, \quad (2.39)$$

One first expands the three-body operator  $\Omega^+$  in terms of the two-body operators  $\omega_{ij}^+$  defined below, and the impulse approximation is obtained by truncating this expansion.

The two-body operators  $\omega_{ij}^+(m)$  ( $i, j = 1, 2, 3; i \neq j$ ) are defined by the equation [4]

$$\omega_{ij}^+(m) \chi_m = \left[ 1 + \frac{1}{E_m - H_0 - V_{ij} + i\epsilon} \right] \chi_m = \psi_m^+(ij), \quad (2.40)$$

provided that

$$\lim_{\epsilon \rightarrow 0^+} \epsilon \psi_m^+(ij) = 0, \quad (2.41)$$

It is clear from Eq. (2.40) that  $\psi_m^+(ij)$  satisfies the differential equation

$$(E_m - H_0 - V_{ij}) \psi_m^+(ij) = 0. \quad (2.42)$$

If  $V_{ij}$  is a Coulomb potential (as in our case), the condition (2.41) is not satisfied[11], in that case Eq. (2.42) rather than Eq. (2.40) will be taken as the equation which defines  $\psi_m^+(ij)$ .

With the help of the operator identity[9]

$$P = Q^{-1} + P^{-1}(Q - P)Q^{-1}, \quad (2.43)$$

where  $P = E - H - i\epsilon$  and  $Q = E_m - H_0 - V_{ij} + i\epsilon$ ,  $G^+$  becomes

$$G^+ = \frac{1}{E_m - H_0 - V_{ij} + i\epsilon} + \frac{1}{E - H - i\epsilon} [(E_m - E) + V_{12} + V_{13} + V_{23} - V_{ij}] \times \frac{1}{E_m - H_0 - V_{ij} + i\epsilon}. \quad (2.44)$$

Therefore

$$G^+ V_{ij} = b_{ij}^+(m) + G^+ [(E_m - E) + V_{12} + V_{13} + V_{23} - V_{ij}] b_{ij}^+(m), \quad (2.45)$$

where

$$b_{ij}^+(m) = \omega_{ij}^+(m) - 1, \quad (2.46)$$

and the plane wave basis is understood. Operating on  $\psi_i$  one now obtains an equation for  $G^+ V_{ij} \psi_i$ , that is

$$G^+ V_{ij} \psi_i = \sum_m G^+ V_{ij} \chi_m \langle \chi_m | \psi_i \rangle, \quad (2.47)$$

$$G^+ V_{ij} \psi_i = \sum_m [b_{ij}^+(m) + G^+ \{(E_m - E) + V_{12} + V_{13} + V_{23} - V_{ij}\} b_{ij}^+(m)] \times \chi_m \langle \chi_m | \psi_i \rangle. \quad (2.48)$$

However

$$\begin{aligned} (E_m - E) \langle \chi_m | \psi_i \rangle &= \langle E_m \chi_m | \psi_i \rangle - \langle \chi_m | E \psi_i \rangle \\ &= \langle \chi_m | H_0 | \psi_i \rangle - \langle \chi_m | H_0 + V_{23} | \psi_i \rangle \\ &= - \langle \chi_m | V_{23} | \psi_i \rangle, \end{aligned} \quad (2.49)$$

and consequently

$$G^+ V_{ij} \psi_i = \{b_{ij}^+(m) + G^+ [V_{23}, b_{ij}^+] + G^+ (V_{12} + V_{13} - V_{ij}) b_{ij}^+\} \psi_i, \quad (2.50)$$

where  $[a, b]$  denotes the commutator of the operators  $a$  and  $b$ , and

$$b_{ij}^+ = \sum b_{ij}^+(m) |\chi_m\rangle \langle \chi_m|. \quad (2.51)$$

Since  $V_i = V_{12} + V_{13}$  it follows that

$$\Omega^+ = (\omega_{13}^+ + \omega_{12}^+ - 1) + G^+ [V_{23}, (b_{13}^+ + b_{12}^+)] + G^+ (V_{13}b_{12}^+ + V_{12}b_{13}^+) \quad (2.52)$$

where

$$\omega_{ij}^+ = b_{ij}^+ + 1 \quad (2.53)$$

Therefore, the matrix elements  $R_{if}$  for any three-particle process may be written as

$$\begin{aligned} R_{if} &= \langle \psi_f | V_f | \Omega^+ \psi_i \rangle \\ &= \langle \psi_f | V_f | (\omega_{13}^+ + \omega_{12}^+ - 1) \psi_i \rangle \\ &\quad + \langle \psi_f | V_f | G^+ [V_{23}, (b_{13}^+ + b_{12}^+)] \psi_i \rangle \\ &\quad + \langle \psi_f | V_f | G^+ (V_{13}b_{12}^+ + V_{12}b_{13}^+) \psi_i \rangle. \end{aligned} \quad (2.54)$$

Since we neglect the binding forces the commutator involving  $V_{23}$  vanishes. This removes the second term on the right-hand side of the above equation. Moreover, it is possible to neglect the expression

$$\langle \psi_f | V_f | G^+ (V_{13}b_{12}^+ + V_{12}b_{13}^+) \psi_i \rangle, \quad (2.55)$$

on the grounds that it is a contribution from multiple scattering. We then obtain the impulse approximation to the matrix element  $R_{if}$ ,

$$R_{if}^I = \langle \psi_f | V_f | (\omega_{13}^+ + \omega_{12}^+ - 1) \psi_i \rangle. \quad (2.56)$$

In the case of heavy-particle impact there is reason to believe that the neglect of terms involving  $V_{12}$  should not in general introduce a serious error. The argument is that if the masses of the projectile and the target nucleus were infinite their interaction potential  $V_{12}$  would be a known function of time and could therefore be removed from the Schrödinger equation by a canonical transformation. Thus, when the projectile is a heavy particle, the contributions to  $R_{if}$  from the potential  $V_{12}$  are expected to be of order  $1/m_2$  compared with the contributions from other potentials, and therefore negligible in general [12]. That is, we can suppose that  $\omega_{12}^+ \rightarrow 1$ . Therefore the impulse approximation to the  $R_{if}$  for a heavy-projectile is given by

$$R_{if}^I = \langle \psi_f | V_f | \omega_{13}^+ \psi_i \rangle. \quad (2.57)$$

## 2.3 Reduction of the Cross Sections

### 2.3.1 Notation

The wave function appropriate to electron capture by an incident particle in the impulse approximation is obtained by replacing the exact wave function  $\Psi_i^+$  in  $R_{if}$  by

$$\Psi_i^I = (\omega_{12}^+ + \omega_{13}^+ - 1)\psi_i, \quad (2.58)$$

which can be decomposed into three terms

$$R_{if}^I = R_{if}^{12} + R_{if}^{13} - R_{if}^B, \quad (2.59)$$

where

$$R_{if}^{12} = \langle \psi_f | V_f | \omega_{12}^+ \psi_i \rangle, \quad (2.60)$$

$$R_{if}^{13} = \langle \psi_f | V_f | \omega_{13}^+ \psi_i \rangle, \quad (2.61)$$

$$R_{if}^B = \langle \psi_f | V_f | \psi_i \rangle, \quad (2.62)$$

$R_{if}^B$  is the first Born approximation of the transition matrix element,  $R_{if}^{12}$  corresponds to the matrix element used in previous applications of the impulse approximation due to charge transfer and  $R_{if}^{13}$  is included to account for the incident particle's motion during the collision.

Each term of the decomposed matrix element will be analyzed separately by means of a suitable mathematical technique. The goal of this analysis is to reduce the matrix elements to form that can readily lend themselves to numerical calculations. In order to simplify the mathematical treatment of  $R_{if}^{13}$  we make the following definition

$$I_{if}(jk, lm) = \langle \psi_f | V_{jk} | \omega_{lm}^+ \psi_i \rangle, \quad (2.63)$$

Since  $V_f = V_{12} + V_{23}$ ,  $R_{if}^{13}$  becomes

$$R_{if}^{13} = I_{if}(12, 13) + I_{if}(23, 13), \quad (2.64)$$

Now  $\omega_{lm}^+ \psi_i$ , in accordance with the definition of the impulse approximation wave function, is

$$\omega_{lm}^+ \psi_i = \sum_n \psi_i^+(lm) \langle \chi_n | \psi_i \rangle, \quad (2.65)$$

where

$$\chi_n = (2\pi)^{-3} \exp [i(\mathbf{k} \cdot \mathbf{x} + \mathbf{k}_1 \cdot \boldsymbol{\rho})], \quad (2.66)$$

which form a convenient set of plane solutions. Now, the summation in Eq. (2.65)

becomes an integration over all values of  $\mathbf{k}$  and  $\mathbf{k}_1$ , and  $\psi_i^+(lm)$  is the solution of the equation

$$\left\{ -\frac{1}{\mu_f} \nabla_\rho^2 - \frac{1}{2a} \nabla_x^2 + \frac{z_1}{x} + E_n \right\} \psi_i^+(lm) = 0, \quad (2.67)$$

where

$$E_n = \frac{1}{2} \left( \frac{k^2}{a} + \frac{k_1^2}{\mu_f} \right). \quad (2.68)$$

The equation for  $\psi_i^+(lm)$  satisfies the outgoing-wave boundary conditions and its explicit form is given by

$$\psi_i^+(lm) = N(\nu) \chi_n {}_1F_1 [i\nu, 1, i(kx - \mathbf{k} \cdot \mathbf{x})], \quad (2.69)$$

with  $\nu = \frac{az_1}{k}$  and

$$N(\nu) = \exp\left(\frac{1}{2}\pi\nu\right) \Gamma(1 - i\nu). \quad (2.70)$$

### 2.3.2 Transition Matrix Element Reduction of Muonium Formation

For heavy particles like  $\mu^+$ , it has been mentioned in Section 2.3.1 that the matrix element appropriate for the formation of *muonium* is given by

$$R_{if} = R_{if}^{13} = I_{if}(12, 13) + I_{if}(23, 13). \quad (2.71)$$

The scalar product in Eq. (2.65) can be evaluated as follows

$$\langle \chi_{m'} | \psi_i \rangle = (2\pi)^2 \int d\mathbf{x}' \int d\mathbf{r}' \exp[-i(\mathbf{k} \cdot \mathbf{x}' + \mathbf{k}_1 \cdot \boldsymbol{\rho})] \exp(i\mathbf{k}_i \cdot \boldsymbol{\sigma}) \phi_i(\mathbf{r}'). \quad (2.72)$$

where the integration over  $\mathbf{x}'$  and  $\mathbf{r}'$  are short for three-dimensional integrals, throughout this report any integration over a vector variable indicate a three-dimensional integral with the region of integration extending over the whole space of that vector variable; unless mentioned otherwise. For example, the integral

$$\int d\mathbf{r} \exp(-r),$$

can be written using polar spherical coordinates as

$$\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \exp(-r).$$

With the help of Eqs. (2.1) and (2.2), Eq. (2.72) becomes

$$\langle \chi_{m'} | \psi_i \rangle = (2\pi)^2 \int d\mathbf{x}' \int d\mathbf{r}' \exp[-i(\mathbf{k} \cdot \mathbf{x}' - a\mathbf{k}_1 \cdot \mathbf{x}' + \mathbf{k}_i \cdot \mathbf{x}')] \exp[i(a\mathbf{r}' \cdot \mathbf{k}_i - \mathbf{r}' \cdot \mathbf{k}_i)] \varphi_i(r'). \quad (2.73)$$

Integrating over  $\mathbf{x}'$  using the standard triple integral [2]

$$\int d\mathbf{r} \exp(\pm i\mathbf{y} \cdot \mathbf{r}) = (2\pi)^3 \delta(\mathbf{y}). \quad (2.74)$$

we obtain

$$\langle \chi_{m'} | \psi_i \rangle = \delta(\mathbf{k}_i + \mathbf{k} - a\mathbf{k}_1) g_i(\mathbf{k} - b\mathbf{k}_i), \quad (2.75)$$

where  $g_i(\mathbf{k} - b\mathbf{k}_i)$  is the *Fourier* transform of the wave function  $\varphi_i(r)$ , (see Appendix B for the definition and evaluation), and the delta function can be expressed as

$$\delta(\mathbf{k}_i + \mathbf{k} - a\mathbf{k}_1) = \frac{1}{a^3} \delta\left[\mathbf{k}_1 - \frac{1}{a}(\mathbf{k}_i + \mathbf{k})\right]. \quad (2.76)$$

Substituting Eq.(2.75) into Eq. (2.65), and then integrating over  $\mathbf{k}_1$ , we obtain

$$\omega_{13}^+ \psi_i = (2\pi a)^{-3} \int d\mathbf{k} N(\nu) g_i(t_1) \exp \left[ i\mathbf{k} \cdot \mathbf{x} + \frac{i}{a} (\mathbf{k}_i + \mathbf{k}) \cdot \boldsymbol{\rho} \right] {}_1F_1 [i\nu, 1, i(kx - \mathbf{k} \cdot \mathbf{x})], \quad (2.77)$$

where  $t_1$  is

$$t_1 = \frac{1}{a} \mathbf{k} + \frac{\mathbf{k}_i}{\mu_i}. \quad (2.78)$$

To evaluate  $I_{if}$  (23, 13) we reverse the order of the momentum and coordinate integrals yielding

$$I_{if}(23, 13) = -(2\pi a)^{-3} z_1 \int d\mathbf{k} N(\nu) g_i(t_1) \int d\mathbf{x} \int d\mathbf{r} \varphi_f(x) \frac{1}{r} \times \exp(i\mathbf{x} \cdot \mathbf{p} + i\mathbf{r} \cdot \mathbf{t}) {}_1F_1 [i\nu, 1, i(kx - \mathbf{k} \cdot \mathbf{x})], \quad (2.79)$$

with

$$\mathbf{t} = \frac{1}{a} (\mathbf{k} - \mathbf{p}). \quad (2.80)$$

The  $\mathbf{r}$  integral in the equation for  $I_{if}$  (23, 13) can be evaluated with the help of [4]

$$\int d\mathbf{r} \frac{\exp(i\mathbf{y} \cdot \mathbf{r})}{r} = \frac{4\pi}{y^2}, \quad (2.81)$$

so that,  $I_{if}$  (23, 13) becomes

$$I_{if}(23, 13) = -(2\pi^2 a^3)^{-1} z_1 \int d\mathbf{k} N(\nu) g_i(t_1) F(1s, \mathbf{k}, \mathbf{p}) t^{-2}, \quad (2.82)$$

where

$$\mathbb{F}(1s, \mathbf{k}, \mathbf{p}) = \int d\mathbf{x} \psi_f(x) \exp(i\mathbf{p} \cdot \mathbf{x}) {}_1F_1 [i\nu, 1, i(kx - \mathbf{k} \cdot \mathbf{x})].$$

Integrals of this kind are normally evaluated by using the integral representation of the confluent hypergeometric function and then, reversing the order of integration with respect to  $\mathbf{x}$ . In our case the final state is an s-state. An expression for  $\mathbb{F}(1s, \mathbf{k}, \mathbf{p})$  may be deduced from Appendix A since

$$\varphi_{1s}(x) = \frac{(az_1)^{3/2}}{\pi^{1/2}} \exp(-az_1 x),$$

it follows from Eq. (A.12) of Appendix A that

$$\mathbb{F}(1s, \mathbf{k}, \mathbf{p}) = -\frac{(az_1)^{3/2}}{\pi^{1/2}} \frac{\partial}{\partial \beta} f(\beta, \nu, \mathbf{k}, \mathbf{p}), \quad (2.83)$$

where the derivative with respect to  $\beta$  is evaluated at  $\beta = az_1$ . This leads to

$$\mathbb{F}(1s, \mathbf{k}, \mathbf{p}) = 8\pi^{1/2}(az_1) \left\{ \frac{(1-i\nu)\beta}{T^2} + \frac{i\nu(\beta-ik)}{T(T-2\delta)} \right\} \left( \frac{T}{T-2\delta} \right)^{i\nu} \quad (2.84)$$

where

$$T = \beta^2 + p^2 \quad (2.85)$$

$$\delta = \mathbf{p} \cdot \mathbf{k} + i\beta k \quad (2.86)$$

The Fourier transformation  $g_i(t_1)$  is found (see Appendix B) to be

$$g_i(t_1) = \frac{8\pi(bz_2)^{5/2}}{\left[ \left( \frac{1}{a}\mathbf{k} + \left( \frac{1}{a} - b \right) \mathbf{k}_i \right)^2 + b^2 z_2^2 \right]^2}, \quad (2.87)$$

Expressing  $\mathbf{k}$  in spherical polar coordinates  $(k, \theta, \phi)$  with  $\cos \theta = \lambda = 0$  along  $\mathbf{p}$ , Eq. (2.87) can be expanded as (see Appendix C)

$$g_i(t_1) = \frac{8\pi(b z_2)^{5/2}}{(A + B \cos \phi)^2}, \quad (2.88)$$

where

$$A = b^2 z_2^2 + \left(\frac{1}{a} - b\right)^2 k_i^2 + a^{-2} k^2 - p^{-1} k \lambda \left\{ \left(\frac{1}{a} - b\right)^2 k_i^2 + b \Delta E + a^{-2} \left(\frac{1}{a} - b\right) p^2 \right\}, \quad (2.89)$$

$$B = k \cdot (\lambda^2 - 1)^{1/2} \left\{ p^{-2} \left[ \left(\frac{1}{a} - b\right)^2 k_i^2 + b \Delta E \right]^2 + a^{-4} (1 - ab)^2 p^2 + 2ba^{-2} (1 - ab) \Delta E - 2a^{-2} (1 + ab)^2 k_i^2 \right\}^{1/2}. \quad (2.90)$$

We carry out the azimuthal integration in Eq. (2.82) by making use of the standard integral [2]

$$\int_0^{2\pi} \frac{d\phi}{(A + B \cos \phi)^2} = \frac{2\pi A}{(A^2 - B^2)^{3/2}}, \quad (2.91)$$

and obtain

$$I_{if}(23, 13) = \frac{-8(bz_2)^{5/2} z_2}{\pi^{1/2} a^3} \int_0^\infty dk k^2 N(\nu) \int_{-1}^1 d\lambda G(k, \lambda) \mathbb{F}(1s, \mathbf{k}, \mathbf{p}) t^{-2}, \quad (2.92)$$

in which

$$G(k, \lambda) = A(A^2 - B^2)^{-3/2}. \quad (2.93)$$

A similar analysis has shown that the matrix element  $I_{if}(12, 13)$  is of order  $O(m_e/m_z)$

times  $I_{if}(23, 13)$ , where  $m_e$  and  $m_z$  are the masses of the electron and nucleus of the hydrogen-like ion respectively. This is confirmed by numerical calculations [1]. Therefore,  $R_{if}$  becomes equal to  $I_{if}(23, 13)$ .

### 2.3.3 Transition Matrix Element Reduction of Positronium Formation

The transition matrix element appropriate to positronium formation in hydrogen like ions, according to the impulse approximation of Section 2.2, is given by Eq. (2.56) which includes  $R_{if}^B$ ,  $R_{if}^{12}$  and  $R_{if}^{13}$ . In the process of derivation of the reduced matrix elements for this case, we adopt a procedure developed by Cheshire [7] which treats  $R_{if}^B$  and  $R_{if}^{12}$  in a unified way. The remaining matrix element  $R_{if}^{13}$  will be treated essentially in the same way as in Section 2.3.2.

In the case of Positronium Formation the incident particle's (positron's) mass is equal to that of the captured electron. For this reason the complexity of the geometry of the problem is simplified. Hence, Figure 2-1 is reduced to Figure 2-2 where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the position vectors of the positron and the electron relative to the massive nucleus, respectively. Now, the initial and final wave functions are

$$\psi_i = \exp(i\mathbf{k}_i \cdot \mathbf{r}_1) \varphi_{1s}(r_2) = \left(\frac{z^3}{\pi}\right)^{1/2} \exp(i\mathbf{k}_i \cdot \mathbf{r}_1) \exp(-zr_2), \quad (2.94)$$

$$\psi_f = \exp\left[i\mathbf{k}_f \cdot \frac{(\mathbf{r}_1 + \mathbf{r}_2)}{2}\right] \eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|) = \left(\frac{1}{8\pi}\right)^{1/2} \exp\left[i\mathbf{k}_f \cdot \frac{(\mathbf{r}_1 + \mathbf{r}_2)}{2}\right] \exp\left[-\frac{1}{2}|\mathbf{r}_1 - \mathbf{r}_2|\right], \quad (2.95)$$

where  $z$  is the charge of the nucleus. In order to find a reduced form of  $R_{if}^B$  and  $R_{if}^{12}$ , we consider  $R_{if}^{B,12}$  which is given by

$$R_{if}^{B,12} = \int \int d\mathbf{r}_1 d\mathbf{r}_2 \exp\left[i\mathbf{k}_f \cdot \frac{(\mathbf{r}_1 + \mathbf{r}_2)}{2}\right] \eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|) \left(\frac{z}{r_1} - \frac{z}{r_2}\right) \psi_{\mathbf{k}_i}^+(\mathbf{r}_1) \varphi_{1s}(r_2). \quad (2.96)$$

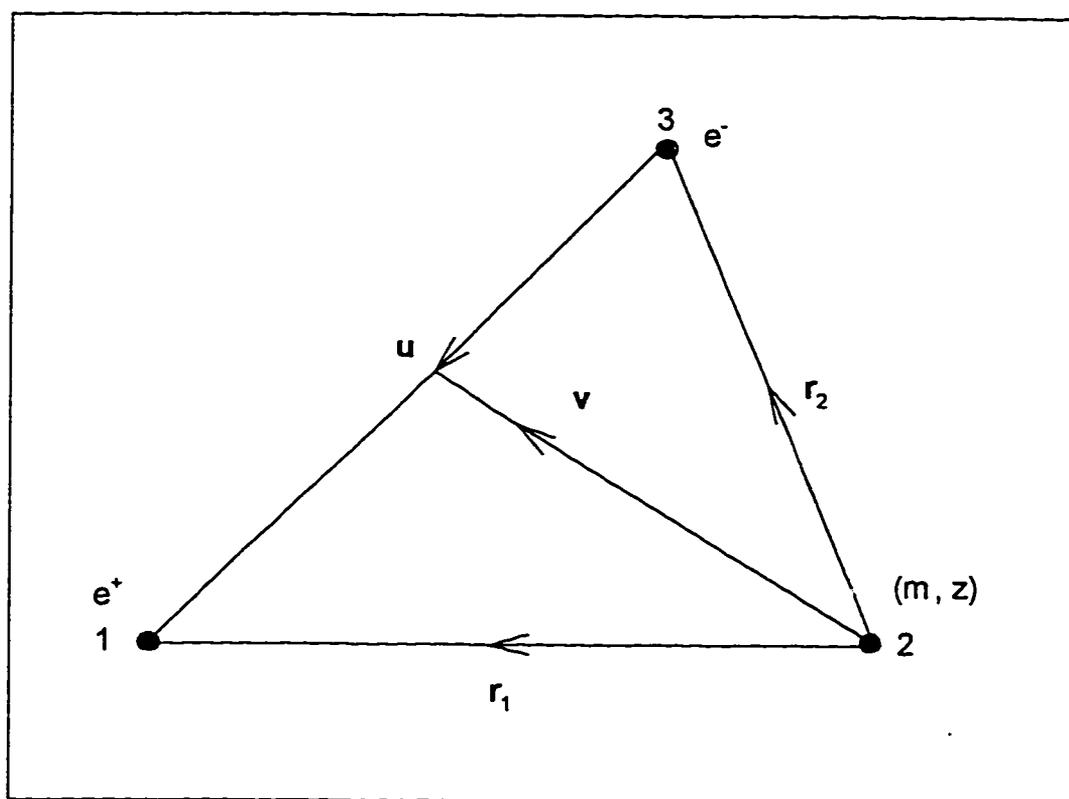


Figure 2-2: Definition of the coordinate system for positronium formation:  $v = \frac{1}{2}(r_1 + r_2)$ ,  $u = r_1 - r_2$ .

This matrix element is reduced to  $R_{if}^B$  if  $\psi_{\mathbf{k}_i}^+(\mathbf{r}_1) = \exp(i\mathbf{k}_i \cdot \mathbf{r}_1)$ ; otherwise  $\psi_{\mathbf{k}_i}^+(\mathbf{r}_1)$  is defined [4] as

$$\psi_{\mathbf{k}_i}^+(\mathbf{r}_1) = \Gamma(1 + i\nu) {}_1F_1[i\nu, 1, i(k_i r_1 - \mathbf{k}_i \cdot \mathbf{r}_1)] \exp(i\mathbf{k}_i \cdot \mathbf{r}_1) \exp\left(-\frac{1}{2}\pi\nu\right), \quad (2.97)$$

with  $\nu = \frac{z}{k_i}$  and the other parameters are similar to those in the previous sections. Now Eq. (2.96) can be expressed as

$$R_{if}^{B,12} = z \int d\mathbf{r}_1 \left(\frac{I_2}{r_1} - I_1\right) \psi_{\mathbf{k}_i}^+(\mathbf{r}_1) \exp\left(\frac{1}{2}i\mathbf{k}_f \cdot \mathbf{r}_1\right). \quad (2.98)$$

where

$$I_1 = \int d\mathbf{r}_2 \exp\left(\frac{1}{2}i\mathbf{k}_f \cdot \mathbf{r}_1\right) \eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|) \varphi_{1s}(r_2) \frac{1}{r_2}, \quad (2.99)$$

$$I_1 = \int d\mathbf{r}_2 \exp\left(\frac{1}{2}i\mathbf{k}_f \cdot \mathbf{r}_1\right) \eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|) \varphi_{1s}(r_2). \quad (2.100)$$

With the help of Fourier transforms of  $\eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|)$ ,  $\varphi_{1s}(r_2)$  and  $\varphi_{1s}(r_2) \frac{1}{r_2}$ , we have

$$\eta_{1s}(|\mathbf{r}_1 - \mathbf{r}_2|) = (2\pi)^{-\frac{5}{2}} \int d\mathbf{P} \exp[i\mathbf{P} \cdot (\mathbf{r}_1 - \mathbf{r}_2)] \left(\frac{1}{4} + P^2\right)^{-2}, \quad (2.101)$$

$$\varphi_{1s}(r_2) = (\pi z)^{-\frac{5}{2}} \int d\mathbf{q} \exp(i\mathbf{q} \cdot \mathbf{r}_2) (z^2 + q^2)^{-2}, \quad (2.102)$$

$$\varphi_{1s}(r_2) \frac{1}{r_2} = 2^{-1} \pi^{-\frac{5}{2}} z^{\frac{3}{2}} \int d\mathbf{q} \exp(i\mathbf{q} \cdot \mathbf{r}_2) (z^2 + q^2)^{-1}. \quad (2.103)$$

Inserting Eqs. (2.101) and (2.103) into Eq. (2.99), we obtain

$$\begin{aligned} I_1 &= 2^{-\frac{7}{2}} \pi^{-5} z^{\frac{3}{2}} \int \int \int d\mathbf{r}_2 d\mathbf{q} d\mathbf{P} \left(\frac{1}{4} + P^2\right)^{-2} (z^2 + q^2)^{-1} \exp(i\mathbf{P} \cdot \mathbf{r}_1) \\ &\quad \times \exp\left(i\mathbf{q} \cdot \mathbf{r}_2 - i\mathbf{P} \cdot \mathbf{r}_2 - \frac{1}{2}i\mathbf{k}_f \cdot \mathbf{r}_2\right). \end{aligned} \quad (2.104)$$

Integrating over  $\mathbf{r}_2$  using Eq. (2.81) we find that

$$I_1 = 2^{-\frac{1}{2}}\pi^{-2}z^{\frac{3}{2}} \int \int d\mathbf{q}d\mathbf{P} \left(\frac{1}{4} + P^2\right)^{-2} (z^2 + q^2)^{-1} \exp(i\mathbf{P} \cdot \mathbf{r}_1) \delta\left(\mathbf{q} - \mathbf{P} - \frac{1}{2}\mathbf{k}_f\right). \quad (2.105)$$

Therefore, it is at once established that

$$I_1 = \frac{z^{\frac{3}{2}}}{\sqrt{2}\pi^2} \int d\mathbf{P} \frac{\exp(i\mathbf{P} \cdot \mathbf{r}_1)}{\left(\frac{1}{4} + P^2\right)^2 \left[z^2 + \left(\mathbf{P} + \frac{1}{2}\mathbf{k}_f\right)^2\right]}. \quad (2.106)$$

A similar analysis can be carried out for  $I_2$  which yield,

$$I_2 = \frac{\sqrt{2}z^{\frac{5}{2}}}{\pi^2} \int d\mathbf{P} \frac{\exp(i\mathbf{P} \cdot \mathbf{r}_1)}{\left(\frac{1}{4} + P^2\right)^2 \left[z^2 + \left(\mathbf{P} + \frac{1}{2}\mathbf{k}_f\right)^2\right]^2}. \quad (2.107)$$

Now, we consider a more general form of Eqs. (2.106) and (2.107), that is

$$f_1 = \int d\mathbf{K} \frac{\exp(i\mathbf{K} \cdot \boldsymbol{\alpha})}{[(\mathbf{K} + \boldsymbol{\beta})^2 + \gamma^2]^2 [(\mathbf{K} + \boldsymbol{\delta})^2 + \nu^2]}, \quad (2.108)$$

$$f_2 = \int d\mathbf{K} \frac{\exp(i\mathbf{K} \cdot \boldsymbol{\alpha})}{[(\mathbf{K} + \boldsymbol{\beta})^2 + \gamma^2]^2 [(\mathbf{K} + \boldsymbol{\delta})^2 + \nu^2]^2}, \quad (2.109)$$

where  $\gamma$  and  $\nu$  are real constants; and  $\boldsymbol{\beta}$  and  $\boldsymbol{\delta}$  are real vectors. Then

$$f_2 = -\frac{1}{2\nu} \frac{\partial}{\partial \nu} f_1, \quad (2.110)$$

Using the formula

$$a^{-2}b^{-1} = \int_0^1 dx \frac{2x}{[ax + b(1-x)]^3}, \quad (2.111)$$

with  $a = (\mathbf{K} + \boldsymbol{\beta})^2 + \gamma^2$  and  $b = (\mathbf{K} + \boldsymbol{\delta})^2 + \nu^2$ ,  $f_1$  can be written as

$$f_1 = \int_0^1 dx \left\{ 2x \int d\mathbf{K} \frac{\exp(i\mathbf{k} \cdot \boldsymbol{\alpha})}{\{[(\mathbf{K} + \boldsymbol{\beta})^2 + \gamma^2]x + (1-x)[(\mathbf{K} + \boldsymbol{\delta})^2 + \nu^2]\}^3} \right\}. \quad (2.112)$$

Next consider the following

$$[(\mathbf{K} + \boldsymbol{\beta})^2 + \gamma^2] x + (1 - x) [(\mathbf{K} + \boldsymbol{\delta})^2 + \nu^2] = (\mathbf{K} + \boldsymbol{\Lambda})^2 + \mu^2, \quad (2.113)$$

where

$$\boldsymbol{\Lambda} = x\boldsymbol{\beta} + (1 - x)\boldsymbol{\delta}, \quad (2.114)$$

and

$$\mu^2 = x\gamma^2 + (1 - x)\nu^2 + x(1 - x)(\boldsymbol{\beta} - \boldsymbol{\delta})^2, \quad (2.115)$$

Therefore, Eq. (2.108) can be rewritten as

$$f_1 = \int_0^1 dx 2x \int d\mathbf{K} \frac{\exp(i\mathbf{k} \cdot \boldsymbol{\alpha})}{[(\mathbf{K} + \boldsymbol{\Lambda})^2 + \mu^2]^3}. \quad (2.116)$$

By making use of the standard result

$$\int d\mathbf{K} \frac{\exp(i\mathbf{k} \cdot \boldsymbol{\alpha})}{(K^2 + \mu^2)^2} = \frac{\pi^2}{\mu} \exp(-\alpha\mu), \quad (2.117)$$

and taking the derivative of both sides of Eq. (2.117) with respect to  $\mu$  and then multiplying both sides by  $\frac{-1}{4\mu}$  we find that

$$\int d\mathbf{K} \frac{\exp(i\mathbf{k} \cdot \boldsymbol{\alpha})}{(K^2 + \mu^2)^3} = \frac{-1}{4\mu} \frac{\partial}{\partial \mu} \frac{\pi^2}{\mu} \exp(-\alpha\mu). \quad (2.118)$$

Now, we can carry out the integration over  $\mathbf{K}$  in Eq. (2.116) by changing the variable of integration from  $\mathbf{K}$  to  $\mathbf{K} + \boldsymbol{\Lambda}$  and using Eq. (2.118), to obtain

$$f_1 = \frac{-\pi}{2} \int_0^1 dx x \exp(i\mathbf{k} \cdot \boldsymbol{\Lambda}) \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right) \frac{1}{\mu} \exp(-\alpha\mu). \quad (2.119)$$

Next, we apply Eq. (2.110) to evaluate  $f_2$ , that is

$$-\frac{1}{2\nu} \frac{\partial}{\partial \nu} \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right) \frac{1}{\mu} \exp(-\alpha\mu) = -\frac{(1-x)}{2} \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \frac{1}{\mu} \exp(-\alpha\mu). \quad (2.120)$$

Combining Eq. (2.119) with Eq. (2.120) we obtain

$$f_2 = \frac{\pi^2}{4} \int_0^1 dx x(1-x) \exp(i\mathbf{k} \cdot \Lambda) \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \frac{1}{\mu} \exp(-\alpha\mu). \quad (2.121)$$

We now make the appropriate substitutions for the parameters  $\alpha$ ,  $\nu$ ,  $\gamma$ ,  $\beta$  and  $\delta$  in Eqs. (2.108) and (2.109) i.e.  $\alpha = r_1$ ,  $\nu = z$ ,  $\gamma = \frac{1}{2}$ ,  $\beta = 0$  and  $\delta = \frac{1}{2}\mathbf{k}_f$  so that

$$\mu^2 = z^2 + (1-4z^2) \frac{x}{2} + \frac{x}{4} (1-x) k_f^2, \quad (2.122)$$

and

$$\Lambda = \frac{1}{2} (1-x) \mathbf{k}_f = -\mathbf{p}. \quad (2.123)$$

Thus

$$I_1 = \frac{-\sqrt{2}z^{\frac{3}{2}}}{4} \int_0^1 dx x \exp \left[ \frac{-1}{2} i (1-x) \mathbf{k}_f \cdot \mathbf{r}_1 \right] \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right) \frac{1}{\mu} \exp(-r_1\mu), \quad (2.124)$$

and

$$I_2 = \frac{\sqrt{2}z^{\frac{5}{2}}}{4} \int_0^1 dx x(1-x) \exp \left[ \frac{-1}{2} i (1-x) \mathbf{k}_f \cdot \mathbf{r}_1 \right] \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \frac{1}{\mu} \exp(-r_1\mu). \quad (2.125)$$

By using the identity

$$\exp(-r_1\mu) = \frac{-1}{r_1} \frac{\partial}{\partial \mu} \exp(-r_1\mu), \quad (2.126)$$

we can express Eq. (2.124) as

$$I_1 = \frac{\sqrt{2}z^{\frac{3}{2}}}{4} \int_0^1 dx x \exp \left[ \frac{-1}{2} i (1-x) \mathbf{k}_f \cdot \mathbf{r}_1 \right] \frac{1}{r_1} \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \exp(-r_1\mu). \quad (2.127)$$

By making use of Eqs. (2.125) and (2.127),  $R_{if}^{B,12}$  becomes

$$R_{if}^{B,12} = \frac{\sqrt{2}z}{4} \int_0^1 dx x \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \left[ \frac{z^{\frac{5}{2}}(1-x)}{\mu} - z^{\frac{3}{2}} \right] \times \int d\mathbf{r}_1 \psi_{\mathbf{k}_i}^+(\mathbf{r}_1) \frac{1}{r_1} \exp \left[ i \left( \frac{x}{2} - 1 \right) \mathbf{k}_f \cdot \mathbf{r}_1 - \mu r_1 \right]. \quad (2.128)$$

Now, in the Born approximation

$$\psi_{\mathbf{k}_i}^+(\mathbf{r}_1) = \exp(i\mathbf{k}_i \cdot \mathbf{r}_1), \quad (2.129)$$

and therefore  $R_{if}^{B,12}$  is reduced to  $R_{if}^B$ . To evaluate the integral over  $\mathbf{r}_1$  in  $R_{if}^B$  we use the integral

$$\int d\mathbf{r} \frac{1}{r} \exp(i\boldsymbol{\omega} \cdot \mathbf{r} - \mu r) = \frac{4\pi}{(\mu^2 + \omega^2)}. \quad (2.130)$$

Taking  $r = r_1$  and  $\boldsymbol{\omega} = \mathbf{k}_i - \mathbf{k}_f + \frac{1}{2}x\mathbf{k}_f$ , then  $R_{if}^B$  becomes

$$R_{if}^B = \sqrt{2}\pi z \int_0^1 dx x \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \left[ \frac{z^{\frac{5}{2}}(1-x)}{\mu} - z^{\frac{3}{2}} \right] \frac{1}{(\mu^2 + \omega^2)}. \quad (2.131)$$

Next, we perform the differentiation in Eq. (2.131)

$$R_{if}^B = \sqrt{2}\pi z^{\frac{5}{2}} \left\{ \int_0^1 dx x(1-x) z \frac{(3A^2 + 4AB + 8B^2)}{B^{\frac{5}{2}}A^3} - 8 \int_0^1 dx \frac{x}{A^3} \right\}, \quad (2.132)$$

where

$$A = \mu^2 + \omega^2, \quad (2.133)$$

and

$$B = \mu^2. \quad (2.134)$$

In order to evaluate  $R_{if}^{12}$  we use Eq. (2.97) as a definition for  $\psi_{\mathbf{k}_i}^+(\mathbf{r}_1)$ , so that the

integral over  $\mathbf{r}_1$  in  $R_{if}^{B,12}$  is evaluated by methods of Appendix A. Thus

$$\int d\mathbf{r}_1 \psi_{\mathbf{k}_i}^+(\mathbf{r}_1) \frac{1}{r_1} \exp \left[ i \left( \frac{x}{2} - 1 \right) \mathbf{k}_f \cdot \mathbf{r}_1 - \mu r_1 \right] = 4\pi\Gamma(1+i\nu) \exp \left[ -\frac{1}{2}\pi\nu \right] \\ \times \left[ \frac{c-id}{\mu^2 + \omega^2} \right]^{i\nu} \\ \times (\mu^2 + \omega^2)^{-1}, \quad (2.135)$$

where

$$c = \mu^2 + \left( \frac{1}{2}x - 1 \right)^2 k_f^2 - k_i^2, \quad (2.136)$$

and

$$d = 2\mu k_i, \quad (2.137)$$

Therefore,

$$R_{if}^{12} = \sqrt{2\pi} z^{\frac{5}{2}} \Gamma(1+i\nu) \exp \left[ -\frac{1}{2}\pi\nu \right] \int_0^1 dx x \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right)^2 \left[ \frac{z(1-x)}{\mu} - 1 \right] \\ \times \left[ \frac{c-id}{\mu^2 + \omega^2} \right]^{i\nu} (\mu^2 + \omega^2)^{-1}. \quad (2.138)$$

Performing the differentiation in  $R_{if}^{12}$  and after some simplification, it is found that

$$R_{if}^{12} = \sqrt{2\pi} z^{\frac{5}{2}} N(\nu) \int_0^1 dx \left\{ \frac{x(1-x)z}{\mu^3} \left[ \frac{3F}{\mu^2} - \frac{3\tilde{F}}{\mu} + \tilde{\tilde{F}} \right] + \frac{x}{\mu^2} \left[ \frac{\tilde{F}}{\mu} - \tilde{\tilde{F}} \right] \right\}, \quad (2.139)$$

where

$$F = (\mu^2 + \omega^2)^{-1} \exp \left[ \nu \arctan \left( \frac{d}{c} \right) + i \frac{\nu}{2} \log \left\{ \frac{c^2 + d^2}{(\mu^2 + \omega^2)^2} \right\} \right], \quad (2.140)$$

$$\tilde{F} = (A_1 + iB_1)(c-id)^{-1}(\mu^2 + \omega^2)^{-1}F, \quad (2.141)$$

$$\tilde{\tilde{F}} = (c-id)^{-1}(\mu^2 + \omega^2)^{-1} \left[ (A_1 + iB_1)(A_2 + iB_2)(c^2 + d^2)^{-1}(\mu^2 + \omega^2)^{-1} + A_3 + iB_3 \right] F, \quad (2.142)$$

with

$$A_1 = -2c^2\mu + 2c(\mu^2 + \omega^2) - 4\mu^2(\mu^2 + \omega^2) - 2d^2\mu, \quad (2.143)$$

$$A_2 = 2(1 - \mu)(\mu^2 + \omega^2) - 4\mu(c + \mu), \quad (2.144)$$

$$A_3 = -2c - 4\mu(1 + \mu), \quad (2.145)$$

$$B_1 = -4\mu^2d + 2d(\mu^2 + \omega^2) + 2c\nu\mu(\mu^2 + \omega^2) - 2\mu\nu c^2, \quad (2.146)$$

$$B_2 = 2(\nu\mu + k_i)(\mu^2 + \omega^2) - 2c\nu\mu + 4\mu d, \quad (2.147)$$

$$B_3 = 2\nu(\mu^2 + \omega^2) - 2\nu c + 4d, \quad (2.148)$$

and

$$\omega^2 = k_i^2 + \left(\frac{1}{2}x - 1\right)^2 k_f^2 + \frac{\left(\frac{1}{2}x - 1\right)}{a} p^2 - a \left(\frac{1}{2}x - 1\right) k_f^2 - \frac{\left(\frac{1}{2}x - 1\right)}{a} k_i^2, \quad (2.149)$$

$$\mu^2 = z^2 + (1 - 4z^2) \frac{x}{2} + \frac{x}{4} (1 - x) k_f^2, \quad (2.150)$$

$$d = 2\mu k_i. \quad (2.151)$$

The reduction of the matrix element  $R_{if}^{13}$  is similar to the techniques employed in Section 2.3.2. We proceed as follows. In accordance with the definition of  $\omega_{13}^{\dagger}$ , the impulse approximation wave function is given by

$$\omega_{13}^{\dagger} \psi_i = \int \int d\mathbf{k}_1 d\mathbf{k}_2 \psi_i^{\dagger}(13) \langle \chi_n | \psi_i \rangle, \quad (2.152)$$

where  $\chi_n$  is a convenient set of plane wave solutions of Eq. (2.67). Here we take

$$\chi_n = (2\pi)^{-3} \exp [i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)], \quad (2.153)$$

and

$$\psi_i^{\dagger}(13) = N(\nu) \chi_n {}_1F_1 [i\nu, 1, i(k_1 u - \mathbf{k}_1 \cdot \mathbf{u})], \quad (2.154)$$

with  $\mathbf{u} = \mathbf{r}_1 - \mathbf{r}_2$  and  $\nu = \frac{-1}{2k_1}$ . We now consider

$$\langle \chi_n | \psi_i \rangle = (2\pi)^{-3} \int \int d\mathbf{r}'_1 d\mathbf{r}'_2 \exp [i(\mathbf{k}_1 \cdot \mathbf{r}'_1 + \mathbf{k}_2 \cdot \mathbf{r}'_2)] \exp (i\mathbf{k}_i \cdot \mathbf{r}'_1) \varphi_{1s}(r_2). \quad (2.155)$$

Substituting Eq.(2.155) into Eq. (2.152) yields

$$\begin{aligned} \omega_{13}^+ \psi_i &= \int \int \int \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{r}'_1 d\mathbf{r}'_2 \psi_{\mathbf{k}_1}^+(\mathbf{u}) \exp \left[ i\mathbf{k}_2 \cdot \mathbf{v} + i\mathbf{r}'_1 \cdot \left( \mathbf{k}_i - \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right) \right] \\ &\quad \times \exp \left[ i\mathbf{r}'_2 \cdot \left( \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right) \right] \varphi_{1s}(r_2), \end{aligned} \quad (2.156)$$

where  $\psi_{\mathbf{k}_1}^+(\mathbf{u})$  is defined by Eq. (2.97) and  $\mathbf{v} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ . Integrating  $\omega_{13}^+ \psi_i$  over  $\mathbf{r}'_2$  with the help of Eq. (B.3), we obtain

$$\begin{aligned} \omega_{13}^+ \psi_i &= 2^{-3} \pi^{-\frac{11}{2}} z^{\frac{5}{2}} \int \int \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{r}'_1 \psi_{\mathbf{k}_1}^+(\mathbf{u}) \exp (i\mathbf{k}_2 \cdot \mathbf{v}) \exp \left[ i\mathbf{r}'_1 \cdot \left( \mathbf{k}_i - \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right) \right] \\ &\quad \times \frac{1}{\left[ \left( \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right)^2 + z^2 \right]^2}. \end{aligned} \quad (2.157)$$

Then we integrate  $\omega_{13}^+ \psi_i$  over  $\mathbf{r}'_1$  by making use of the three-dimensional delta integral in Eq. (2.74), so that

$$\omega_{13}^+ \psi_i = \frac{z^{\frac{5}{2}}}{\pi^{\frac{5}{2}}} \int \int d\mathbf{k}_1 d\mathbf{k}_2 \psi_{\mathbf{k}_1}^+(\mathbf{u}) \exp (i\mathbf{k}_2 \cdot \mathbf{v}) \delta \left( \mathbf{k}_i - \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right) \frac{1}{\left[ \left( \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right)^2 + z^2 \right]^2}. \quad (2.158)$$

Next we integrate  $\omega_{13}^+ \psi_i$  over  $\mathbf{k}_2$ , in doing so one should note that

$$\delta \left( \mathbf{k}_i - \mathbf{k}_1 - \frac{1}{2}\mathbf{k}_2 \right) = 8 \delta [\mathbf{k}_2 - 2(\mathbf{k}_i - \mathbf{k}_1)]. \quad (2.159)$$

Carrying out the integration over  $\mathbf{k}_2$ , Eq. (2.158) becomes

$$\omega_{13}^+ \psi_i = \frac{8z^{\frac{5}{2}}}{\pi^{\frac{5}{2}}} \int d\mathbf{k} \psi_{\mathbf{k}}^+(\mathbf{u}) \exp [2i(\mathbf{k}_i - \mathbf{k}) \cdot \mathbf{v}] \frac{1}{\left[ (2\mathbf{k} - \mathbf{k}_i)^2 + z^2 \right]^2}, \quad (2.160)$$

where we have replaced  $\mathbf{k}_1$  by  $\mathbf{k}$  to simplify the notation and to be consistent with that of Section 2.3.3.

Now, we are ready to evaluate  $R_{if}^{13}$ , that is

$$R_{if}^{13} = \langle \psi_f | V_{13} + V_{23} | \omega_{13}^+ \psi_i \rangle, \quad (2.161)$$

where  $V_{13}$  and  $V_{12}$  are given by

$$V_{13} = \frac{z}{r_1} = \frac{z}{|\mathbf{v} + \frac{1}{2}\mathbf{u}|}, \quad (2.162)$$

$$V_{23} = \frac{-z}{r_2} = \frac{z}{|\mathbf{v} - \frac{1}{2}\mathbf{u}|}. \quad (2.163)$$

Substitution of Eqs. (2.160), (2.162) and (2.163) into Eq. (2.161) yields

$$\begin{aligned} R_{if}^{13} &= \frac{8z^{\frac{7}{2}}}{\pi^{\frac{5}{2}}} \int \int \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{k} \eta_{1s}(u) \psi_{\mathbf{k}}^+(\mathbf{u}) \exp[2i(\mathbf{k}_i - \mathbf{k}) \cdot \mathbf{v}] [(2\mathbf{k} - \mathbf{k}_i)^2 + z^2]^{-2} \\ &\quad \times \left[ \frac{1}{|\mathbf{v} + \frac{1}{2}\mathbf{u}|} - \frac{1}{|\mathbf{v} - \frac{1}{2}\mathbf{u}|} \right]. \end{aligned} \quad (2.164)$$

Changing the integration variables in  $R_{if}^{13}$  from  $\mathbf{r}_1$  and  $\mathbf{r}_2$  to  $\mathbf{u}$  and  $\mathbf{v}$  with the help of following equations

$$\mathbf{r}_1 = \mathbf{v} + \frac{1}{2}\mathbf{u}, \quad (2.165)$$

$$\mathbf{r}_2 = \mathbf{v} - \frac{1}{2}\mathbf{u}, \quad (2.166)$$

we integrate the right hand side of  $R_{if}^{13}$  over  $\mathbf{v}$  using the integral

$$\int d\mathbf{r} \frac{\exp(i\mathbf{q} \cdot \mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} = \frac{4\pi}{q^2} \exp(i\mathbf{q} \cdot \mathbf{r}'), \quad (2.167)$$

with  $\mathbf{q} = 2\mathbf{k}_i - \mathbf{k}_f - 2\mathbf{k}$ ,  $\mathbf{r} = \mathbf{v}$  and  $\mathbf{r}' = \frac{1}{2}\mathbf{u}$  in the first term and  $\mathbf{r}' = -\frac{1}{2}\mathbf{u}$  in the second

term Eq. (2.164) . After carrying out the integration over  $\mathbf{v}$  we obtain

$$R_{if}^{13} = \frac{8z^{\frac{7}{2}}}{\pi^{\frac{3}{2}}} \int d\mathbf{k} [I(\mathbf{k}, \mathbf{k} - \mathbf{p}) - I(\mathbf{k}, \mathbf{p} - \mathbf{k})] (\mathbf{k} - \mathbf{p})^{-2} [(2\mathbf{k} - \mathbf{k}_i)^2 + z^2]^{-2}, \quad (2.168)$$

where

$$I[\mathbf{k}, t(\mathbf{k} - \mathbf{p})] = \int d\mathbf{u} \eta_{1s}(u) \psi_{\mathbf{k}}^+(\mathbf{u}) \exp[i t(\mathbf{k} - \mathbf{p}) \cdot \mathbf{u}], \quad (2.169)$$

and  $\mathbf{p}$  is the momentum transfer vector defined by Eq. (2.28). Now, to evaluate the Integral in Eq. (2.169) we use the results obtained in Appendix A, and the techniques of differentiation under the integral to find that

$$I[\mathbf{k}, t(\mathbf{k} - \mathbf{p})] = \sqrt{\frac{\pi}{2}} N(\nu) \frac{\partial}{\partial \gamma} \left[ \left( \frac{c - id}{\gamma^2 + \omega^2} \right)^{i\nu} (\gamma^2 + \omega^2)^{-1} \right]_{\gamma=\frac{1}{2}}, \quad (2.170)$$

where the parameters are given by  $d = 2k \gamma$ ,  $c = \gamma^2 - k^2 + t(\mathbf{k} - \mathbf{p})^2$  and  $\omega^2 = [\mathbf{k} + t(\mathbf{k} - \mathbf{p})]^2$ . In order to evaluate the azimuthal integral of  $\mathbf{k}$  in Eq. (2.168) we take the polar coordinates for  $\mathbf{k}$  with  $\mathbf{p}$  as the z-axis; a procedure similar to that of Section 2.3.2 gives

$$R_{if}^{13} = 32\sqrt{2}z^{7/2} \int_0^\infty dk N(\nu) \int_{-1}^1 d\lambda \frac{A[X(1) - X(-1)]}{(A^2 - B^2)^{3/2} (k^2 + p^2 - 2kp\lambda)}, \quad (2.171)$$

where

$$X(t) = \frac{k^2 \exp[-\nu \arctan(d/c)]}{(c^2 + k^2) (\frac{1}{4} + \omega^2)^2} [XR - YS + i(XS + YR)]. \quad (2.172)$$

Here

$$X = \cos \Theta, Y = \sin \Theta, \quad (2.173)$$

$$\Theta = \frac{\nu}{2} \log \left[ \frac{c^2 + k^2}{(\frac{1}{4} + \omega^2)} \right], \quad (2.174)$$

$$R = f_1 + f_2\lambda + f_3\lambda^2, S = f_4 + f_5\lambda + f_6\lambda^2, \quad (2.175)$$

and

$$f_1 = p^4 + \frac{1}{4}p^2 + (1+t)p^2k^2 + \frac{1}{4}(1-t)k^2, \quad (2.176)$$

$$f_2 = -(4+t)p^3k - \frac{1}{4}(2-t)pk - 2(1+t)pk^3, \quad (2.177)$$

$$f_3 = 4p^3k^2(1 + \frac{1}{2}t), \quad (2.178)$$

$$f_4 = -\frac{1}{8}tk + (1+t)k^3 + (1 + \frac{1}{2}t)kp^2, \quad (2.179)$$

$$f_5 = -\frac{1}{8}tp - 2(1+t)pk^2 - \frac{1}{2}tp^3, \quad (2.180)$$

$$f_6 = tp^2k, \quad (2.181)$$

with

$$\omega^2 = p^2 + 2(1+t)k^2 - 2(1+t)kp\lambda, \quad (2.182)$$

$$c = \frac{1}{4} + p^2 - 2kp\lambda, \quad (2.183)$$

and

$$A = z^2 + 4k^2 + k_i^2 - (k_i^2 + \frac{1}{2} + 2p^2)\frac{k\lambda}{p}, \quad (2.184)$$

$$B^2 = \frac{k^2}{4p^2}(\lambda^2 - 1)(4k_i^4 + 1 + 16p^2 - 48k_i^2p^2 + 4k_i^2 + 8p^2). \quad (2.185)$$

# Chapter 3

## Numerical Methods

### 3.1 Introduction

Numerical integrations of functions of several variables, over regions with dimension greater than one, are usually difficult to evaluate. There are two reasons for this. First, the number of function evaluations needed to sample an  $N$ -dimensional space increases as the  $N$ -th power of the number needed to do a one-dimensional integral [23]. For example, if a one-dimensional integral computed by 10 function evaluations, then, it is likely an order of  $10^3$  evaluations needed to achieve the same accuracy for a similar three-dimensional integral [27]. Second, the region of integration in  $N$ -dimensional space is defined by an  $N - 1$  dimensional boundary which can itself be prohibitively complicated: it need not be convex or simply connected. By contrast, the boundary of a one-dimensional integral consists of two numbers, its upper and lower limits.

If the integrand is not strongly peaked in very small regions, and the boundary is complicated, then the problem can be suitable for Monte Carlo integration, or methods of sampling [25]. This method is very straightforward to implement and program. Unfortunately, the accuracy obtained from these methods is low compared with other techniques available in the case of integration with dimensions less than eight. However, for dimensions greater than eight sampling methods compete well with other integration

algorithms.

If the boundary is *simple* and the integrand is relatively *smooth*, then breaking up the problem into repeated one-dimensional integrals, will be effective and relatively fast.

The problem at hand involves both two-dimensional and three-dimensional integrals with simple boundaries. Hence, we will apply the method of breaking integrals into repeated one-dimensional integrals.

## 3.2 Complex Gamma Function

Complex Gamma Functions occur in the expressions of the transition matrix elements derived in Chapter. 2. Since the gamma function is not a standard function in most popular programming languages such as Fortran, Basic and C, it is necessary to code a routine or program to calculate the function in a given range of arguments.

The gamma function is defined by the integral

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t} dt. \quad (3.1)$$

The gamma function satisfies the recurrence relation

$$\Gamma(z + 1) = z \Gamma(z). \quad (3.2)$$

If the function is known for arguments  $z > 1$  or, more generally in the half complex plane  $\text{Re}(z) > 1$  it can be obtained for  $z < 1$  or  $\text{Re}(z) > 1$  by the reflection formula [13]

$$\Gamma(1 - z) = \frac{\pi}{\Gamma(z) \sin(\pi z)} = \frac{\pi z}{\Gamma(z + 1) \sin(\pi z)}. \quad (3.3)$$

Notice that  $\Gamma(z)$  has a pole at  $z = 1$ , and at all negative integer values of  $z$ .

There are a variety of methods in use for calculating the function  $\Gamma(z)$  numerically, however we adapt the method derived by Lanczos [48], since it avoids direct evaluation

of the integral in Eq. (3.1) and its ease of implementation. We will not attempt to derive the approximation, but only state the resulting formula: For certain integer choices of  $\gamma$  and  $N$ , and for certain coefficients  $c_1, c_2, \dots, c_N$ , the gamma function is given by

$$\Gamma(z+1) = \sqrt{2\pi} \left(z + \gamma + \frac{1}{2}\right)^{z+\frac{1}{2}} e^{-(z+\gamma+\frac{1}{2})} \left[ c_0 + \sum_{i=1}^N \frac{c_i}{z+i} + \epsilon \right] \quad (z > 0). \quad (3.4)$$

The error term is parametrized by  $\epsilon$ . For  $\gamma = 1$ ,  $N = 6$  and a certain set of  $c$ 's, the error is smaller than  $|\epsilon| < 2 \times 10^{-10}$ . Notice that this formula applies as well for the complex gamma function, *everywhere* in the half complex plane  $\text{Re}(z) > 0$ .

It is better to implement  $\ln \Gamma(z)$  than  $\Gamma(z)$ , since the latter will overflow many computers floating-point representation at quite modest values of  $|z|$ . The implementation is incorporated as a subroutine in the program to calculate the total cross sections given in Appendix D.

### 3.3 Quadrature Rules

Numerical quadrature is the mathematical process of obtaining approximate numerical values for definite one-dimensional integrals. Quadrature rules are the building blocks upon which quadrature schemes and algorithms are based.

The numerical computation of a single integral is called mechanical quadrature, that of a double integral, mechanical cubature and so on. In mechanical quadrature, a given function  $f(x)$  on the interval  $[a, b]$  is replaced by an interpolating or approximating function  $\varphi(x)$  of a simple kind (usually a polynomial) and approximately setting

$$\int_a^b f(x) dx = \int_a^b \varphi(x) dx. \quad (3.5)$$

As is the case when  $\varphi(x)$  is a polynomial,  $\varphi(x)$  must be such that the integral can be evaluated directly by an analytical method. For this purpose, we choose the function

$\varphi(x)$  to be the Lagrange interpolation polynomial  $L_n(x)$  [29]. Assuming, for the function  $y = f(x)$ , that we know the corresponding values at  $n + 1$  points  $x_0, x_1, x_2, \dots, x_n$  in  $[a, b]$ :

$$f(x_i) = y_i \quad (i = 0, 1, 2, \dots, n). \quad (3.6)$$

It is required to find approximately

$$\int_a^b y \, dx = \int_a^b f(x) \, dx, \quad (3.7)$$

We use the given values  $y_i$  to construct the Lagrange polynomial

$$L_n(x) = \sum_{i=1}^n \frac{\Pi_{n+1}(x)}{(x - x_i) \Pi'_{n+1}(x)} y_i, \quad (3.8)$$

where

$$\Pi_{n+1}(x) = (x - x_0)(x - x_1) \dots (x - x_n), \quad (3.9)$$

and

$$L_n(x_i) = y_i \quad (i = 0, 1, 2, \dots, n). \quad (3.10)$$

Replacing the function  $f(x)$  by the polynomial  $L_n(x)$ , we get

$$\int_a^b f(x) \, dx = \int_a^b L_n(x) \, dx + R_n[f], \quad (3.11)$$

where  $R_n[f]$  is the error in the quadrature formula (3.11) (the remainder term). From this, using Eq. (3.8), we obtain the approximate quadrature formula

$$\int_a^b y \, dx = \sum_{i=0}^n w_i y_i, \quad (3.12)$$

where

$$w_i = \int_a^b \frac{\Pi_{n+1}(x)}{(x - x_i) \Pi'_{n+1}(x)} \, dx \quad (i = 0, 1, 2, \dots, n). \quad (3.13)$$

If the limits of integration  $a$  and  $b$  are interpolation points, then the quadrature formula (3.12) is of the *closed type*; otherwise it is of the *open type*.

We note that

- The coefficients  $w_i$  are independent of the choice of the function  $f(x)$  for a given arrangement of points.
- For a polynomial of degree  $n$ , formula (3.12) is exact because in that case  $L_n(x) \equiv f(x)$ ; hence, formula (3.12) is exact for  $y = x^k$  ( $k = 0, 1, 2, \dots, n$ ); that is,  $R_n[x^k] = 0$  for  $k = 0, 1, 2, \dots, n$ .

If the interpolation points are equally spaced points on the interval  $[a, b]$  including the end points, then

$$x_0 = a, \quad x_i = x_0 + i h \quad (i = 0, 1, 2, \dots, n-1) \quad x_n = b, \quad (3.14)$$

with

$$h = \frac{b-a}{n},$$

Letting

$$y_i = f(x_i) \quad (i = 0, 1, 2, \dots, n), \quad (3.15)$$

and replacing the function  $y$  by an appropriate Lagrange interpolation polynomial, we obtain the approximate quadrature formula

$$\int_{x_0}^{x_n} y \, dx = \sum_{i=0}^n w_i y_i, \quad (3.16)$$

where  $w_i$  are given by Eq. (3.13).

In order to derive explicit expression for the coefficients  $w_i$ , we express  $L_n(x)$  as

$$L_n(x) = \sum_{i=0}^n p_i(x) y_i, \quad (3.17)$$

where

$$p_i(x) = \frac{(x - x_0)(x - x_1) \dots (x - x_{i-1})(x - x_{i+1}) \dots (x - x_n)}{(x_i - x_0)(x_i - x_1) \dots (x_i - x_{i-1})(x_i - x_{i+1}) \dots (x_i - x_n)}.$$

Defining

$$q = \frac{x - x_0}{h}, \quad (3.18)$$

and using the notation [29]

$$q^{[n+1]} = q(q-1) \dots (q-n), \quad (3.19)$$

in Eq. (3.17), we find that

$$L_n(x) = \sum_{i=0}^n \frac{(-1)^{n-i}}{i! (n-1)!} \frac{q^{[n+1]}}{q-i} y_i. \quad (3.20)$$

In Eq. (3.16) we replace the function  $y$  by the polynomial  $L_n(x)$  and obtain with the help of Eq. (3.20) and Eq. (3.19)

$$w_i = h \frac{(-1)^{n-i}}{i! (n-1)!} \int_0^h \frac{q^{[n+1]}}{q-i} dq \quad (i = 0, 1, 2, \dots, n), \quad (3.21)$$

and since

$$h = \frac{b-a}{n},$$

we ordinarily put

$$w_i = (b-a) H_i, \quad (3.22)$$

where

$$H_i = \frac{1}{n} \frac{(-1)^{n-i}}{i! (n-1)!} \int_0^h \frac{q^{[n+1]}}{q-i} dq \quad (i = 0, 1, 2, \dots, n), \quad (3.23)$$

are constants called Cotes coefficients [28].

Therefore,

$$\int_a^b y \, dx = (b - a) \sum_{i=0}^n H_i y_i, \quad (3.24)$$

where

$$y_i = f(a + i h) \quad (i = 0, 1, 2, \dots, n).$$

It can be shown that the following relations are true:

$$\sum_{i=0}^n H_i = 1, \quad (3.25)$$

and

$$H_i = H_{n-i}, \quad (3.26)$$

Applying formula (3.16) to the case  $n = 1$ , we find that

$$\int_{x_0}^{x_1} y \, dx = \frac{h}{2} (y_0 + y_1), \quad (3.27)$$

This is the Trapezoidal rule for approximating a definite integral, the trapezoidal rule can be derived in different ways.

The remainder term (the error) of the trapezoidal formula is given by

$$R = \int_{x_0}^{x_1} y \, dx - \frac{h}{2} (y_0 + y_1), \quad (3.28)$$

If we assume that  $y(x)$  possesses a continuous second derivative,  $R$  can be expressed (see, for example, [28]) as

$$R = -\frac{h^3}{12} y''(\xi), \quad (3.29)$$

where  $\xi \in (x_0, x_1)$ .

To evaluate the integral

$$\int_a^b y \, dx,$$

we divide the interval of integration  $[a, b]$  into  $n$  equal parts  $[x_0, x_1], [x_1, x_2], \dots,$

$[x_{n-1}, x_n]$  and to each we apply the trapezoidal formula (3.27). Setting  $h = \frac{b-a}{n}$  and denoting the values of the integrand at the points  $x_i$  by  $y_i = f(x_i)$  ( $i = 0, 1, 2, \dots, n$ ), we obtain

$$\int_a^b y \, dx = \frac{h}{2} (y_0 + y_1) + \frac{h}{2} (y_1 + y_2) + \dots + \frac{h}{2} (y_{n-1} + y_n),$$

or

$$\int_a^b y \, dx = h \left( \frac{y_0}{2} + y_1 + y_2 + \dots + y_{n-2} + y_{n-1} + \frac{y_n}{2} \right). \quad (3.30)$$

This formula is called the extended trapezoidal rule or simply just the trapezoidal rule.

If the function  $y(x)$  possesses a continuous second derivative on the interval  $[a, b]$ , then the remainder term  $R$  of the trapezoidal rule is given by [29]

$$R = -\frac{(a-b)h^3}{12} y''(\xi) \quad (3.31)$$

where  $\xi \in [a, b]$ .

### 3.3.1 Simpson's Rule

Applying formula (3.16) to the case  $n = 2$ , we obtain

$$\int_{x_0}^{x_1} y \, dx = \frac{h}{3} (y_0 + 4y_1 + y_2), \quad (3.32)$$

which is Simpson's quadrature formula. Geometrically, the same result can be obtained by replacing the curve  $y = f(x)$  by a parabola  $y = L_2(x)$  passing through three points  $M_0(x_0, y_0)$ ,  $M_1(x_1, y_1)$  and  $M_2(x_2, y_2)$ .

The remainder term  $R$  of Simpson's formula is defined as

$$R = \int_{x_0}^{x_1} y \, dx - \frac{h}{3} (y_0 + 4y_1 + y_2), \quad (3.33)$$

Assuming that the function  $y(x)$  possesses a fourth derivative on the interval  $[a, b]$ , a

simpler expression for  $R$  can be obtained (see, for example, [24]), that is,

$$R = -\frac{h^5}{90} y^{(4)}(\xi). \quad (3.34)$$

We can easily see from Eq. (3.34) that the formula (3.32) is exact for polynomials not only of degree two but of degree three as well, which means that Simpson's formula has a rather high accuracy for a relatively small number of points.

The extended Simpson's rule for an odd number of points can be obtained as follows: Let  $n = 2m$  be an even number and let  $y_i = f(x_i)$  ( $i = 0, 1, 2, \dots, n$ ) be the values of the function for equally spaced points  $a = x_0, x_1, \dots, x_n = b$ , then

$$h = \frac{b-a}{n} = \frac{b-a}{2m}.$$

Applying Simpson's formula to each interval  $[x_0, x_2], [x_2, x_4], \dots, [x_{2m-2}, x_{2m}]$  of length  $2h$ , we get

$$\begin{aligned} \int_a^b y \, dx &= \frac{h}{3} (y_0 + 4y_1 + y_2) + \frac{h}{3} (y_2 + 4y_3 + y_4) + \dots \\ &\quad \dots + \frac{h}{3} (y_{2m-2} + 4y_{2m-1} + y_{2m}), \end{aligned}$$

or

$$\begin{aligned} \int_a^b y \, dx &= \frac{h}{3} [ (y_0 + y_{2m}) + 4 (y_1 + y_3 + \dots + y_{2m-1}) \\ &\quad + 2 (y_2 + y_4 + \dots + y_{2m-2}) ]. \end{aligned} \quad (3.35)$$

Defining

$$\sigma_1 = y_1 + y_3 + \dots + y_{2m-1},$$

$$\sigma_2 = y_2 + y_4 + \dots + y_{2m-2},$$

we can write (3.35) more compactly as

$$\int_a^b y \, dx = \frac{h}{3} [(y_0 + y_{2m}) + 4 \sigma_1 + 2 \sigma_2]. \quad (3.36)$$

This is Simpson's quadrature rule and its remainder term is given by [28]

$$R = -\frac{(b-a) h^4}{180} y^{(4)}(\xi), \quad (3.37)$$

where  $\xi \in [a, b]$  and it is assumed that  $y^{(4)}(\xi)$  exists on the interval  $[a, b]$ .

In many cases, it is extremely difficult to estimate the error in Simpson's rule (3.36) using (3.37). There are many reasons for this, for example, the real number  $\xi$  is not specified exactly. If we were able to find  $\xi$  exactly, then, we would add the remainder term  $R$  to its quadrature formula and obtain an exact result for the integral. In fact, we merely try to estimate an upper bound on the remainder term, and even this can not be achieved except for a few simple functions. In practice, a double computation is carried out with spacing  $h$  and  $2h$ , and it is taken that the coincident decimals belong to the exact value of the integral.

### 3.3.2 The Gauss-Legendre Rule

The requirement that the integration points  $x_0, x_1, x_2, \dots, x_n$  must be equally spaced limits the degree of exactness that can be obtained from a quadrature rule. In order to derive an optimum rule, we need to remove this requirement. By special placement of the points the accuracy of the numerical integration process could be increased.

Let  $P_{n+1}(t)$  be a polynomial of degree  $n + 1$  such that

$$\int_{-1}^1 t^k P_n(t) \, dt = 0, \quad (3.38)$$

where  $k = 1, 2, \dots, n$ . If we let  $t_0, t_1, \dots, t_n$  be the zeros of  $P_{n+1}(t)$ , it can be shown

[28] that

$$\int_{-1}^1 f(t) dt = \sum_{i=0}^n w_i f(t_i), \quad (3.39)$$

where

$$w_i = \int_{-1}^1 \frac{\Pi_{n+1}(x)}{(x - x_i) \Pi'_{n+1}(x)} dt, \quad (3.40)$$

with  $\Pi_{n+1}(x)$  given by (3.8) and  $f(t)$  the function to be integrated with  $t_i$ 's as integration points. This formula is exact for all polynomials of degree at most  $2n + 1$ .

The family of polynomials  $P_n(t)$  that satisfies (3.38) and  $P_n(1) = 1$ , are called Legendre polynomials. The requirement that  $P_n(1) = 1$  must be imposed, because the zeros of a polynomial determine its coefficients only to within a multiplication factor.

Legendre polynomials have the following properties [13]:

1.  $P_n(x) = \frac{1}{2^n} \frac{d^n}{dx^n} [(x^2 - 1)^n]$ , ( $n = 0, 1, 2, \dots$ )
2.  $P_n(1) = 1$ ,  $P_n(-1) = (-1)^n$ , ( $n = 0, 1, 2, \dots$ )
3.  $\int_{-1}^1 P_n(x) Q_k(x) dx = 0$ , ( $k < n$ ), where  $Q_k(x)$  is any polynomial of degree  $k$ .
4. The Legendre polynomial  $P_n(x)$  has  $n$  distinct real roots lying in the interval  $(-1, 1)$ .

To evaluate the integral

$$\int_a^b f(x) dx,$$

we make a change of variables,

$$x = \frac{b+a}{2} + \frac{b-a}{2} t, \quad (3.41)$$

to obtain

$$\int_a^b f(x) dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b+a}{2} + \frac{b-a}{2} t\right) dt. \quad (3.42)$$

Applying the Gauss-Legendre quadrature rule with  $n$  points (3.39) to this last integral,

we obtain

$$\int_a^b f(x) dx = \frac{b-a}{2} \sum_{i=0}^{n-1} w_i f(x_i), \quad (3.43)$$

where

$$x_i = \frac{b+a}{2} + \frac{b-a}{2} t_i, \quad (i = 0, 1, 2, \dots, n),$$

and  $t_i$ 's are the zeros of the Legendre polynomial  $P_n(t)$ .

The remainder term  $R_n$  of the Gauss-Legendre rule with  $n$  points is given by (see, for example, [29])

$$R_n = \frac{(b-a)^{2n+1} (n!)^4 f^{(2n)}(\xi)}{[(2n)!]^3 (2n+1)}, \quad (3.44)$$

provided that  $f^{(2n)}(x)$  exists on the interval of integration.

Note that the Legendre-Gauss quadrature rule is of the open type, that is, the end-points of the interval  $[a, b]$  are not included. This is due to the fact that the zeros of Legendre polynomials lie entirely within the interval  $(-1, 1)$ .

### 3.4 Approximation of Improper Integrals

An integral is called proper if the interval of integration  $[a, b]$  is *finite* and the integrand  $f(x)$  is *continuous* on  $[a, b]$ , otherwise the integral is improper.

First, we consider the approximation of the improper integral

$$\int_a^\infty f(x) dx, \quad (3.45)$$

where the function  $f(x)$  is continuous on the interval  $[a, \infty)$ . The integral (3.45) is convergent if

$$\lim_{b \rightarrow \infty} \int_a^b f(x) dx, \quad (3.46)$$

exists and is finite. If the limit (3.46) does not exist, then the integral (3.45) is divergent. Therefore, before attempting to evaluate an improper integral one must make sure, using familiar convergence tests, that the integral converges.

To evaluate the convergent improper integral (3.45) to a given accuracy  $\epsilon$ , we rewrite it in the form

$$\int_a^\infty f(x) dx = \int_a^b f(x) dx + \int_b^\infty f(x) dx. \quad (3.47)$$

Since the integral converges, the number  $b$  may be chosen such that the inequality

$$\left| \int_b^\infty f(x) dx \right| < \frac{\epsilon}{2}, \quad (3.48)$$

is satisfied.

The remaining proper integral

$$\int_a^b f(x) dx, \quad (3.49)$$

may be computed using one of the quadrature rules. If  $S$  is an approximation to the value of the integral (3.49) to an accuracy of  $\frac{\epsilon}{2}$ ; that is

$$\left| \int_a^b f(x) dx - S \right| < \frac{\epsilon}{2}, \quad (3.50)$$

then from (3.47), (3.48) and (3.50) we have

$$\left| \int_a^\infty f(x) dx - S \right| < \epsilon. \quad (3.51)$$

Next, we consider the improper integral

$$\int_a^b f(x) dx, \quad (3.52)$$

where the interval of integration  $[a, b]$  is finite and the integrand  $f(x)$  has at most a finite number of discontinuities on  $[a, b]$ . Since the interval of integration may be partitioned into subintervals with a single discontinuity point of the integrand, it is enough to examine the case when there is a single discontinuity point  $c$  of the function

$f(x)$  on  $[a, b]$ .

If  $c$  is an interior point of the interval  $[a, b]$ , then by definition [29] we put

$$\int_a^b f(x) dx = \lim_{\substack{\delta_1 \rightarrow +0 \\ \delta_2 \rightarrow +0}} \left\{ \int_a^{c-\delta_1} f(x) dx + \int_{c-\delta_2}^b f(x) dx \right\}, \quad (3.53)$$

and if the limit exists the integral is convergent, otherwise it is divergent.

A similar definition holds for the improper integral (3.52) if the discontinuity point  $c$  coincides with one of the endpoints of the integration interval  $[a, b]$  (see, for example, [28]).

In order to obtain the required accuracy  $\epsilon$  for the convergent improper integral (3.53) with the point of discontinuity  $c \in (a, b)$ , one chooses positive numbers  $\delta_1$  and  $\delta_2$  so small that the inequality

$$\left| \int_{c-\delta_1}^{c+\delta_2} f(x) dx \right| < \frac{\epsilon}{2}, \quad (3.54)$$

holds. Then, by applying one of the quadrature rules, one approximately calculates the proper integrals

$$\int_a^{c-\delta_1} f(x) dx, \quad (3.55)$$

and

$$\int_b^{c+\delta_2} f(x) dx. \quad (3.56)$$

If  $S_1$  and  $S_2$  are approximate values of the integrals (3.55) and (3.56) respectively to within  $\frac{\epsilon}{2}$  each, then

$$\int_a^b f(x) dx = S_1 + S_2, \quad (3.57)$$

is satisfied to an accuracy of  $\epsilon$ . If the discontinuity point  $c$  of the integrand  $f(x)$  is an endpoint the interval of integration  $[a, b]$ , then the computational procedure is modified accordingly.

### 3.5 Error Analysis

In numerical integration, we usually replace the value of an integral by a finite sum  $\sum_{i=1}^n w_i f(x_i)$ , and in so doing we allow two sorts of error to enter. First, there is the remainder term or truncation error  $R_t$  which is due to the fact that the finite sum is only approximately equal to the integral

$$\int_a^b f(x) dx = \sum_{i=1}^n w_i f(x_i) + R_t. \quad (3.58)$$

In the second place, there is the roundoff error  $R_r$  which arises from the fact that we compute  $\sum_{i=1}^n w_i f(x_i)$  only approximately, due to the limitation on the accuracy of the computer. Hence, the actual value  $\sum^*$  we obtain from computing the sum is

$$\sum^* = \sum_{i=1}^n w_i f(x_i) + R_r. \quad (3.59)$$

Therefore, the estimate of the total error is

$$\left| \int_a^b f(x) dx - \sum^* \right| \leq |R_t| + |R_r|. \quad (3.60)$$

In practice exact error analysis is usually omitted. There are many reasons for this:

1. it is difficult or impossible to carry out;
2. many of the mathematical theorems are irrelevant to machine computation [31];
3. the estimates are too pessimistic [24].

Before we consider practical error estimation methods, we define two important quantities which measure the deviation of an estimate value from its exact value.

If  $\alpha$  and  $\beta$  are two numbers, of which one is approximately equal to the other, the absolute error of  $\beta$  as an approximation to  $\alpha$  is  $|\alpha - \beta|$  and the relative error of  $\beta$  as an approximation to  $\alpha$  is  $|\alpha - \beta| / |\alpha|$ . The relative error of  $\beta$  as an approximation to

$\alpha$  is related to the number of correct digits in  $\beta$  which is given by the integral part of the real number

$$-\log \left| \frac{\alpha - \beta}{\alpha} \right|, \quad (3.61)$$

where the base of the logarithm being taken is the same as the base for the digits system [31].

Mainly, we seek an estimate,  $EST$ , for the integral  $\int_a^b f(x) dx$ , which satisfies

$$\left| \int_a^b f(x) dx - EST \right| \leq \max(\varepsilon_{abs}, \varepsilon_{rel} \int_a^b f(x) dx), \quad (3.62)$$

where  $\varepsilon_{abs}$  and  $\varepsilon_{rel}$  are the absolute and relative accuracies desired, respectively.

By considering the following method, we can deduce an estimate for the integral  $\int_a^b f(x) dx$ . One calculates two estimates  $EST_r$  and  $EST_s$ , which satisfy

$$\int_a^b f(x) dx = EST_r + C_r f^{(r)}(\xi_r), \quad (3.63)$$

and

$$\int_a^b f(x) dx = EST_s + C_s f^{(s)}(\xi_s), \quad (3.64)$$

given that  $f(x)$  is *sufficiently smooth* [25], and  $C_r$  and  $C_s$  are some constants. Also, the numbers  $\xi_r$  and  $\xi_s$  are in the interval  $[a, b]$ , and  $r$  and  $s$  are two integers such that  $s > r$ . Since, in practice, the values  $f^{(r)}(\xi_r)$  and  $f^{(s)}(\xi_s)$  are not available or extremely difficult to obtain, one is left with the information that  $EST_s$  is a higher-order estimate than  $EST_r$  and therefore, a much better estimate than  $EST_r$ , so that

$$\left| \int_a^b f(x) dx - EST_r \right| \approx |EST_s - EST_r|. \quad (3.65)$$

Therefore,  $EST_s$  being better than  $EST_r$ , we have

$$\left| \int_a^b f(x) dx - EST_s \right| < |EST_s - EST_r|. \quad (3.66)$$

The result (3.66) suggests a way to satisfy the requirement in (3.62), that is, a sequence of estimates  $R_1(f)$ ,  $R_2(f)$ ,  $\dots$ ,  $R_n(f)$  is generated based on one of the quadrature rules such that  $R_{i+1}(f)$  is a much better estimate to the value  $\int_a^b f(x) dx$  than  $R_i(f)$ . Then,  $R_{i+1}(f)$  is accepted as an approximation to the integral to the required accuracy, if

$$|R_{i+1}(f) - R_i(f)| < \varepsilon_{abs}, \quad (3.67)$$

or

$$|R_{i+1}(f) - R_i(f)| < \varepsilon_{rel} |R_{i+1}(f)|, \quad (3.68)$$

and the value  $|R_{i+1}(f) - R_i(f)|$  is taken as the error in the estimate  $R_{i+1}(f)$ .

Next, we consider the problem of approximating the double integral

$$I = \int_a^b \left[ \int_c^d g(x, y) dx \right] dy \equiv \int_a^b F(y) dy, \quad (3.69)$$

with

$$F(y) = \int_c^d g(x, y) dx,$$

to absolute accuracy  $\varepsilon_{tot}$ . We denote the approximation obtained for the inner integral by  $Q_2(y)$  and its error by  $E_2(y)$  and the approximation to  $\int_a^b Q_2(y) dy$  by  $Q_1$  and its error by  $E_1$ . Then, the integral  $I$  can be written as

$$I = \int_a^b [Q_2(y) + E_2(y)] dy,$$

or

$$I = Q_1 + E_1 + \int_a^b E_2(y) dy, \quad (3.70)$$

This suggests imposing the condition

$$|I - Q_1| \leq \varepsilon_{outer} + |b - a| \varepsilon_{inner} = \varepsilon_{tot}, \quad (3.71)$$

on the absolute accuracy  $\varepsilon_{outer}$  and  $\varepsilon_{inner}$  for  $Q_1$  and  $Q_2(y)$ , respectively. One way to satisfy (3.71) is to assign [24]

$$\varepsilon_{outer} = \frac{\varepsilon_{tot}}{2}, \quad \varepsilon_{inner} = \frac{\varepsilon_{tot}}{2|b-a|}, \quad (3.72)$$

This is not necessarily the optimum assignment [21]. But, it has the property that if both accuracies  $\varepsilon_{outer}$  and  $\varepsilon_{inner}$  are achieved, then the required accuracy  $\varepsilon_{tot}$  is also achieved [30].

The above discussion can be generalized to a multiple integral over a rectangular region (the limits of integration do not depend on the variables of integration) [26]. For example, to approximate the triple integral

$$\int_a^b \left( \int_c^d \left[ \int_e^k f(x, y, z) dx \right] dy \right) dz,$$

to absolute accuracy  $\varepsilon_{tot}$ , we should assign

$$\varepsilon_z = \frac{\varepsilon_{tot}}{2}, \quad \varepsilon_y = \frac{\varepsilon_{tot}}{4|b-a|}, \quad \varepsilon_x = \frac{\varepsilon_{tot}}{4|b-a||d-c|}, \quad (3.73)$$

where  $\varepsilon_z$ ,  $\varepsilon_y$  and  $\varepsilon_x$  are the absolute accuracy assigned to the integrals over  $z$ ,  $y$  and  $x$ , respectively.

In addition to the problem of roundoff error, one must be aware of other computational noise, which can contaminate the numerical estimates. These include overflow, underflow and loss of significance [22]. One way to remedy such sorts of problems is to carry out the computations on machines that use extended-precision arithmetic. If such facilities are not available, one should first analyze the expressions to be computed. For example, if the integrand, over  $[-1, 1]$ , involves a factor of the form  $(1-x)^\alpha(1+x)^\beta$ , the direct computation of  $1 \pm x_i$  for  $|x_i|$  close to one would lead to loss of significance. One compensation for this loss of significance is the fact that weight associated with a point close to an endpoint is very small; nevertheless it can cause considerable trouble

especially if  $\alpha$  and  $\beta$  are negative [31].

### 3.6 Numerical Integration Procedures

A multiple integral can be evaluated numerically by applying a one-dimensional integration scheme for each one-dimensional integral in the multiple integral. The implementation of this method needs an interface subroutine to link the successive integration schemes [21].

A numerical integration scheme consists of three main parts:

1. An algorithm for dividing the interval of integration into subintervals;
2. A quadrature rule for estimating the integral over each subinterval;
3. A strategy for estimating the error over each subinterval.

An integration scheme or routine is called *adaptive* if the position of the integration points of the  $n$ -th iterate depends on the information gathered from iterates  $1, \dots, n-1$ . This is usually achieved by a successive partitioning of the original interval, such that many points are located in the neighborhoods of difficult spots of the integrand [26]. In *non-adaptive* integration routines, the sequence of integration points is chosen according to a fixed pattern independent of the nature of the integrand; the number of such points however, depends on the integrand [31].

An integration routine can be classified as *iterative* or *non-iterative*. In an iterative routine, successive approximations to the integral are computed until the required accuracy is achieved [22]. In a non-iterative routine, the information from the first approximation is used to generate a second approximation, which is taken as the final result [30].

### 3.7 Mathematical Analysis of the Reduced Transition Matrix Elements

In attempting to evaluate an integral numerically, one should try to confirm the existence of the integral and reduce it to simplest form. Also, one needs to decide in advance the accuracy to which numerical values are to be given. In Section 2.3.2 we obtained an expression for the transition matrix element  $R_{if}$  of the muonium formation process, that is

$$R_{if} = \frac{-8(bz_2)^{5/2}z_2}{\pi^{1/2}a^3} \int_0^\infty dk k^2 N(\nu) \int_{-1}^1 d\lambda G(k, \lambda) \mathbb{F}(1s, \mathbf{k}, \mathbf{p}) t^{-2}, \quad (3.74)$$

where the parameters and functions in the expression are defined in Section 2.3.2.

Examining the integrand as a function of  $\lambda$ , we see that it has singularities in the neighborhood of  $\lambda = 1$  when  $k = p$  in the factor  $t^{-2}$ . In order to test the convergence of the  $\lambda$ -integral, we make the following transformation:

$$\lambda = x_0(p, x) - x, \quad (3.75)$$

where

$$x_0(p, x) = \frac{k^2 + p^2}{2k p},$$

and  $x$  is the new variable of integration. The transformed integral becomes

$$\int_{x_0(p, x)-1}^{x_0(p, x)+1} d\lambda G(k, x) \mathbb{F}(1s, \mathbf{k}, \mathbf{p}) (2a^2 p k x)^{-1}. \quad (3.76)$$

The integral (3.76) can be written as

$$\int_{x_0(p, x)-1}^{x_0(p, x)+1} = \int_{x_0(p, x)-1}^{-\epsilon} + \int_{-\epsilon}^{\epsilon} + \int_{\epsilon}^{x_0(p, x)+1}, \quad (3.77)$$

where it is understood that for simplicity the integrand in (3.77) is omitted, and  $\epsilon$  is

any sufficiently small positive real number. Next, we define

$$I(\varepsilon) \equiv \int_{x_0(p,x)-1}^{-\varepsilon} + \int_{\varepsilon}^{x_0(p,x)+1}. \quad (3.78)$$

If indeed the integral (3.76) exists, it must equal  $\lim_{\varepsilon \rightarrow 0} I(\varepsilon)$ . Each part of the integral (3.78) is proper and can be evaluated by the methods that have been developed in the previous sections of this chapter. Since  $I(\varepsilon)$  can not be evaluated analytically, the only available technique at our disposal is to examine the behavior of  $I(\varepsilon)$  for a sequence of  $\varepsilon_j$  which has a *limit* of zero (for example,  $\varepsilon_j = 10^{-j}$ ,  $j = 1, \dots, n$ ). Substituting all the parameters involved, the evaluation of the integrals  $I(\varepsilon_j)$  shows convergence and hence, an evidence of the existence of the  $\lambda$ -integral in (3.74).

Because of the factor  $N(\nu)$ , difficulties may arise since it oscillates very rapidly for small values of  $k$ . The explicit form of the factor  $N(\nu)$  is given by

$$N(\nu) = \exp\left(\frac{1}{2\pi\nu}\right) \Gamma(1 - i\nu).$$

In order to examine the behavior of  $N(\nu)$ , we express it in the polar form

$$N(\nu) = \exp\left(\frac{1}{2\pi\nu}\right) |\Gamma(1 - i\nu)| \exp(i\phi), \quad (3.79)$$

where  $\phi$  is the argument (angle) of the complex gamma function  $\Gamma(1 - i\nu)$ . The magnitude  $|\Gamma(1 - i\nu)|$  can be written in terms of elementary functions with the help of the identity [14]

$$|\Gamma(1 - i\nu)| = \sqrt{\frac{\pi\nu}{\sinh(\pi\nu)}}. \quad (3.80)$$

Further, the hyperbolic sine can be expressed as

$$\sinh(\pi\nu) = \frac{\exp(\pi\nu) - \exp(-\pi\nu)}{2}, \quad (3.81)$$

and since  $\nu = \frac{\alpha}{k}$ , Eq. (3.79) becomes

$$N(k) = \sqrt{\frac{\pi \alpha}{2k}} \exp\left(\frac{\pi \alpha}{2\pi}\right) \frac{\exp(i \phi)}{[\exp(\frac{\pi \alpha}{k}) - \exp(-\frac{\pi \alpha}{k})]^{1/2}}. \quad (3.82)$$

For  $k \ll 1$ , the negative exponential in the denominator of Eq. (3.82) goes to zero, and therefore,

$$N(k) = \sqrt{\frac{\pi \alpha}{2k}} \exp(i \phi). \quad (3.83)$$

Hence, the real and imaginary parts of  $N(k)$  oscillate rapidly between  $\pm \sqrt{\frac{\pi \alpha}{2k}}$  for small values of  $k$ .

To carry out the integration over  $k$  in (3.74), we split the integration interval as follows:

$$\int_0^{\infty} = \int_0^{k_0} + \int_{k_0}^{\infty}, \quad (3.84)$$

where  $k_0$  is an arbitrary value at which the integrand is *well-behaved*. Each part of the integral is improper and therefore, they should be analyzed separately [27].

The first integral on the right-hand side of (3.84) can be written as

$$\int_0^{k_0} dk k^2 N(k) F(p, k), \quad (3.85)$$

where

$$F(p, k) = \int_{-1}^1 d\lambda G(k, \lambda) \mathbb{F}(1s, \mathbf{k}, \mathbf{p}) t^{-2}. \quad (3.86)$$

Because of the rapid oscillatory behavior of  $N(k)$  in the neighborhood of small values of  $k$ , the integral can not be evaluated directly by the methods that have been developed previously in this chapter. We avoid this difficulty by splitting the integration interval in (3.85) as

$$\int_0^{k_0} = \int_0^{\epsilon} + \int_{\epsilon}^{k_0}. \quad (3.87)$$

Taking  $\epsilon$  small enough such that the rapid oscillatory behavior is included in the interval  $[0, \epsilon]$  and truncating the integration over  $k$  in (3.85) at  $\epsilon$ , the truncating error incurred

will not exceed

$$\left| \int_0^\epsilon dk k^2 N(k) F(p, k) \right|. \quad (3.88)$$

Similarly, the  $k$ -integral over the interval  $[k_0, \infty)$  is estimated by truncating the integral for a large of  $k = k_t$ . In doing so we allow for a truncating error which does not exceed

$$\left| \int_{k_t}^\infty dk k^2 N(k) F(p, k) \right|. \quad (3.89)$$

The overall truncating error  $R_{tot}$  of the  $k$ -integration is

$$R_{tot} = \left| \int_0^\epsilon dk k^2 N(k) F(p, k) \right| + \left| \int_{k_t}^\infty dk k^2 N(k) F(p, k) \right|. \quad (3.90)$$

The total cross section  $Q$  for the muonium formation is computed from the formula

$$Q = \frac{1}{2\pi^2 a v^2} \left( \frac{\mu_f}{\mu_i} \right) \int_{p_{\min}}^{p_{\max}} dp p |R_{if}|^2 (\pi a_0^2),$$

here the usual angular integration has been replaced by the more convenient integral over  $p$  (for more details, see Section 2.1).

# Chapter 4

## Results and Discussion

### 4.1 Introduction

Positronium and muonium formation have unique properties. They provide a useful test of quantum electrodynamics. Collision phenomena associated with positronium and muonium are unusual in many respects and offer a severe challenge to both theory and experiment.

To an increasing extent, it is possible to study the behavior of positive muons in gases, including muonium formation. Comparison and contrast between the behavior of positrons, muons and protons in interaction with gas atoms and molecules should help distinguish the nature of the effects involved, including chemical reactions.

Positrons and positive muons are used as probes in the study of condensed matter. One expects to get some insight into the properties of dense gases from observations of positrons and positronium decay rates and the fractional production of positronium. Assistance in the analysis of the complicated effects which occur can be obtained from experiments with muons under similar conditions.

Apart from the intrinsic importance of positronium ( $Ps$ ) formation as the only scattering channel peculiar to positrons, knowledge of the cross sections for the formation process ( $Q_{Ps}$ ) is essential in

- (a) the interpretation of observations on annihilation radiation from some galactic centers;
- (b) the partitioning of the total scattering cross section ( $Q_{tot}$ ) into various elastic and inelastic channels;
- (c) the understanding of measurement of  $Ps$  formation fractions in high-density gases;
- (d) the comparison of electron and positron total cross sections at intermediate energies as a test of the validity of the Born approximation in that range.

The Born approximation for the capture process involves the following assumptions [4]:

- (a) the electron is regarded as free for the duration of the collision, but its momentum distribution is taken to be that of the appropriate bound state;
- (b) the interaction between the projectile particle and the electron is so weak that the two-particle scattering is adequately described by the Born approximation.

The impulse approximation retains the assumption that the electron can be regarded as free but removes the second restriction. Replacing the Born two-particle matrix element by the exact matrix element for the same process, this was taken to imply that whenever the Born approximation is valid so does the impulse approximation. The latter is also valid when the two-particle interaction cannot be assumed to be weak (provided the target binding forces can be neglected [9]).

A special element of interest relevant to our study is whether or not the impulse approximation is an improvement on the Born approximation. As we will show, *the impulse approximation is worse than the Born approximation in the energy range relevant for experiment*. We find, here, that the same statement applies for the electron capture by positrons, and probably for positive muons. However, features appear in

the differential cross sections in the impulse approximation may be more consistent with observations than in the Born approximation.

Positronium atoms can be in a triplet ( $S = 1$ ) spin state, in which case it is called orthopositronium, or in a singlet ( $S = 0$ ) spin state, known as parapositronium. If we neglect the small spin dependent forces that determine the fine structure, these two states are degenerate in energy. The magnitude of splitting between the ortho and para positronium has been calculated and found to be  $8.45 \times 10^{-4}$  eV [4], so it is a very good approximation to neglect the splitting in the present context.

Systems composed of two electrons and a positron and two positrons and an electron or two positrons and two electrons are all possible, but while positronium formation in positron-atom collisions can occur readily, the formation of these more complicated systems is quite unlikely and will not be considered. On the other hand the existence of stable positive ions formed by the attachment of a positron to a neutral atom would have important implications on the scattering problem. It has been shown that no bound states of a positron with hydrogen can exist [4].

However a bound state of a singly charged particle with a hydrogen atom exists when the mass of the particle is greater than 2.625 electron masses [9]. As a consequence, a bound state of a  $\mu^+$  muon with a hydrogen atom can exist.

Among the positronium atoms formed, one quarter will be in the singlet spin state (parapositronium) and will annihilate rapidly, but the remaining three quarters will be in the triplet state (orthopositronium) and these will decay slowly through three photon annihilation. The decay of the orthopositronium is suitable for experimental observations. These experiments have been conducted with variable degrees of success. Charlton [41] has published experimental data for the energy dependence of the total cross sections for He, Ar, H<sub>2</sub> and CH<sub>4</sub> and also other data are available for various gases from different authors. The availability of mono-energetic positron beams of reasonable intensity has made it possible to compare the cross sections computed from collision theory and experiment directly. A number of experimental investigations have

been carried out (see, for example [40] and [45]) in an attempt to measure positronium formation cross sections in  $e^+ - H$  collision. The importance of positronium itself as a target has been emphasized in a review article by Charlton [32]. Humberston *et al* [33] have proposed a way of producing antihydrogen atoms in the laboratory by antiproton-positronium collisions.

The integrated cross sections have been calculated by several methods [49] for positronium formation in  $e^+ - H$  collision and there are obvious differences among existing results. The differential cross sections have been calculated by Mandal *et al* [34] and Nahar [35] using the distorted-wave approximation, by Roberts [36] using the second-order Faddeev-Watson approximation and by Mukherjee [37] using the closed-coupling approximation.

Calculation of the differential and integrated cross sections are repeated in the present study for electron capture from various hydrogen-like ions (including hydrogen) by positrons and  $\mu^+$  muons using the impulse approximation. Discussion and comparisons of the present results with the theoretical and experimental data are made.

## 4.2 Positronium Formation

Total cross sections are computed at various incident positron energies up to a maximum of 544 eV. These are calculated in three approximations,  $Q^B$  (Born),  $Q^{13}$  (see below for its definition) and  $Q^I$  (impulse), corresponding to the matrix elements  $R_{if}^B$ ,  $R_{if}^{13}$  and  $R_{if}^I$ . The results are given in Table 4.1 for H and in Table 4.2 for  $He^{+1}$ . Cross sections for ortho and para positronium may be obtained by multiplying the tabulated cross sections by the factors  $\frac{3}{4}$  and  $\frac{1}{4}$ , respectively. In Figure 4-1 the total cross sections for the electron capture process from the ground state of atomic hydrogen is given in the various approximations mentioned above. The following physical interpretation of these results is suggested. The cross section  $Q^{13}$  includes only the distortion from the interaction between the electron and the positron. Since the corresponding interaction

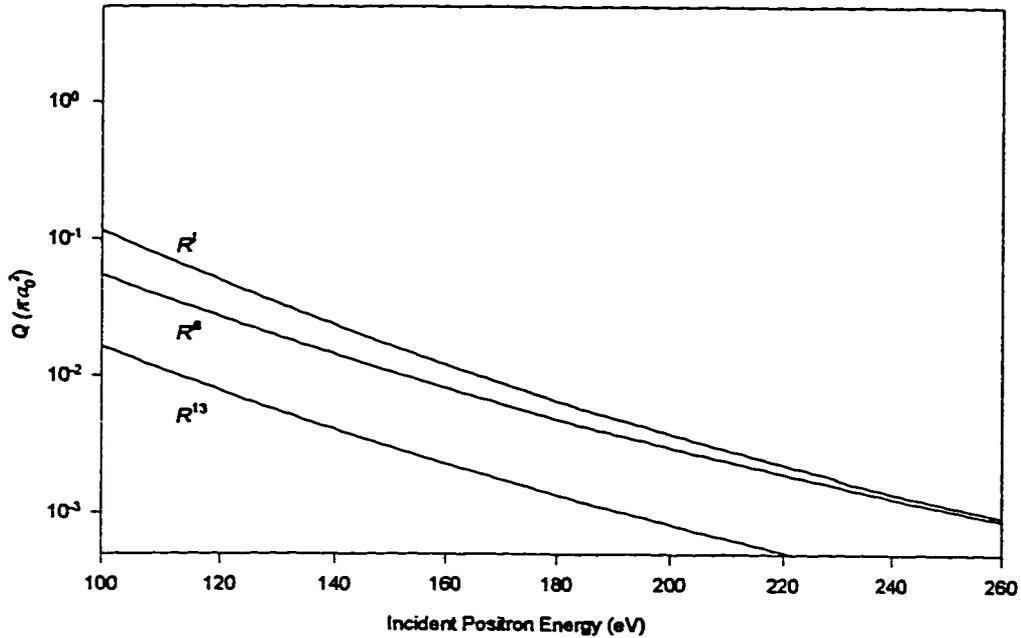


Figure 4-1: Total cross sections of positronium formation in the ground state from atomic hydrogen in the ground state in the Born ( $R^B$ ),  $R^{13}$  and impulse  $R^I$  approximations versus incident positron energies in the range 100–260 eV.

is attractive, the velocity of the positron will increase and hence reduce the capture probability. Moreover, above 200 eV the Born approximation has reached an almost steady rate of fall-off, suggesting that the increase in the positron speed will have a steady effect above this energy.

The total impulse approximation cross section  $Q^I$  takes account of both the positron-proton and positron-electron distortions. Since the static unperturbed hydrogen atom is repulsive, this suggests that the positron speed will be reduced and the resultant capture probability increased. This may explain why  $Q^I$  is greater than  $Q^B$  at low incident positron energies but above 14 eV, since in this region  $Q^B$  falls off more rapidly than anywhere else.

$E$ (eV)	$Q^{13}$ ( $\pi a_0^3$ )	$E$ (eV)	$Q^I$ ( $\pi a_0^3$ )	$E$ (eV)	$Q^B$ ( $\pi a_0^3$ )
10.2	3.50	7.0	4.25,1	10.2	4.47
13.6	3.16	8.0	7.38,1	12.2	4.85
17.0	2.45	10.2	6.84,1	13.6	4.78
27.2	1.00	12.0	5.65,1	15.0	4.54
68.0	6.28,-2	13.6	4.70,1	16.3	4.23
136.0	3.80,-3	17.0	3.17,1	17.7	3.90
244.8	2.49,-4	20.0	2.26,1	19.0	3.57
353.6	4.01,-5	27.2	1.08,1	20.4	3.25
462.4	1.01,-5	30.0	8.25	21.8	2.96
544.0	4.31,-6	35.0	5.27	23.1	2.68
		40.0	3.47	24.5	2.44
		45.0	2.35	25.8	2.21
		50.0	1.63	27.2	2.01
		55.0	1.15	29.9	1.66
		61.0	7.78,-1	32.6	1.37
		62.0	7.31,-1	35.4	1.14
		63.0	6.87,-1	38.1	9.58,-1
		65.0	6.07,-1	40.8	8.05,-1
		72.0	4.03,-1	95.2	5.52,-2
		73.0	3.80,-1	108.8	3.31,-2
		75.0	3.40,-1	122.4	2.08,-2
		80.0	2.59,-1	136.0	1.35,-2
		85.0	2.00,-1	163.2	6.20,-3
		90.0	1.23,-1	190.4	3.13,-3
		95.0	1.23,-1	217.6	1.70,-3
		100.0	9.72,-2	244.8	9.79,-4
		110.0	6.27,-2	272.0	5.92,-4
		120.0	4.16,-2	299.2	3.72,-4
		136.0	2.27,-2	326.4	2.42,-4
				353.6	1.63,-4
				380.8	1.12,-4
				170.0	7.36,-3
				180.0	5.47,-3
				190.0	4.12,-3
				200.0	3.14,-3
				210.0	2.42,-3
				220.0	1.89,-3
				230.0	1.48,-3
				244.8	1.05,-3
				353.6	1.34,-4
				462.4	2.82,-5

Table 4.1: Total cross sections of positronium formation in the ground state from atomic hydrogen in the ground state at several incident positron energies  $E_i$  in the three approximations  $Q^B$ ,  $Q^{13}$  and  $Q^I$ . The notation  $a, b$  stands for  $a \times 10^b$ .

Energy (eV)	$Q^{13}$ ( $\pi a_0^2$ )	Energy (eV)	$Q^I$ ( $\pi a_0^2$ )	Energy (eV)	$Q^B$ ( $\pi a_0^2$ )
48	5.51,-2	48	1.24	48.96	4.21,-1
55	1.58,-1	55	3.45	54.4	6.69,-1
60	1.57,-1	60	3.35	59.84	6.50,-1
65	1.45,-1	65	3.02	65.28	5.75,-1
70	1.30,-1	70	2.65	70.72	4.92,-1
75	1.15,-1	80	1.98	76.16	4.15,-1
80	1.01,-1	85	1.70	81.6	3.47,-1
85	8.86,-2	100	1.08	87.04	2.90,-1
100	5.98,-2	115	6.99,-1	92.48	2.40,-1
115	4.10,-2	125	5.30,-1	97.92	2.04,-1
125	3.22,-2	140	3.56,-1	103.36	1.72,-1
140	2.27,-2	150	2.76,-1	108.8	1.45,-1
150	1.82,-2	160	2.16,-1	119.68	1.05,-1
160	1.47,-2	170	1.71,-1	130.56	7.00,-2
170	1.19,-2	180	1.36,-1	141.44	5.70,-2
180	9.78,-3	200	8.84,-2	152.32	4.30,-2
190	8.06,-3	210	7.20,-2	163.2	3.29,-2
200	6.68,-3	220	5.90,-2	190.4	1.77,-2
210	5.57,-3	230	4.86,-2	217.6	1.01,-2
220	4.67,-3	240	4.03,-2	244.8	6.14,-3
230	3.94,-3	250	3.36,-2		
240	3.33,-3	260	2.81,-2		
250	2.83,-3	300	1.45,-2		
260	2.42,-3				

Table 4.2: Same as Table 4-1 but for  $\text{He}^{+1}$  as a target.

In order to compare these results with the experimental data available for the case of hydrogen, it is necessary to make the following assumption: a hydrogen molecule can be regarded as a pair of independent atoms [47]. Also, the theoretical cross section is multiplied by a factor of 1.202 to take into account the capture into excited states of the positronium atom. This factor comes about because of the  $n^{-3}$  rule [42] which states that the electron capture cross section of an excited state with a principle quantum number  $n$  is estimated as  $n^{-3}$  times the cross section of the ground state of the positronium. Hence, by summing  $n^{-3}$  over all states of the positronium we obtain  $\sum_{n=1}^{\infty} n^{-3} \approx 1.202$ .

In Figure 4-2 the current theoretical values for the case of hydrogen are compared with the experimental data of Coleman *et al* [40] and Fornari *et al* [46]. It is evident that the energy dependence of the theoretical cross sections is very different from the experimental trend and it is difficult to judge the reliability of the experimental data from the theoretical side. The impulse approximation is not able to produce the experimental shape of data at low energies since the impulse approximation is not expected to hold when the velocity of the incident particle is comparable with the characteristic speed of the target. The measured  $Q_{P_s}$  decreases at intermediate energies. It seems that there is a small probability that a broad secondary peak in  $Q_{P_s}$  between 100 and 175 eV. Neither the impulse nor Born approximation predict such features.

In the case of He, one needs additional theoretical assumptions to compare with experimental results. The interaction between the two electrons of He can be neglected and they equally contribute to the capture cross section, that is, we multiply the theoretical cross sections obtained for  $\text{He}^{+1}$  by a factor of 2. Therefore, an overall factor of  $2 \times 1.202$  is needed. The comparison is given in Figures 4-7 and 4-3. The general trend of the experimental data is similar to that of  $\text{H}_2$  except that the secondary maximum is somewhat stronger between 90 and 200 eV and a third one between 200 and 250 eV. No such maxima are predicted by any of the three theoretical approximations.

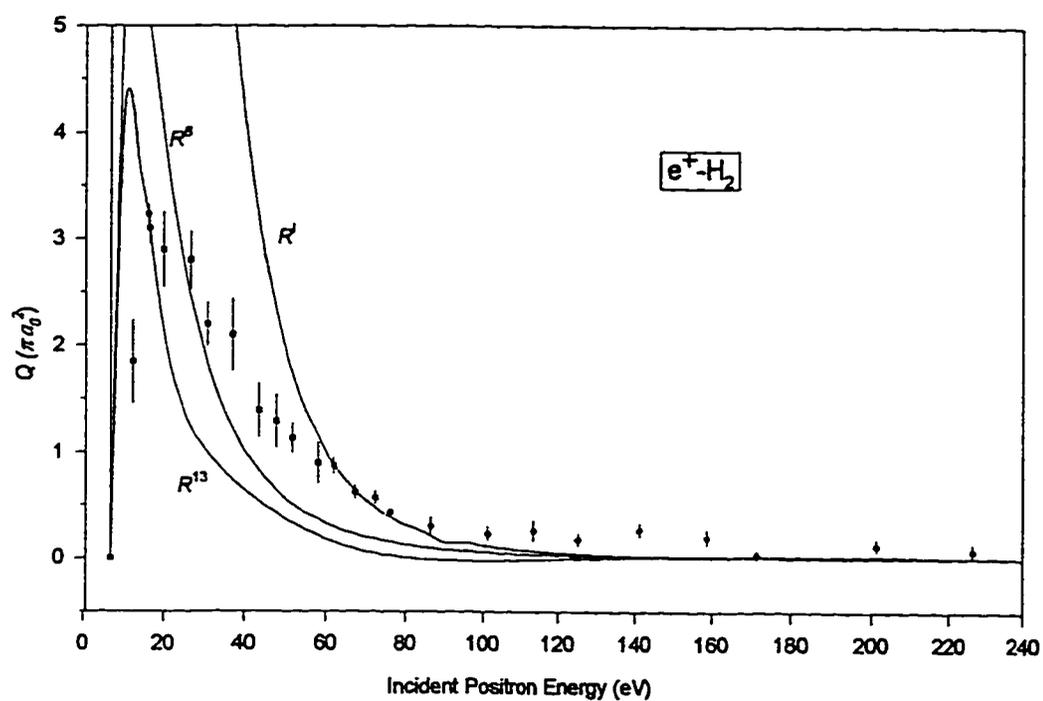


Figure 4-2: Total cross sections of positronium formation from atomic hydrogen in the present approximations corrected for capture into the excited states of the positronium atom and the experimental data for the same process from [40] (circles) and [46] (squares).

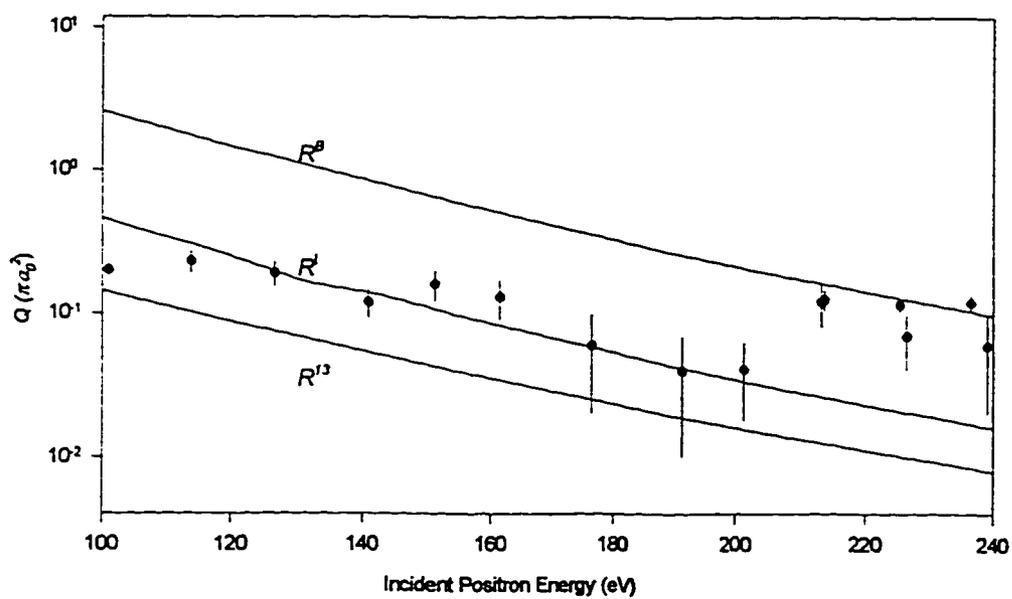


Figure 4-3: Total cross sections of positronium formation from atomic helium in the present approximations corrected for capture into the excited states of the positronium atom and the experimental data for the same process from [40] (circles), in the energy range 100–240 eV.

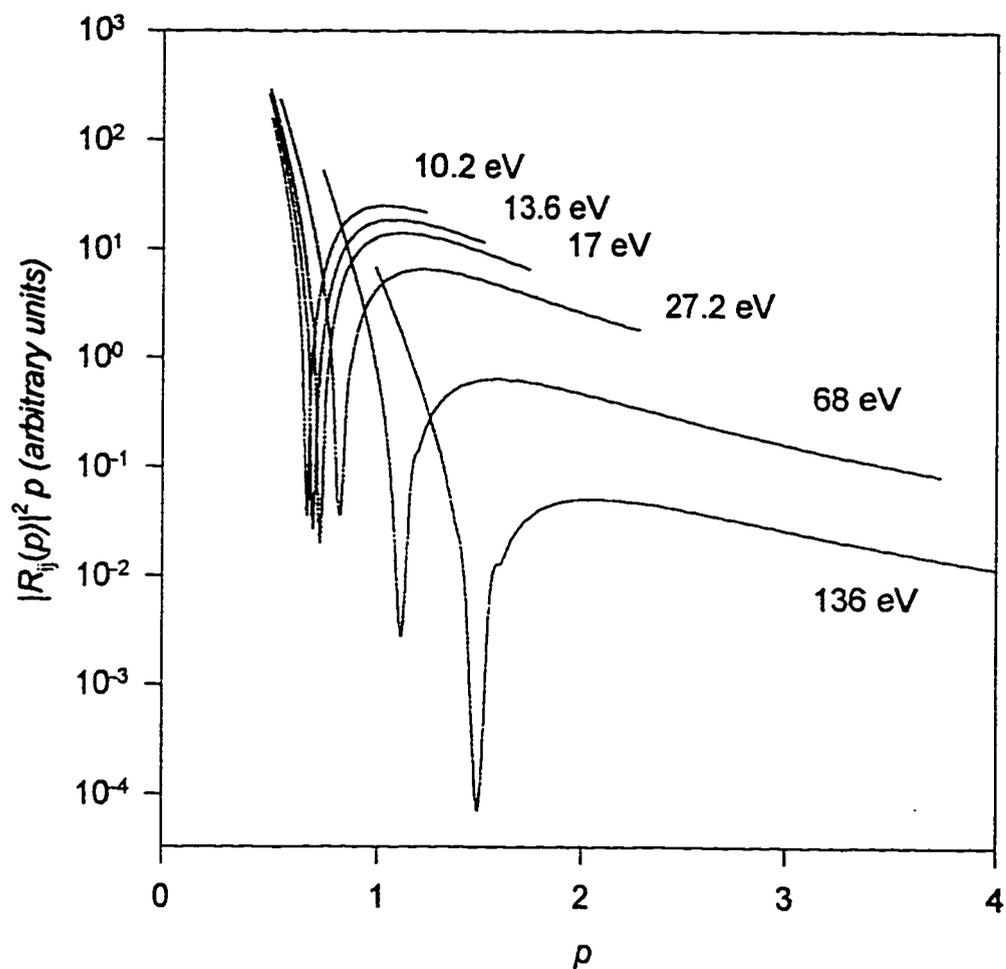


Figure 4-4: Angular distribution for positronium formation in the ground state from atomic hydrogen in the ground state calculated at various incident positron energies in the Born approximation.

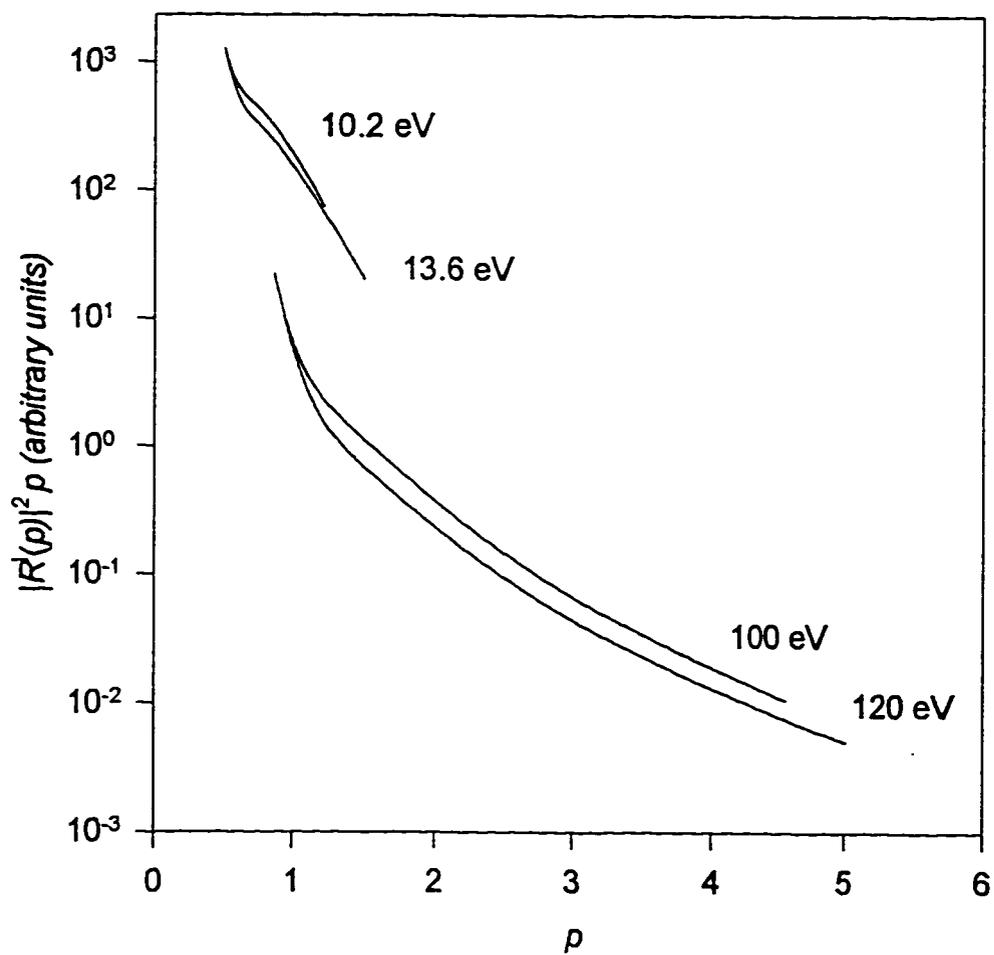


Figure 4-5: Same as Figure 4-4 but in the impulse approximation.

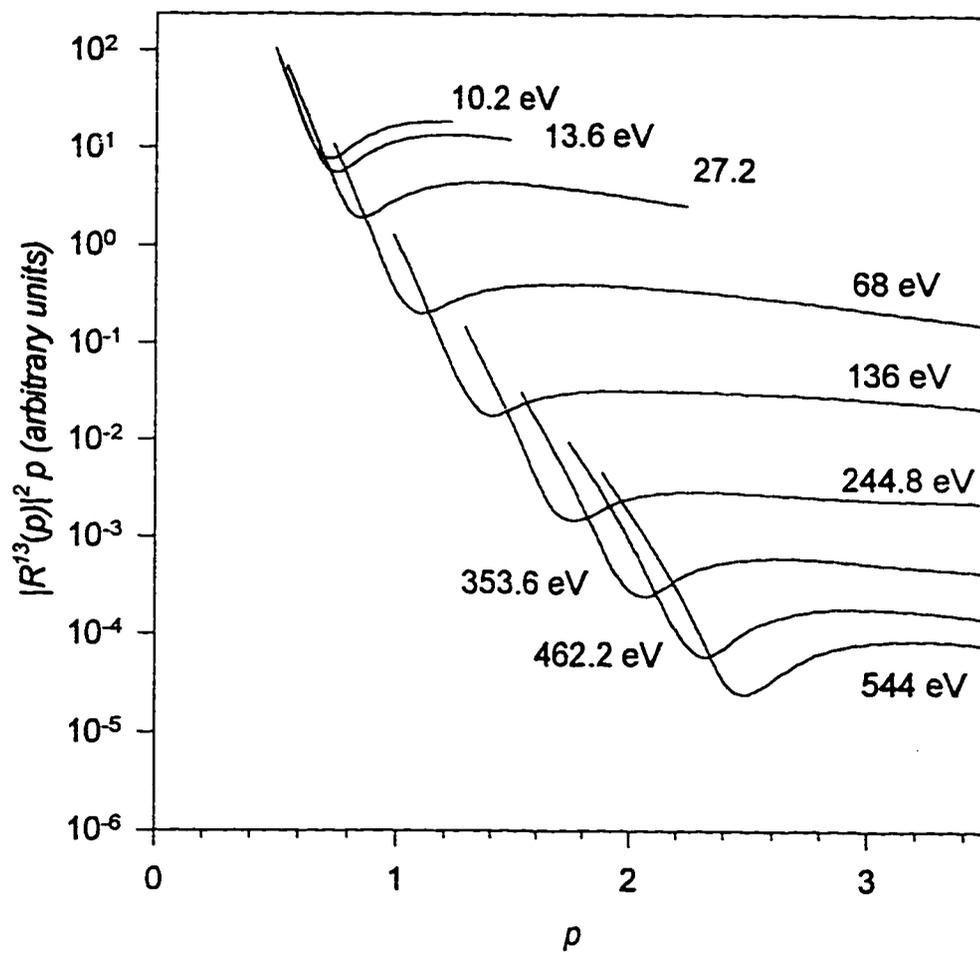


Figure 4-6: Same as Figure 4-4 but in the  $R^{13}$  approximation.

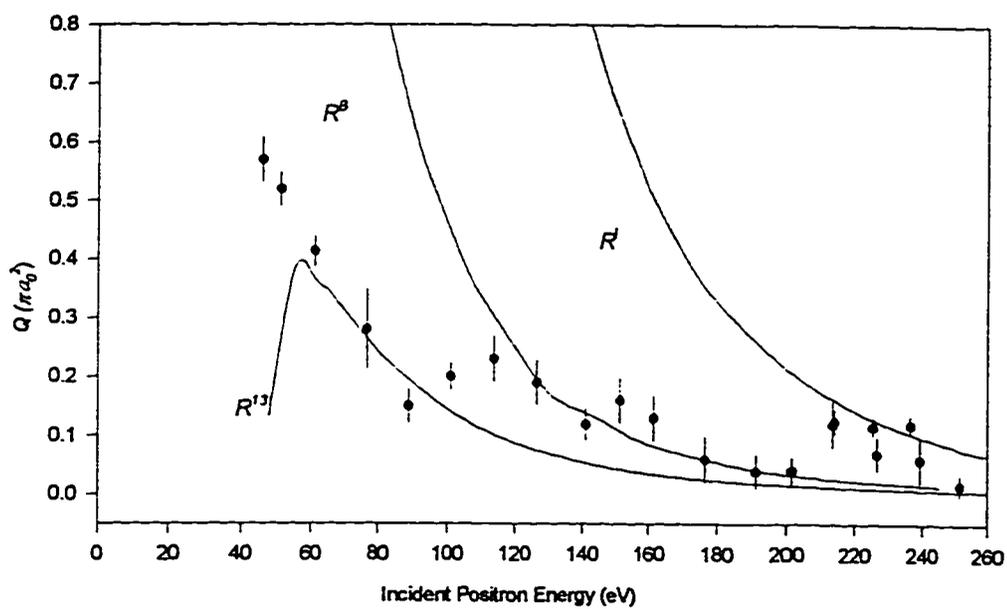


Figure 4-7: Total cross sections of positronium formation from atomic helium in the present approximations corrected for capture into the excited states of the positronium atom and the experimental data for the same process from [40] (circles).

As given in Chapter 2, differential cross sections are related to the transition matrix element by

$$\frac{d\sigma}{d\Omega} = \frac{1}{2\pi^2} \frac{k_f}{k_i} |R_{if}|^2.$$

Angular distributions  $|R_{if}(p)|^2$  versus  $p$  is shown in Figure 4-4 for various incident positron energies on hydrogen in the Born approximation, where  $p$  is related to the angle of scattering  $\theta$  by

$$p^2 = k_i^2 + \frac{1}{4}k_f^2 - k_i k_f \cos \theta$$

The general feature of the distributions shows a steep slope in the forward direction followed by a deep dip and a weak maximum followed by a tail and a relatively high probability of capture in the backward direction. Figures 4-6 and 4-5 show the angular distribution for various incident energies in  $R^{13}$  and impulse approximations. The general feature of the distribution of the  $R^{13}$  shows a large slope in the forward direction followed by a broader maximum and a tail similar to that of the Born approximation. In contrast with this behavior the angular distribution of the impulse approximation decreases monotonically from its maximum value in the forward direction. The angular distribution predicted by  $R^I$  seems to be physically more reasonable than that predicted by  $R^B$ , and since the above features are little altered with increasing positron energy it is, to some extent, surprising that the cross sections  $Q^I$  and  $Q^B$  should be in such close agreement at high energies. We are not aware of any experimental data available for positronium formation differential cross sections.

### 4.3 Muonium Formation

We have calculated the total cross sections of muonium formation in the ground state at several incident energies. In Table 4.3 we have tabulated the values of ground state capture cross sections for various hydrogenic targets using the impulse approximation. Before we discuss these theoretical data we would like to mention that to the best

$E_i$ (KeV)	H	He <sup>+1</sup>	Li <sup>+2</sup>	C <sup>+5</sup>	N <sup>+6</sup>	O <sup>+7</sup>	Fe <sup>+25</sup>
25	1.74,-3	5.11,-3	3.16,-3	6.99,-5	1.62,-5	3.92,-6	2.01,-13
56	3.95,-5	2.84,-4	4.18,-4	8.09,-5	3.14,-5	1.15,-5	7.26,-12
100	2.05,-6	2.25,-5	5.27,-5	3.93,-5	2.27,-5	1.17,-5	6.13,-11
200	5.08,-8	7.75,-7	2.65,-6	6.79,-6	5.98,-6	4.61,-6	4.86,-10
400	1.11,-9	2.11,-8	9.20,-8	5.27,-7	6.31,-7	6.70,-7	2.04,-9
900	1.16,-11	2.57,-10	1.35,-9	1.38,-8	2.03,-8	2.71,-8	3.70,-9
1100	3.72,-12	8.44,-11	4.57,-10	5.20,-9	7.96,-9	1.10,-8	3.45,-9

Table 4.3: Total cross sections of muonium formation in the ground state from the ground states of various hydrogenic targets in the energy range 25–1100 KeV calculated by the impulse approximation.

of our knowledge the experimental data for the process is not available. One reason for such shortage is the relative rarity of muons [38] compared to positrons where the experimental investigation are relatively abundant.

Figure 4-8 shows the total cross sections computed using the impulse approximation for hydrogenic targets. The curves of the total cross section can be put into three groups. The first one is hydrogen and the low-charged target (He<sup>+1</sup> and Li<sup>+2</sup>) in which the total cross sections exhibit a rapid monotonic decrease as the incident muon energy increases with no apparent minima and maxima. In this group the rapid fall-off decreases as the charge on the target increases. The second group includes C<sup>+5</sup>, N<sup>+6</sup> and O<sup>+7</sup> in which the total cross section shows a small peak at about 56-KeV. The tail curves of the second groups exhibit the same behavior as that of the first group except that they are larger and tightly packed together. The third group (Fe<sup>+25</sup>) has a very different trend from the other groups, that is, the total cross section increases rapidly in the energy range 25–300 KeV and then increases smoothly and asymptotically approaching that of the second group from below.

Figure 4-9 shows the total cross sections for muonium formation and electron capture by protons [1] in the ground states from hydrogen calculated using the impulse approximation. It should be noted that for low energies the muonium formation cross section falls off more rapidly with increasing energies than the cross section for electron

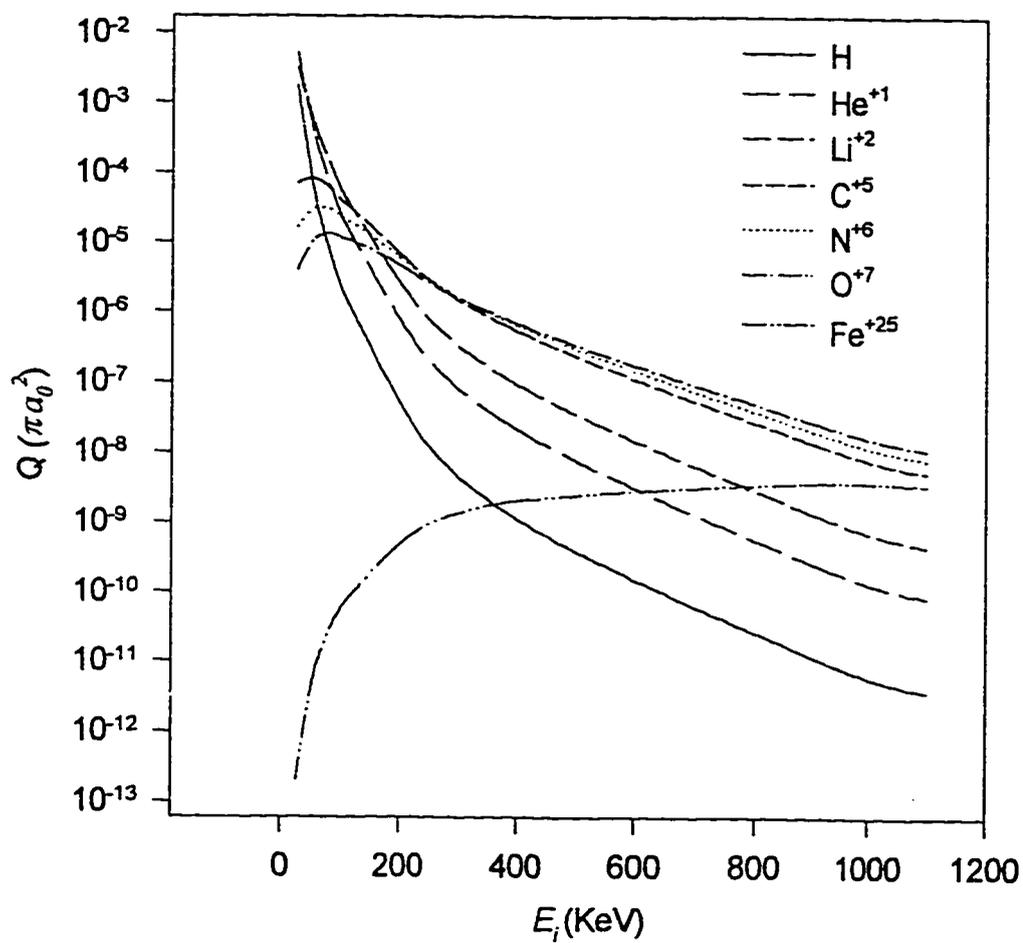


Figure 4-8: Total cross sections of muonium formation in the ground state from the ground states of various hydrogenic targets in the energy range 25–1100 KeV calculated by the impulse approximation.

capture by protons, and its value is less than that of electron capture by protons in the energy range considered.

The features of the differential cross section from various hydrogenic targets at several incident energies are presented in Figure 4-10 through Figure 4-13. Although, there are slight differences from one figure to another, they all exhibit certain common features in the form of *shoulders* when the incident muon energy is low and become broad *resonances* at high energies. Figure 4-14 shows a comparison between the angular distribution of the impulse, Born [45] and OBK (the Born approximation without the projectile-nucleus interaction) [9] approximations for an incident muon energy of 25 KeV.

## 4.4 Conclusion

The classical impulse approximation replaces the effect of long range interactions by an effective impulsive force, and as its name indicates, acting over a short duration. This is a reasonable good approximation for sufficiently high energies. The same procedure, however, is invalid for quantum systems as the exchange force cannot be neglected. The quantum impulse approximation was introduced as a modification of the Born approximation which would be better at sufficiently high energies.

Comparison with experimental results shows that the Born approximation is systematically better than the impulse approximation for the total cross section of electron scattering off various atoms. Since the impulse approximation was introduced as an improvement of the Born approximation, this is surprising. It means that some thing is wrong with the extra assumption made in the impulse approximation. One could simply abandon the impulse approximation. However, the question remains, "what is wrong with it and how can it be corrected (if at all)?" . One would like to improve the understanding of the physics of this process.

There are two inter-related possibilities that come to mind. It may be that the

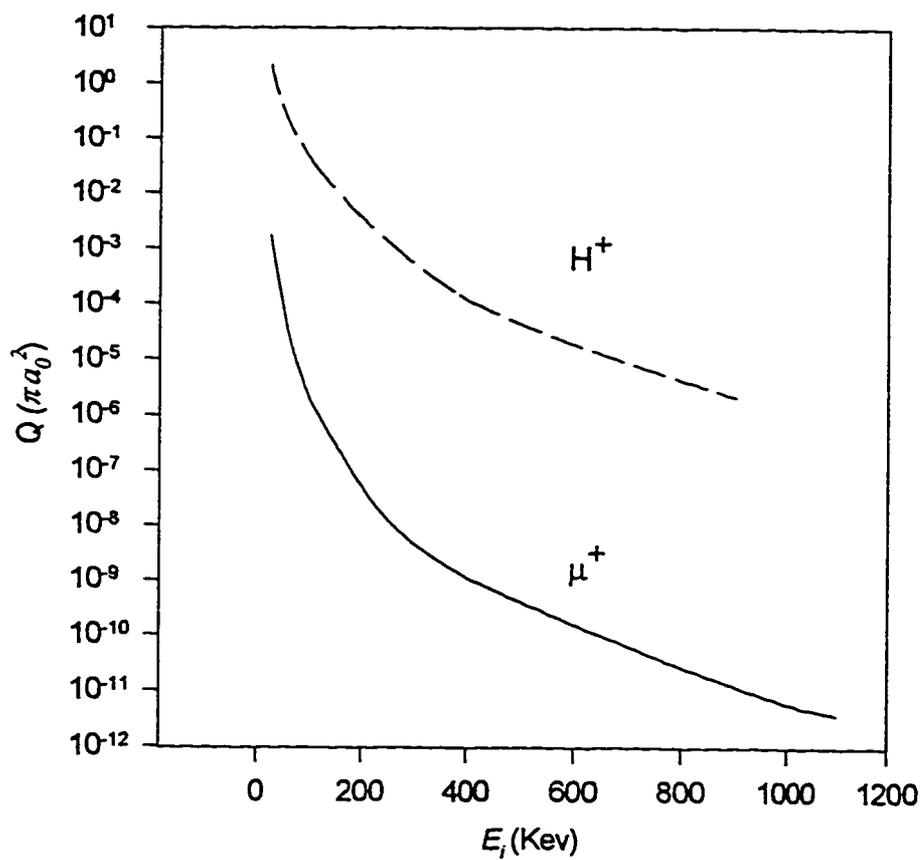


Figure 4-9: Total cross sections of electron capture from atomic hydrogen in the ground state by  $\mu^+$  muons and protons into the ground state at incident particle energies  $E_i$ .

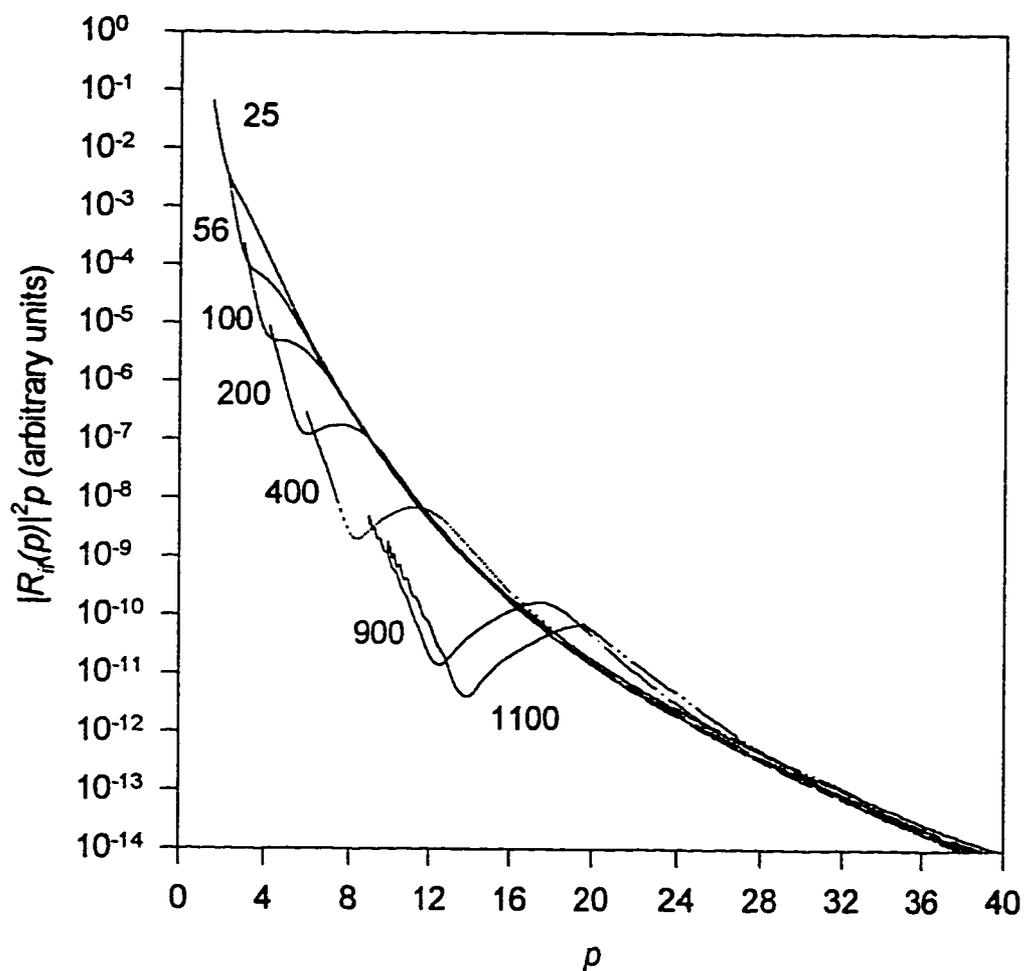
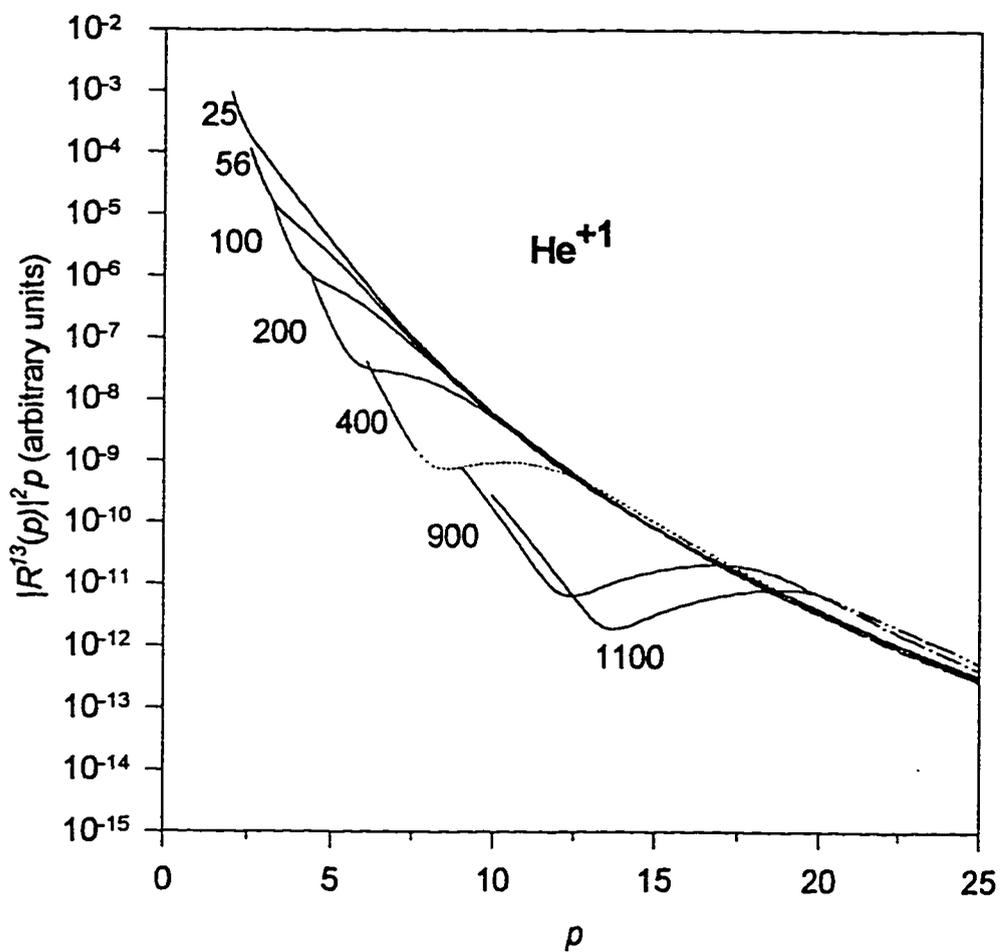
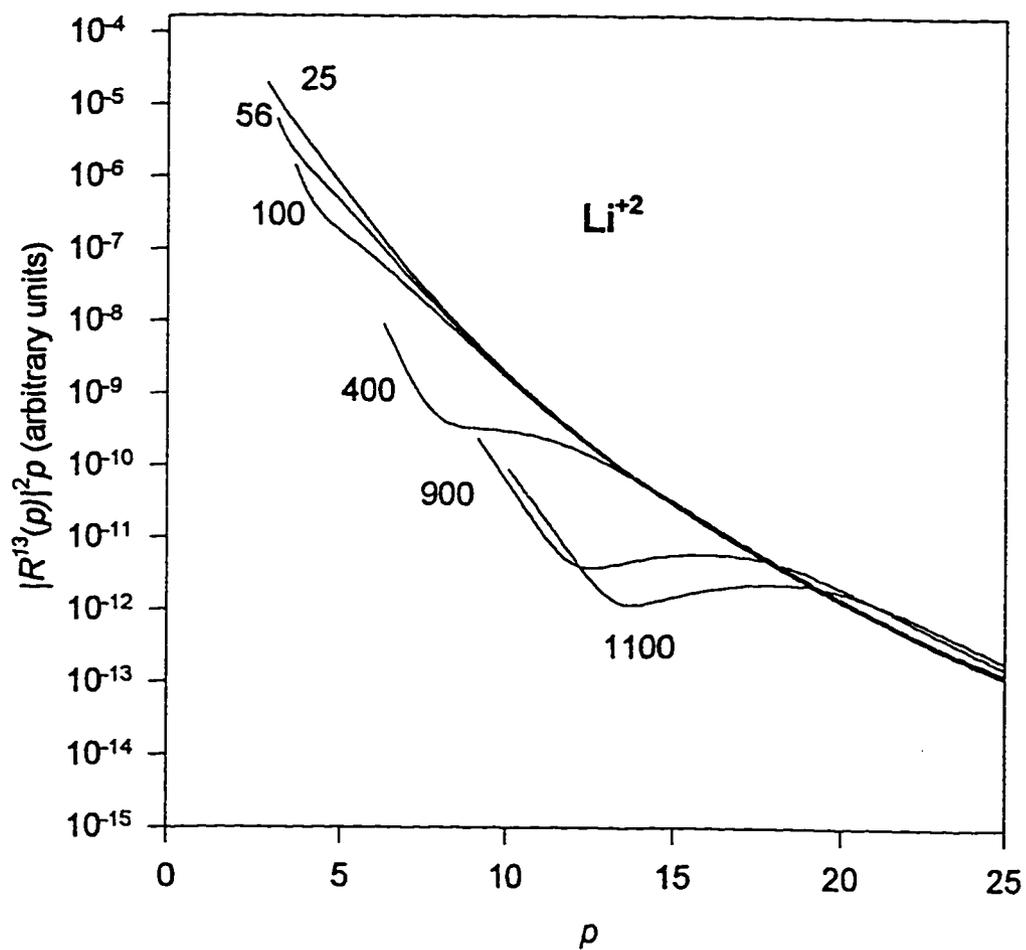


Figure 4-10: The impulse approximation angular distributions of muonium formation in the ground state from atomic hydrogen in the ground state. The number adjacent to each curve indicates the incident muon energies for that curve.  $p$  is related to the angle of scattering as  $p^2 = k_i^2 + k_f^2 - 2k_i k_f \cos \theta$ .

Figure 4-11: Same as Figure 4-10 but for  $\text{He}^{+1}$ .

Figure 4-12: Same as Figure 4-10 but for  $\text{Li}^{+2}$ .

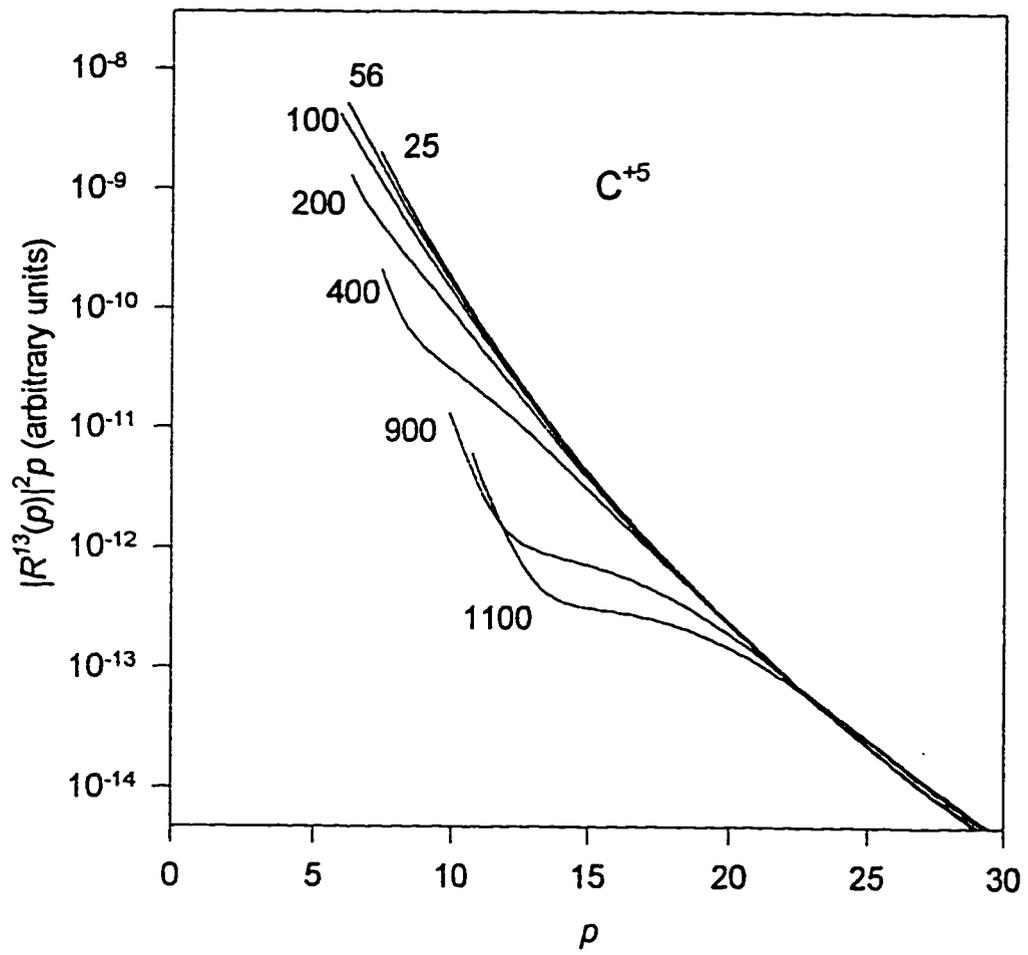


Figure 4-13: Same as Figure 4-10 but for  $C^{+5}$ .

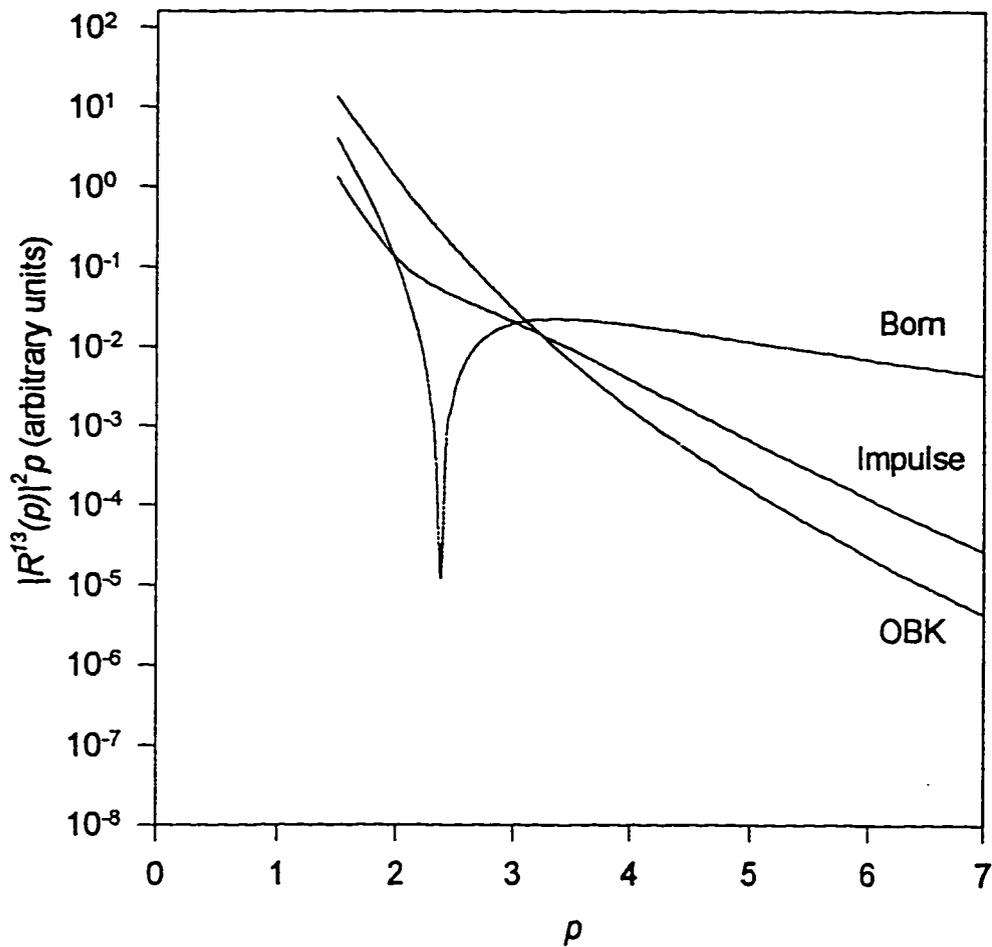


Figure 4-14: Angular distribution of muonium formation in the ground state from hydrogen in the ground state calculated using the Born, OBK and impulse approximation at an incident muon energy of 25 KeV.

fact of the exchange-force being non-classical plays a vital role. The quantum impulse approximation is supposed to account for this difference while omitting the nucleus-electron interaction in the target. It may not be accounting for it correctly though. The other possibility is that it may simply not be a valid assumption to neglect the large intra-target potential quantum mechanically. In other words, the mean field resulting from the intra-target potential may play a role in the scattering of the electron.

The simplest procedure would be to avoid using identical particles in the interaction. This may be done by using positrons and muons as projectiles. In the latter case there would be little difference except that the mass being greater one needs to adjust the relevant energy range. The major difference in both cases is that from the experimental side we are not able to obtain data as easily, since in one case the particle is likely to be annihilated and while in the other it might decay. However, this experiment, though more difficult should be feasible.

There is, as yet, no data available on muon scattering off atoms and scanty data for positrons, which is ambiguous. Though one experiment appears to be better described by the Born approximation, the other appears to favor the impulse approximation. In the hope that more experimental data will be available in the future, we have computed the total cross sections for the positronium and muonium formation in the relevant energy range.

It turned out that the earlier calculations [7] for the process  $e^+ + H(1s) \longrightarrow (e^+e^-)(1s) + H^+$  had not been sufficiently refined as regards the numerical evaluation of an improper integral near the points where the singularities arose. As such the differential cross sections could not be meaningfully evaluated. We have refined the calculation and obtained the differential cross sections as well. Features appear in it in the form of *shoulders* when the differential cross section is relatively large and becoming broad *resonances* for lower energies. This discussion has also been presented. We have found that the experimental data of the total cross sections for the process favors the theoretical values calculated in the Born approximation, to a certain extent, rather than

the impulse approximation, even in intermediate energy range. Since there is no experimental data for higher energies range, where the impulse approximation is expected to be better than the Born approximation, we can only speculate about such cases. Suggesting that incorporation of the mean field into the calculation defeats the case for the impulse approximation. However, it may be that while the mean field is relevant for the total cross section it can get appropriately *cancelled out* for the differential cross section. Even if it still enters into the cross section, it could hardly wipe out the features predicted. *The test for the utility of the impulse approximation is likely to be the differential cross section, if it can be measured.*

# Appendix A

## Coeffluent Hypergeometric Function Integral

Consider the following integral which involves the confluent hypergeometric function  ${}_1F_1$ , an exponential and a plane wave, that is

$$f(\beta, \nu, \mathbf{k}, \mathbf{p}) = \int d\mathbf{r} \frac{\exp(-\beta r)}{r} \exp(i\mathbf{p} \cdot \mathbf{r}) {}_1F_1[i\nu, 1, i(kr - \mathbf{k} \cdot \mathbf{r})], \quad (\text{A.1})$$

where  $\beta$ ,  $\nu$  and  $k$  are real, and  $\beta > 0$ . In order to evaluate this integral we replace the confluent hypergeometric function  ${}_1F_1$  by its contour integral representation [13]

$${}_1F_1[a, 1, z] = \frac{1}{2\pi i} \oint_C dt \exp(tz) t^{a-1} (t-1)^{-a}. \quad (\text{A.2})$$

Here  $C$  is a closed contour which starts at the origin and encircles the point  $t = 1$  once in the anti-clockwise sense.

Substituting Eq. (A.2) into Eq. (A.1) and then, reversing the order of integration with respect  $\mathbf{r}$ , we obtain

$$f(\beta, \nu, \mathbf{k}, \mathbf{p}) = \frac{1}{2\pi i} \oint_C dt t^{i\nu-1} (t-1)^{-i\nu} \Phi(t), \quad (\text{A.3})$$

where

$$\Phi(t) = \int dr \frac{\exp[it(\mathbf{p}-t\mathbf{k}) \cdot \mathbf{r}]}{r} \exp[-(\beta - itk)r]. \quad (\text{A.4})$$

To evaluate  $\Phi(t)$  we use the integral

$$\int dr \frac{\exp(i\mathbf{y} \cdot \mathbf{r})}{r} \exp(-\mu r) = \frac{4\pi}{y^2 + \mu^2}, \quad (\text{A.5})$$

which yields

$$\Phi(t) = \frac{4\pi}{(\mathbf{p}-t\mathbf{k})^2 + (\beta - itk)^2}, \quad (\text{A.6})$$

or

$$\Phi(t) = \frac{4\pi}{\beta^2 + p^2 - 2t(i\beta\mathbf{k} - \mathbf{p} \cdot \mathbf{k})}, \quad (\text{A.7})$$

and consequently

$$f(\beta, \nu, \mathbf{k}, \mathbf{p}) = \frac{1}{2i} \oint_C dt \frac{t^{i\nu-1} (t-1)^{-i\nu}}{\beta^2 + p^2 - 2t(i\beta\mathbf{k} - \mathbf{p} \cdot \mathbf{k})}. \quad (\text{A.8})$$

The integrand on the right-hand side of Eq. (A.8) has branch points at  $t = 0$  and  $t = 1$ , and a simple pole at

$$t = T_0 \equiv \frac{\beta^2 + p^2}{2t(i\beta\mathbf{k} - \mathbf{p} \cdot \mathbf{k})}, \quad (\text{A.9})$$

but no other singularity. Clearly

$$\text{Im } T_0 = \frac{-\beta\mathbf{k}(\beta^2 + p^2)}{2[(\mathbf{p} \cdot \mathbf{k})^2 + \beta^2 k^2]}, \quad (\text{A.10})$$

and therefore,

$$\beta + 2k \text{Im } T_0 = \frac{-\beta[p^2 k^2 - (\mathbf{p} \cdot \mathbf{k})^2]}{(\mathbf{p} \cdot \mathbf{k})^2 + \beta^2 k^2} < 0, \quad (\text{A.11})$$

This is the condition of convergence and it follows that the point  $t = T_0$  lies outside

the contour  $C$ . Cauchy's residue theorem [14] may be applied to give

$$f(\beta, \nu, \mathbf{k}, \mathbf{p}) = \frac{4\pi}{\beta^2 + p^2} \left\{ \frac{(\mathbf{p} + \mathbf{k})^2 - (\mathbf{k} + i\beta)^2}{\beta^2 + p^2} \right\}^{i\nu}. \quad (\text{A.12})$$

# Appendix B

## Fourier Transform of the Wave Functions

The Fourier transform definition may vary slightly from one textbook to another, here we adopt the following form

$$g(\mathbf{k}) = \int d\mathbf{r} \exp(-i\mathbf{k} \cdot \mathbf{r}) \varphi_{1s}(\mathbf{r}), \quad (\text{B.1})$$

which defines a Fourier transform of the function  $\varphi_{1s}(\mathbf{r})$  which can be any well-behaved function, in our case it is the ground state of a hydrogen like-ion given by

$$\varphi_{1s}(\mathbf{r}) = \frac{(az_1)^{3/2}}{\pi^{1/2}} \exp(-az_1 r). \quad (\text{B.2})$$

Carrying out the integration over  $\mathbf{r}$  with the help of Bethe's integral,

$$\int d\mathbf{r} \exp(\pm i\mathbf{y} \cdot \mathbf{r} - \mu r) = \frac{8\pi\mu}{(y^2 + \mu^2)^2}, \quad (\text{B.3})$$

with  $\mu = az$  and  $\mathbf{y} = \mathbf{k}$ , we readily find that

$$g(\mathbf{k}) = 8\pi \frac{(az)^{5/2}}{(k^2 + a^2 z^2)^2}. \quad (\text{B.4})$$

# Appendix C

## Evaluation of the Azimuthal Integrand

Consider the denominator in Eq. (2.87). Expanding the term involving  $\mathbf{k}$  and  $\mathbf{k}_i$ , the denominator becomes

$$\left[ \frac{1}{a^2} k^2 + \left( \frac{1}{a} - b \right)^2 k_i^2 + 2 \left( \frac{1}{a^2} - \frac{b}{a} \right) \mathbf{k} \cdot \mathbf{k}_i + b^2 z_2^2 \right]^2. \quad (\text{C.1})$$

Now, notice that

$$\mathbf{k} \cdot \mathbf{k}_i = k k_i \cos \theta''. \quad (\text{C.2})$$

Expressing  $\mathbf{k}$  in spherical polar coordinates  $(k, \theta, \phi)$  and selecting the  $z$ -axis to be along  $\mathbf{p}$ , we obtain

$$\mathbf{k} \cdot \mathbf{p} = k p \cos \theta, \quad (\text{C.3})$$

with

$$\mathbf{k} = k(\sin \theta \cos \phi \hat{\mathbf{x}} + \sin \theta \sin \phi \hat{\mathbf{y}} + \cos \theta \hat{\mathbf{z}}), \quad (\text{C.4})$$

Also, we can express  $\mathbf{k}_i$  in spherical polar coordinates  $(k_i, \theta', \phi')$ . Without loss of

generality we can put  $\phi' = 0$ , then

$$\mathbf{k}_i = k_i(\sin \theta' \hat{\mathbf{x}} + \cos \theta' \hat{\mathbf{z}}), \quad (\text{C.5})$$

so that

$$\mathbf{k} \cdot \mathbf{k}_i = k k_i \cos \theta' = k k_i (\sin \theta' \sin \theta \cos \phi + \cos \theta \cos \theta'), \quad (\text{C.6})$$

where, it is clear that

$$\cos \theta' = \frac{\mathbf{k}_i \cdot \mathbf{p}}{k_i p}. \quad (\text{C.7})$$

From the definition of  $\mathbf{p}$ , we obtain

$$p^2 = a^2 k_f^2 + k_i^2 - 2a \mathbf{k}_i \cdot \mathbf{k}_f, \quad (\text{C.8})$$

which implies

$$\mathbf{k}_i \cdot \mathbf{k}_f = -\frac{p^2}{2a} + \frac{a k_f^2}{2} + \frac{k_i^2}{2a}. \quad (\text{C.9})$$

Next, we evaluate the dot product  $\mathbf{k}_i \cdot \mathbf{p}$  with the help of Eq. (2.28) and using the result for  $\mathbf{k}_i \cdot \mathbf{k}_f$ , we obtain

$$\mathbf{k}_i \cdot \mathbf{p} = -\frac{p^2}{2} + \frac{a^2 k_f^2}{2} + \frac{3k_i^2}{2}. \quad (\text{C.10})$$

Notice that  $k_i^2$  and  $k_f^2$  are related by Eq. (2.35).

Using Eq. (C.10) in Eq. (C.7), and substituting the resulting equation into (C.6), we eliminate  $\mathbf{k} \cdot \mathbf{k}_i$  from Eq. (C.1) with the help the resulting equation from the previous step and obtain

$$\left[ \frac{1}{a^2} k^2 + \left( \frac{1}{a} - b \right)^2 k_i^2 + 2 \left( \frac{1}{a^2} - \frac{b}{a} \right) \mathbf{k} \cdot \mathbf{k}_i + b^2 z_2^2 \right]^2 = [A + B \cos \phi]^2, \quad (\text{C.11})$$

where

$$A = b^2 z_2^2 + \left(\frac{1}{a} - b\right)^2 k_i^2 + a^{-2} k^2 - p^{-1} k \lambda \left\{ \left(\frac{1}{a} - b\right)^2 k_i^2 + b \Delta E + a^{-2} (1 - ab) p^2 \right\}, \quad (\text{C.12})$$

and

$$\begin{aligned} B = & k(\lambda^2 - 1)^{1/2} \left\{ p^{-2} \left[ \left(\frac{1}{a} - b\right)^2 k_i^2 + b \Delta E \right]^2 + a^{-4} (1 - ab)^2 p^2 \right. \\ & \left. + 2ba^{-2} (1 - ab) \Delta E - 2a^{-2} (1 + ab)^2 k_i^2 \right\}^{1/2}, \end{aligned} \quad (\text{C.13})$$

with  $\lambda = \cos \theta$ .

# Appendix D

## Computer Programs

Here we give the computer programs used in evaluating and calculating the cross sections. We also include Mathematica Notebook in which the differentiation involved in Eq. (2.138) is performed analytically and the result is converted to Fortran forms. The following programs are included:

1. Fortran source code to calculate the total cross sections of positronium formation in the first Born approximation;
2. Fortran source code to calculate the total cross sections of positronium formation in the  $R^{13}$  approximation;
3. Fortran source code to calculate the total cross sections of muonium formation in the impulse approximation;
4. Mathematica Notebook mentioned above.

```

*
*                                     Program 1
* This program calculates the total cross section of positronium
* formation in the Born approximation and when modified can be used
* together with program 2 to calculate the cross sections in
* the impulse approximation.
  REAL AX,BX,AY,BY,RESLT1,RESLT2,RESLT3,RESLT4,
&RESULT,C,RIJ,RTOL
  REAL A,B,M1,M2,Z1,Z2,UI,UF,ZB2,ZA1,DE,
&KI,KF,PMAX,PMIN,V,PI
  INTEGER N,K
  EXTERNAL RIJ
  COMMON /ENRGN/ F
  COMMON /MASS1N/ M1
  COMMON /MASS2N/ M2
  COMMON /CH1N/ Z1
  COMMON /CH2N/ Z2
  COMMON /PBORN/AX,BX
  COMMON /POINT/N
  OPEN(UNIT=4,FILE='r13test2.in',STATUS='UNKNOWN')
99 PRINT*, 'ENTER M1 M2 Z1 Z2'
  READ(*,*)M1,M2,Z1,Z2
  PRINT*, 'ENTER INCEDINT ENERGY'
  READ(*,*)F
  A=M1/(1.0+M1)
  B=M2/(1.0+M2)
  UI=M1*(M2+1.0)/(1.0+M1+M2)
  UF=M2*(M1+1.0)/(1.0+M1+M2)
  ZB2=Z2*B
  ZA1=Z1*A
  DE=-A*Z1**2+B*Z2**2
  KI=SQRT(UI**2*F*1.0E3/(M1*13.6))
  IF ((UF*KI**2/UI-UF*DE).LE.0.0) GO TO 99
  KF=SQRT(UF*KI**2/UI-UF*DE)
  PMAX=(A*KF+KI)
  PMIN=ABS(A*KF-KI)
  PRINT*, 'LIMIT P ', PMIN, PMAX
  V=KI/UI
  PI=3.14159
  PRINT*, 'ENTER AX BX'
  READ(*,*)AX,BX
  IF (AX .EQ. BX) GOTO 33
  PRINT*, 'ENTER AY BY'
  READ(*,*)AY,BY
  AY=PMIN
  BY=PMAX
  PRINT*, 'ENTER NUMBER OF POINTS FOR THE P-INTEGRAL'
  READ(*,*)N

```

```

      RTOL=1.0E-3
      CALL SIMPY(RIJ,AY,BY,N,RESULT)
      C=1.0/(2.0*PI**2*A*V**2)*(UF/UI)
      RESULT=C*RESULT
      PRINT*, ' INCIEDENT ENERGY', ' CROSS SECTION'
      PRINT*, F, RESULT
      GO TO 99
33  END
-----
* Simpson's rule
  SUBROUTINE SIMPX(F,A,B,RTOL,RESULT)
    REAL F,A,B,RTOL,RESULT,WX,
+OSUMX,HX,SUMX
    INTEGER I,M
    M=0
    OSUMX=-1.E30
77  M=M+2
    HX=(B-A)/REAL(2**M*20)
    SUMX=0.0
    DO 22 I=0,2**M*20
      WX=4.0
      IF (MOD(I,2).EQ.0) WX=2.0
      IF (I.EQ.0.OR.I.EQ.2**M*20) WX=1.0
      SUMX=SUMX+HX*WX*F(A+HX*I)
22  CONTINUE
    SUMX=SUMX/3.0
    IF ((ABS(SUMX-OSUMX).LT.RTOL*ABS(OSUMX))) GOTO 40
    IF (I.GT.1000) GOTO 50
    OSUMX=SUMX
    GOTO 77
50  PRINT*, 'WARNING : '
    PRINT*, 'FAILS TO REACH THE REQUIRED EPSX '
    PRINT*, 'ERROR FOR P-INT. ',ABS(SUMX-OSUMX)
40  RESULT=SUMX
    RETURN
    END
-----
  SUBROUTINE SIMPY(F,A,B,M,RESULT)
    REAL F,A,B,RESULT,WX,
+HX,SUMX
    INTEGER I,M
    HX=(B-A)/REAL(M)
    SUMX=0.0
    DO 22 I=0,M
      WX=4.0
      IF (MOD(I,2).EQ.0) WX=2.0
      IF (I.EQ.0.OR.I.EQ.M) WX=1.0
      SUMX=SUMX+HX*WX*F(A+HX*I)

```

```

22  CONTINUE
    RESULT=SUMX/3.0
    RETURN
    END

```

```

-----
* Gamma function subroutine
  FUNCTION gammln(xx)
    COMPLEX gammln,xx
    INTEGER j
    DOUBLE PRECISION stp,cof(6)
    DOUBLE COMPLEX ser,tmp,x,y
    SAVE cof,stp
    DATA cof,stp/76.18009172947146d0,-86.50532032941677d0,
&24.01409824083091d0,-1.231739572450155d0,.1208650973866179d-2,
&-.5395239384953d-5,2.5066282746310005d0/
    x=xx
    y=x
    tmp=x+5.5d0
    tmp=(x+0.5d0)*log(tmp)-tmp
    ser=1.000000000190015d0
    do 11 j=1,6
      y=y+1.d0
      ser=ser+cof(j)/y
11  continue
    gammln=tmp+log(stp*ser/x)
    return
    END

```

```

-----
  COMPLEX FUNCTION R13B(P,X)
  COMPLEX R1,NC,ZZ,RT,F3,DF3,DDF3,I
  REAL P,X,KIKF,W2,U2,C,CC,U,V,Y,F1,
&DF1,DDF1,F2,DF2,DDF2,DC,DDC
  REAL A,B,M1,M2,Z1,Z2,UI,UF,ZB2,ZA1,DE,
&KI,KF,PMAX,PMIN,VI,PI
  COMPLEX GAMMLN,Z
  EXTERNAL GAMMLN
  COMMON /ENRGN/ F
  COMMON /MASS1N/ M1
  COMMON /MASS2N/ M2
  COMMON /CH1N/ Z1
  COMMON /CH2N/ Z2
  A=M1/(1.0+M1)
  B=M2/(1.0+M2)
  UI=M1*(M2+1.0)/(1.0+M1+M2)
  UF=M2*(M1+1.0)/(1.0+M1+M2)
  ZB2=Z2*B
  ZA1=Z1*A
  DE=-A*Z1**2+B*Z2**2

```

```

KI=SQRT(UI**2*F*1.0E3/(M1*13.6))
KF=SQRT(UF*KI**2/UI-UF*DE)
PMAX=(A*KF+KI)
PMIN=ABS(A*KF-KI)
VI=KI/UI
PI=3.14159
I=(0.0,1.0)
V=Z2/KI
KIKF=(A**2*KF**2+KI**2-P**2)/(2.0*A)
W2=KI**2+(X/2.0-1.0)**2*KF**2+(X-2.0)*KIKF
U=SQRT(ZB2**2+(0.25-ZB2**2)*X+X/4.0*(1.0-X)*KF**2)
U2=ZB2**2+(0.25-ZB2**2)*X+X/4.0*(1.0-X)*KF**2
C=U2+(1.0-0.5*X)**2*KF**2-KI**2
DC=2.0*U
DDC=2.0
Y=U**2 + W2
RT=C - 2.0*I*KI*U
F1=-1.0 + (1.0 - X)*Z2/U
F2=1.0/(Y)
F3=RT/(Y)
DF1=-((1.0 - X)*Z2/U**2)
DF2=-2.0*U/(Y)**2
DF3=-2.0*U*(RT)/
- (Y)**2 +
- (DC - 2.0*I*KI)/(Y)
DDF1=2.0*(1.0 - X)*Z2/U**3
DDF2=8.0*U**2/(Y)**3 -
- 2.0/(Y)**2
DDF3=8.0*U**2*(RT)/
- (Y)**3 -
- 4.0*(DC - 2.0*I*KI)*U/
- (Y)**2 -
- 2.0*(RT)/
- (Y)**2 +
- DDC/(Y)
R1=(-((DF2*F1*F3**(I*V) +
- DF1*F2*
- F3**(I*V) +
- I*DF3*F1*F2*
- F3**(-1.0 + I*V)*V)
- /U**2) +
- (2.0*DF1*DF2*F3**(I*V) +
- DDF2*F1*F3**(I*V) +
- DDF1*F2*F3**(I*V) +
- 2.0*I*DF2*DF3*F1*
- F3**(-1.0 + I*V)*V +
- 2.0*I*DF1*DF3*F2*
- F3**(-1.0 + I*V)*V +

```

```

-      I*DDF3*F1*F2*
-      F3**(-1.0 + I*V)*V +
-      I*DF3**2*F1*F2*
-      F3**(-2.0 + I*V)*
-      (-1.0 + I*V)*V)/U)/U

```

```

Z=1.0+I*V
ZZ=GAMMLN(Z)
NC=CEXP((-PI/2.0*V)+ZZ)
CC=SQRT(2.0)*PI*SQRT(Z2)**5
R13B=X*CC*NC*R1
RETURN
END

```

\*-----

```

REAL FUNCTION RF(P,X)
REAL P,X
COMPLEX Z,R13B
Z=R13B(P,X)
RF=REAL(Z)
RETURN
END

```

\*-----

```

REAL FUNCTION IMF(P,X)
REAL P,X
COMPLEX Z,R13B
Z=R13B(P,X)
IMF=IMAG(Z)
RETURN
END

```

\*-----

```

REAL FUNCTION RF2(X)
REAL D,RF
COMMON /XVAL1/ D
RF2=RF(D,X)
RETURN
END

```

\*-----

```

REAL FUNCTION RF3(P)
REAL P,D,RF2,AX,BX,RESULT,RTOL
INTEGER N
EXTERNAL RF2
COMMON /XVAL1/ D
COMMON /PBORN/AX,BX
COMMON /POINT/N
D=P
RTOL=1.0E-4
CALL SIMPX(RF2,AX,BX,RTOL,RESULT)
RF3=RESULT
RETURN

```

END

```

*-----
REAL FUNCTION IMF2(X)
REAL D, IMF
COMMON /XVAL2/D
IMF2=IMF(D,X)
RETURN
END

```

```

*-----
REAL FUNCTION IMF3(P)
REAL P,D, IMF2, AX, BX, RESULT, RTOL
INTEGER N
EXTERNAL IMF2
COMMON /XVAL2/ D
COMMON /PBORN/AX, BX
COMMON /POINT/N
D=P
RTOL=1.0E-4
CALL SIMPX(IMF2, AX, BX, RTOL, RESULT)
IMF3=RESULT
RETURN
END

```

```

*-----
REAL FUNCTION FCT(P,X)
REAL P,X,KIKF,W2,U2,C,D,CC
REAL A,B,M1,M2,Z1,Z2,UI,UF,ZB2,ZA1,DE,
&KI,KF,PMAX,PMIN,V,PI
COMMON /ENRGN/ F
COMMON /MASS1N/ M1
COMMON /MASS2N/ M2
COMMON /CH1N/ Z1
COMMON /CH2N/ Z2
A=M1/(1.0+M1)
B=M2/(1.0+M2)
UI=M1*(M2+1.0)/(1.0+M1+M2)
UF=M2*(M1+1.0)/(1.0+M1+M2)
ZB2=Z2*B
ZA1=Z1*A
DE=-A*Z1**2+B*Z2**2
KI=SQRT(UI**2*F*1.0E3/(M1*13.6))
KF=SQRT(UF*KI**2/UI-UF*DE)
PMAX=(A*KF+KI)
PMIN=ABS(A*KF-KI)
V=KI/UI
PI=3.14159
KIKF=(A**2*KF**2+KI**2-P**2)/(2.0*A)
W2=KI**2+(X/2.0-1.0)**2*KF**2+(X-2.0)*KIKF
U2=ZB2**2+(0.25-ZB2**2)*X+X/4.0*(1.0-X)*KF**2

```

```

C=U2+W2
D=U2
CC=SQRT(2.0)*PI*Z2*(SQRT(ZB2))**3
FCT=CC*(X*(1.0-X)*ZB2*(3.0*C**2+4.0*C*D+8.0*D**2)/
&((SQRT(D))**5*C**3)-8.0*X/C**3)
RETURN
END

```

```

*-----
REAL FUNCTION V12I(X)
REAL D,FCT
COMMON /XVAL/ D
V12I=FCT(D,X)
RETURN
END

```

```

*-----
REAL FUNCTION BORN(P)
REAL P,D,V12I,AX,BX,RESULT,RTOL
INTEGER N
EXTERNAL V12I
COMMON /XVAL/ D
COMMON /PBORN/AX,BX
COMMON /POINT/N
D=P
RTOL=1.0E-4
CALL SIMPX(V12I,AX,BX,RTOL,RESULT)
BORN=RESULT
RETURN
END

```

```

*-----
REAL FUNCTION RIJ(P)
REAL IMF3,RF3,BORN
*   RIJ=(IMF3(P)**2+(RF3(P)-BORN(P))**2)*P
RIJ=(BORN(P))**2*P
PRINT*,'P=',P,' RIJ=',RIJ
RETURN
END

```

```

*                                     Program 2
* This program calculates the total cross sections of positronium
* formation in the R13 approximation.
*-----
  REAL RIJ,RESULT,M1,M2,A,Z1,Z2,ZB2,ZA1,
&KF,DE,F,
&AZ,BZ,AY,BY,AX,BX,PMAX,PMIN,KI,UI,UF,PI,V
  INTEGER N1,N2,N3,K1,K2,K3
  EXTERNAL RIJ
  COMMON /PARM/AZ,BZ,AY,BY,AX,BX,N1,N2,N3,K1,K2,K3
  OPEN(UNIT=7,FILE='gauss5md.out',STATUS='UNKNOWN')
  PI=4.0*ATAN(1.0)
  M1=1836.0
  M2=1836.0
  A=M1/(1.0+M1)
  B=M2/(1.0+M2)
  UI=M1*(M2+1.0)/(1.0+M1+M2)
  UF=M2*(M1+1.0)/(1.0+M1+M2)
  Z1=1.0
  Z2=1.0
  ZB2=Z2*B
  ZA1=Z1*A
  DE=-A*Z1**2+B*Z2**2
  F=25.0
  KI=SQRT(UI**2*F*10.0**3/(M1*13.6))
  KF=SQRT(UF*KI**2/UI-UF*DE)
  PMAX=(A*KF+KI)
  PMIN=ABS(A*KF-KI)
  PRINT*, 'PMAX=', PMAX, 'PMIN=', PMIN
  V=KI/UI
99 PRINT*, 'ENTER INTERVAL ENDPOINTS FOR X-INTEGRATION OR 0 0
& TO QUIT'
  PRINT*, 'KI=', KI
  PRINT*, 'PI=', PI
  PRINT*, 'KF', KF
  READ*, AX, BX

  IF ((AX-BX).NE. 0) THEN

    PRINT*, 'ENTER INTERVAL ENDPOINTS FOR Y-INTEGRATION'
    READ*, AY, BY
    PRINT*, 'ENTER INTERVAL ENDPOINTS FOR Z-INTEGRATION'
    READ*, AZ, BZ
    PRINT*, 'ENTER NUMBER OF POINTS FOR EACH INTEGRAL'
    READ*, N1,N2,N3
    PRINT*, 'TYPE 2 2 2 FOR SIMPSONS RULE'

```

```

PRINT*, 'TYPE 3 3 3 FOR GAUSS RULE'
PRINT*, 'PMAX=', PMAX, ' PMIN=', PMIN
READ*, K1, K2, K3
AZ=PMIN
IF (K1.EQ.1) THEN
    CALL TRAP3Z(RIJ, AZ, BZ, N1, RESULT)

ELSE
    CALL SIMPS3(RIJ, AZ, BZ, N1, RESULT)
END IF
C1=-8.0*(SQRT(A*Z2))**5*Z2/SQRT(PI)/A**2
C2=1.0/(2*PI**2*A*V**2)*(UF/UI)
RESULT=C1**2*C2*RESULT
WRITE(7,*) '          RESULTS          '
WRITE(7,*) RESULT
GO TO 99
ENDIF
END

```

---

```

COMPLEX*16 FUNCTION SBR13(X1, K1, P1)
REAL*8 X1, K1, P1
REAL*8 PI, M1, M2, A, B, UI, UF, Z1, Z2, ZB2, ZA1, DE, KI, KF,
+PMAX, PMIN, K, ALFA, P, X, AC, T, TC, F, BC, GC, V
COMPLEX*16 GAMMLN, DELTA, FC, I, NC, Z, II, SBR
EXTERNAL GAMMLN
I=(0.0d0, 1.0d0)
II=(1.0d0, 0.0d0)
PI=4.0d0*ATAN(1.0d0)
M1=1836.0d0
M2=1836.0d0
A=M1/(1.0d0+M1)
B=M2/(1.0d0+M2)
UI=M1*(M2+1.0d0)/(1.0d0+M1+M2)
UF=M2*(M1+1.0d0)/(1.0d0+M1+M2)
Z1=1.0d0
Z2=1.0d0
ZB2=Z2*B
ZA1=Z1*A
DE=-A*Z1**2+B*Z2**2
F=25.0d0
KI=SQRT(UI**2*F*1.0d3/(M1*13.6d0))
KF=SQRT(UF*KI**2/UI-UF*DE)
PMAX=(A*KF+KI)
PMIN=ABS(A*KF-KI)
V=KI/UI
X=X1
K=K1
P=P1

```

```

ALFA=A*Z1/K
AC=B**2*Z2**2+V**2+K**2/A**2-
&K*X/P*(V**2+B*DE+(1.0d0-A*B)/A**2*P**2)
BC=K**2*(X**2-1.0d0)*(1.0d0/P**2*(V**2+B*DE
&)**2+1.0/A**4*(1.0-A*B)**2*P**2+
&2.0d0*B/A**2*(1.0d0-A*B)*DE-
&2.0d0/A**2*(1.0d0+A*B)*V**2)
GC=AC*(SQRT(AC**2-BC))**(-3)
Z=1.0d0-I*ALFA
NC=EXP((PI/2.0d0*ALFA)+(GAMMLN(Z)))
T=1.0d0/A**2*(K**2+P**2-2.0d0*P*K*X)
DELTA=P*K*X+I*Z1*K
TC=Z1**2+P**2
FC=8.0d0*SQRT(PI)*(SQRT(A*Z1))**3*
&((1.0d0-I*ALFA)*(A*Z1)/TC**2+
&I*ALFA*(A*Z1-I*K)/(TC*(TC-2.0d0*DELTA)))*
&(TC/(TC-2.0d0*DELTA))**(I*ALFA)
SBR=K**2*NC*GC*FC*1.0d0/T
SBR13=SBR
RETURN
END

```

```

-----
FUNCTION gammln(xx)
COMPLEX*16 gammln,xx
INTEGER j
DOUBLE PRECISION stp,cof(6)
DOUBLE COMPLEX ser,tmp,x,y
SAVE cof,stp
DATA cof,stp/76.18009172947146d0,-86.50532032941677d0,
&24.01409824083091d0,-1.231739572450155d0,.1208650973866179d-2,
&- .5395239384953d-5,2.5066282746310005d0/
x=xx
y=x
tmp=x+5.5d0
tmp=(x+0.5d0)*log(tmp)-tmp
ser=1.000000000190015d0
do 11 j=1,6
  y=y+1.d0
  ser=ser+cof(j)/y
11 continue
gammln=tmp+log(stp*ser/x)
return
END

```

```

-----
REAL*8 FUNCTION F(X,Y,Z)
REAL*8 X,Y,Z
COMPLEX*16 Z2, SBR13
Z2=SBR13(X,Y,Z)

```

```

F=DREAL(Z2)
RETURN
END

```

```

-----*
REAL*8 FUNCTION F2(X,Y,Z)
REAL*8 X,Y,Z
COMPLEX*16 Z2,SBR13
Z2=SBR13(X,Y,Z)
F2=DIMAG(Z2)
RETURN
END

```

```

-----*
SUBROUTINE SIMPS(FUNC,A,B,N,SS)
REAL A,B,S,SS,H,X
INTEGER I,N,LS,W
S=0
SS=0
H=(B-A)/N
IF (N/2*2.EQ.N) THEN
  LS=0
  GO TO 35
END IF
LS=3
DO 31 I=0,3
  X=A+H*I
  W=3
  IF (I.EQ.0 .OR. I.EQ.3) W=1
  SS=SS+W*FUNC(X)
31 CONTINUE
SS=SS*H*3/H
IF (N.EQ.3) RETURN
35 DO 40 I=0,N-LS
  X=A+H*(I+LS)
  W=2
  IF (INT(I/2)*2+1.EQ.I) W=4
  IF (I.EQ.0 .OR. I.EQ.N-LS) W=1
  S=S+W*FUNC(X)
40 CONTINUE
SS=SS+S*H/3
RETURN
END

```

```

-----*
SUBROUTINE SIMPS2(FUNC,A,B,N,SS)
REAL A,B,S,SS,H,X
INTEGER I,N,LS,W
S=0
SS=0
H=(B-A)/REAL(N)

```

```

      IF (N/2*2.EQ.N) THEN
        LS=0
        GO TO 35
      END IF
      LS=3
      DO 31 I=0,3
        X=A+H*I
        W=3
        IF (I.EQ.0 .OR. I.EQ.3) W=1
        SS=SS+W*FUNC(X)
31  CONTINUE
      SS=SS*H*3/H
      IF (N.EQ.3) RETURN
35  DO 40 I=0,N-LS
        X=A+H*(I+LS)
        W=2
        IF (INT(I/2)*2+1.EQ.I) W=4
        IF (I.EQ.0 .OR. I.EQ.N-LS) W=1
        S=S+W*FUNC(X)
40  CONTINUE
      SS=SS+S*H/3
      RETURN
      END

```

---

```

SUBROUTINE SIMPS3(FUNC,A,B,N,SS)
REAL A,B,S,SS,H,X
INTEGER I,N,LS,W
S=0
SS=0
H=(B-A)/N
IF (N/2*2.EQ.N) THEN
  LS=0
  GO TO 35
END IF
LS=3
DO 31 I=0,3
  X=A+H*I
  W=3
  IF (I.EQ.0 .OR. I.EQ.3) W=1
  SS=SS+W*FUNC(X)
31 CONTINUE
SS=SS*H*3/H
IF (N.EQ.3) RETURN
35 DO 40 I=0,N-LS
  X=A+H*(I+LS)
  W=2
  IF (INT(I/2)*2+1.EQ.I) W=4
  IF (I.EQ.0 .OR. I.EQ.N-LS) W=1

```

```

        S=S+W*FUNC(X)
40    CONTINUE
      SS=SS+S*H/3
      RETURN
      END
*-----
      SUBROUTINE gauleg(a,b,x,w,n)
      INTEGER n
      REAL*8 x(n),w(n),a,b
      DOUBLE PRECISION EPS
      PARAMETER (EPS=3.d-16)
      INTEGER i,j,m
      DOUBLE PRECISION p1,p2,p3,pp,xl,xm,z,z1
      m=(n+1)/2
      xm=0.5d0*(b+a)
      xl=0.5d0*(b-a)
      do 12 i=1,m
        z=cos(3.141592654d0*(i-.25d0)/(n+.5d0))
1      continue
        p1=1.d0
        p2=0.d0
        do 11 j=1,n
          p3=p2
          p2=p1
          p1=((2.d0*j-1.d0)*z*p2-(j-1.d0)*p3)/j
11       continue
        pp=n*(z*p1-p2)/(z*z-1.d0)
        z1=z
        z=z1-p1/pp
        if(abs(z-z1).gt.EPS)goto 1
        x(i)=xm-xl*z
        x(n+1-i)=xm+xl*z
        w(i)=2.d0*xl/((1.d0-z*z)*pp*pp)
        w(n+1-i)=w(i)
12      continue
      return
      END
*-----
      SUBROUTINE GAUSS(H,A1,B1,N,XI1)
      INTEGER J,N
      REAL*8 H,X,A1,B1,XI1
      REAL*8 QW(99),QX(99),A,B,XI
      EXTERNAL GAULEG
      A=A1
      B=B1
      CALL GAULEG(A,B,QX,QW,N)
      XI=0.0d0
      DO 30 J=1,N

```

```

        X=QX(J)
        XI=XI+H(X)*QW(J)
30 CONTINUE
    XI1=XI
    RETURN
    END

```

```

* -----
    REAL*8 FUNCTION FF(S1)
    REAL*8 S1,F,Y,Z
    COMMON /FUNCN1/D1,D
    Y=D1
    Z=D2
    FF=F(S1,Y,Z)
    RETURN
    END

```

```

* -----
    REAL FUNCTION G(YZ,ZZ)
    REAL YZ,ZZ,RESULT,D1,D2,ERREST
    REAL*8 AX1,BX1,RESLT1,RESLT2,FF
    EXTERNAL FF
    COMMON /FUNCN1/D1,D2
    COMMON /PARM/AZ,BZ,AY,BY,AX,BX,N1,N2,N3,K1,K2,K3
    D1=YZ
    D2=ZZ
    AX1=AX
    BX1=BX
    IF (K3.EQ.1) THEN
        CALL TRAPZ(FF,AX,BX,N3,RESULT)
    ELSE IF (K3.EQ.2) THEN
        CALL SIMPS(FF,AX,BX,N3,RESULT)
    ELSE
        CALL GAUSS(FF,AX1,0.5D0,N3,RESLT1)
        CALL GAUSS(FF,0.5D0,BX1,N3,RESLT2)
        RESULT=REAL(RESLT1+RESLT2)
    END IF
    G=RESULT
    RETURN
    END

```

```

* -----
    REAL FUNCTION GG(S2)
    REAL S2,G
    COMMON/FUNCN2/D3
    GG=G(S2,D3)
    RETURN
    END

```

```

* -----
    REAL FUNCTION U(ZZZ)
    REAL ZZZ,RESULT,D3

```

```

EXTERNAL GG
COMMON /FUNCN2/D3
COMMON /PARM/AZ, BZ, AY, BY, AX, BX, N1, N2, N3, K1, K2, K3
D3=ZZZ
IF (K2.EQ.1) THEN
  CALL TRAP2Z(GG, AY, BY, N2, RESULT)
ELSE
  CALL SIMPS2(GG, AY, BY, N2, RESULT)
END IF
U=RESULT
RETURN
END

```

```

* -----
REAL*8 FUNCTION FF2(S1)
REAL*8 S1, F2, Y, Z
COMMON /FUNCN1/D1, D2
Y=D1
Z=D2
FF2=F2(S1, Y, Z)
RETURN
END

```

```

* -----
REAL FUNCTION G2(YZ, ZZ)
REAL YZ, ZZ, RESULT, D1, D2
REAL*8 RESULT1, RESULT2, FF2, AX1, BX1
EXTERNAL FF2
COMMON /FUNCN1/D1, D2
COMMON /PARM/AZ, BZ, AY, BY, AX, BX, N1, N2, N3, K1, K2, K3
D1=YZ
D2=ZZ
AX1=AX
BX1=BX
IF (K3.EQ.1) THEN
  CALL TRAPZ(FF2, AX, BX, N3, RESULT)
ELSE IF (K3.EQ.2) THEN
  CALL SIMPS(FF2, AX, BX, N3, RESULT)
ELSE
  CALL GAUSS(FF2, AX1, 0.5D0, N3, RESULT1)
  CALL GAUSS(FF2, 0.5D0, BX1, N3, RESULT2)
  RESULT=REAL(RESULT1+RESULT2)
END IF
G2=RESULT
RETURN
END

```

```

* -----
REAL FUNCTION GG2(S2)
REAL S2, G2
COMMON/FUNCN2/D3

```

```
GG2=G2(S2,D3)
RETURN
END
```

\*-----

```
REAL FUNCTION U2(ZZZ)
REAL ZZZ,RESULT,D3
EXTERNAL GG2
COMMON /FUNCN2/D3
COMMON /PARM/AZ,BZ,AY,BY,AX,BX,N1,N2,N3,K1,K2,K3
D3=ZZZ
IF (K2.EQ.1) THEN
  CALL TRAP2Z(GG2,AY,BY,N2,RESULT)
ELSE
  CALL SIMPS2(GG2,AY,BY,N2,RESULT)
END IF
U2=RESULT
RETURN
END
```

\*-----

```
REAL FUNCTION RIJ(P)

REAL P,U,U2
RIJ=(U(P)**2+U2(P)**2)*P
WRITE(7,*) 'P=',P, ' RIJ=',RIJ
PRINT*, 'P=',P, ' RIJ=',RIJ
RETURN
END
```

\* Program 3  
 \* This program calculates the total cross sections of muonium  
 \* formation in the impulse approximation.

```

-----
      REAL RIJ, RESULT, M1, M2, A, Z1, Z2, ZB2, ZA1,
&KF, DE, F, RTOL, RESULT1, RESULT2, RESULT3,
&AZ, BZ, AY, BY, AX, BX, PMAX, PMIN, KI, UI, UF, PI, V
      REAL*8 AY1, BY1, FF, MM1, MM2, ZZ1, ZZ2
      INTEGER N1, N2, N3, K1, K2, K3
      EXTERNAL RIJ
      COMMON /YLIMIT/AY1, BY1
      COMMON /ENRG/ FF
      COMMON /MASS1/ MM1
      COMMON /MASS2/ MM2
      COMMON /CH1/ ZZ1
      COMMON /CH2/ ZZ2
      PRINT*, 'ENTER F M1 M2 Z1 Z2'
      READ(*, *) F, M1, M2, Z1, Z2
      FF=F
      MM1=M1
      MM2=M2
      ZZ1=Z1
      ZZ2=Z2
      PI=4.0*ATAN(1.0)
      A=M1/(1.0+M1)
      B=M2/(1.0+M2)
      UI=M1*(M2+1.0)/(1.0+M1+M2)
      UF=M2*(M1+1.0)/(1.0+M1+M2)
      ZB2=Z2*B
      ZA1=Z1*A
      DE=-A*Z1**2+B*Z2**2
      KI=SQRT(UI**2*F*10.0**3/(M1*13.6))
      KF=SQRT(UF*KI**2/UI-UF*DE)
      PMAX=(A*KF+KI)
      PMIN=ABS(A*KF-KI)
      V=KI/UI
99 PRINT*, 'ENTER INTERVAL ENDPOINTS FOR X-INTEGRATION OR
&0 0 TO QUIT'
      READ*, AX, BX
      IF ((AX-BX).NE. 0) THEN
          PRINT*, 'ENTER INTERVAL ENDPOINTS FOR Y-INTEGRATION'
          READ*, AY, BY
          AY1=AY
  
```

```

BY1=BY
PRINT*, 'AY1 BY1',AY1,BY1
PRINT*, 'ENTER INTERVAL ENDPOINTS FOR Z-INTEGRATION'
READ*, AZ, BZ
PRINT*, 'ENTER NUMBER OF POINTS FOR EACH INTEGRAL'
READ*, N1,N2,N3
PRINT*, 'TYPE 2 2 2 FOR SIMPSONS RULE'
PRINT*, 'TYPE 3 3 3 FOR GAUSS RULE'
PRINT*, 'PMAX=',PMAX,' PMIN=',PMIN
READ*,K1,K2,K3
AZ=PMIN
IF (K1.EQ.1) THEN
    PRINT*, 'RIJ(PMIN)=' ,RIJ(PMIN)
ELSE IF (K1.EQ.2) THEN
    RTOL=0.001
    CALL SIMPS3(RIJ,AZ,AZ+1.0,N3,RESLT1)
    CALL SIMPS3(RIJ,AZ+1.0,AZ+2.5,N3,RESLT2)
    CALL SIMPS3(RIJ,AZ+2.5,BZ,N3,RESLT3)
    RESULT=RESLT1+RESLT2+RESLT3
ELSE IF (K1.EQ.2) THEN
    PRINT*, 'NOT AVAILBLE'
ELSE
    PRINT*, 'NOT AVAILBLE'
END IF
C1=-8.0*(SQRT(A*Z2))**5*Z2/SQRT(PI)/A**2
C2=1.0/(2*PI**2*A*V**2)*(UF/UI)
RESULT=C1**2*C2*RESULT
PRINT*, 'FINAL RESUTL=',RESULT
PRINT*, '===== '
GO TO 99
ENDIF
END

```

```

-----
COMPLEX*16 FUNCTION SBR13(X1,K1,P1)
REAL*8 X1,K1,P1
REAL*8 PI,M1,M2,A,B,UI,UF,Z1,Z2,ZB2,ZA1,DE,KI,KF,
+PMAx,PMIN,K,ALFA,P,X,AC,T,TC,F,BC,GC,V
COMPLEX*16 GAMMLN,DELTA,FC,I,NC,Z,II
EXTERNAL GAMMLN
COMMON /ENRG/ F
COMMON /MASS1/ M1
COMMON /MASS2/ M2
COMMON /CH1/ Z1
COMMON /CH2/ Z2
X=X1
K=K1
P=P1
I=(0.0d0,1.0d0)

```

```

II=(1.0d0,0.0d0)
PI=4.0d0*ATAN(1.0d0)
A=M1/(1.0d0+M1)
B=M2/(1.0d0+M2)
UI=M1*(M2+1.0d0)/(1.0d0+M1+M2)
UF=M2*(M1+1.0d0)/(1.0d0+M1+M2)
ZB2=Z2*B
ZA1=Z1*A
DE=-A*Z1**2+B*Z2**2
KI=SQRT(UI**2*F*1.0d3/(M1*13.6d0))
KF=SQRT(UF*KI**2/UI-UF*DE)
PMAX=(A*KF+KI)
PMIN=ABS(A*KF-KI)
V=KI/UI
ALFA=A*Z1/K
AC=B**2*Z2**2+V**2+K**2/A**2-
&K*X/P*(V**2+B*DE+(1.0d0-A*B)/A**2*P**2)
BC=K**2*(X**2-1.0d0)*(1.0d0/P**2*(V**2+B*DE
&)**2+1.0d0/A**4*(1.0d0-A*B)**2*P**2+
&2.0d0*B/A**2*(1.0d0-A*B)*DE-
&2.0d0/A**2*(1.0d0+A*B)*V**2)
GC=AC*(SQRT(AC**2-BC))**(-3)
Z=1.0d0-I*ALFA
NC=EXP((PI/2.0d0*ALFA)+(GAMMLN(Z)))
T=1.0d0/A**2*(K**2+P**2-2d0*P*K*X)
DELTA=P*K*X+I*ZA1*K
TC=ZA1**2+P**2
FC=8.0d0*SQRT(PI)*(SQRT(A*Z1))**3*
&((1.0d0-I*ALFA)*(A*Z1)/TC**2+
&I*ALFA*(A*Z1-I*K)/(TC*(TC-2.0d0*DELTA)))*
&(TC/(TC-2.0d0*DELTA))** (I*ALFA)
SBR13=K**2*NC*GC*FC*1.0d0/T
RETURN
END

```

```

*-----
FUNCTION gammln(xx)
COMPLEX*16 gammln,xx
INTEGER j
DOUBLE PRECISION stp,cof(6)
DOUBLE COMPLEX ser,tmp,x,y
SAVE cof,stp
DATA cof,stp/76.18009172947146d0,-86.50532032941677d0,
&24.01409824083091d0,-1.231739572450155d0,.1208650973866179d-2,
&- .5395239384953d-5,2.5066282746310005d0/
x=xx
y=x
tmp=x+5.5d0
tmp=(x+0.5d0)*log(tmp)-tmp

```

```

        ser=1.000000000190015d0
        do 11 j=1,6
            y=y+1.d0
            ser=ser+cof(j)/y
11      continue
        gammln=tmp+log(stp*ser/x)
        return
        END
*-----
      REAL*8 FUNCTION F(X,Y,Z)
      REAL*8 X,Y,Z
      COMPLEX*16 Z2, SBR13
      Z2=SBR13(X,Y,Z)
      F=DREAL(Z2)
      RETURN
      END
*-----
      REAL*8 FUNCTION F2(X,Y,Z)
      REAL*8 X,Y,Z
      COMPLEX*16 Z2,SBR13
      Z2=SBR13(X,Y,Z)
      F2=DIMAG(Z2)
      RETURN
      END
*-----
      REAL*8 FUNCTION FF(X,K)
      REAL*8 X,K,P,F
      COMMON /PP1/ P
      FF=F(X,K,P)
      RETURN
      END
*-----
      REAL*8 FUNCTION FF2(X,K)
      REAL*8 X,K,P,F2
      COMMON /PP2/ P
      FF2=F2(X,K,P)
      RETURN
      END
*-----
      SUBROUTINE DGAUSS(F,A,B,C,D,EPSX,EPSY,RESULT)
      REAL*8 SUMY,SUMX,A,B,C,D,EPSX,EPSY,
&OSUMX,OSUMY,F,QW(3000),QX(3000),RESULT,
&QWY(3000),QY(3000)
      INTEGER J,I,N,M
      N=0
      OSUMY=-1.D30
33     N=N+1

```

```

SUMY=0.0D0
CALL gauleg(C,D,QY,QWY,2**N*8)
DO 11 J=1,2**N*8
  M=0
  OSUMX=-1.D30
77  M=M+1
  SUMX=0.0D0
  CALL gauleg(A,B,QX,QW,2**M*8)
  DO 22 I=1,2**M*8
    SUMX=SUMX+QW(I)*F(QX(I),QY(J))
22  CONTINUE
  IF ((ABS(SUMX-OSUMX).LT.EPSX*ABS(OSUMX))) GOTO 40
  IF (I.GT.1000) GOTO 50
  OSUMX=SUMX
  GOTO 77
50  PRINT*, 'WARNING : '
  PRINT*, 'FAIL TO REACH THE REQUIRED EPSX FOR '
  PRINT*, 'Y=', QWY(J)
  PRINT*, 'ERROR FOR Y', ABS(SUMX-OSUMX)
  PRINT*, 'SUMX', SUMX, ' OSUMX', OSUMX
  PRINT*, ' '
40  SUMY=SUMY+QWY(J)*SUMX
11  CONTINUE
  PRINT*, 'SUMY', SUMY, ' OSUMY', OSUMY
  IF ((ABS(SUMY-OSUMY).LT.EPSY*ABS(OSUMY))) GOTO 80
  IF (J.GT.2000) GOTO 71
  OSUMY=SUMY
  GOTO 33
71  PRINT*, 'THE PROGRAM FAILS TO REACH THE REQUIRED ACCURACY'
80  PRINT*, 'THE REQUIRED RESULT=', SUMY
  PRINT*, 'FUNCTIONAL EVALUATIONS ARE', J, I
  RESULT=SUMY
  RETURN
  END
-----
SUBROUTINE gauleg(a,b,x,w,n)
  INTEGER n
  REAL*8 x(n),w(n),a,b
  DOUBLE PRECISION EPS
  PARAMETER (EPS=3.d-16)
  INTEGER i,j,m
  DOUBLE PRECISION p1,p2,p3,pp,x1,xm,z,z1
  m=(n+1)/2
  xm=0.5d0*(b+a)
  x1=0.5d0*(b-a)
  do 12 i=1,m
    z=cos(3.14159265358979d0*(i-.25d0)/(n+.5d0))
1  continue

```

```

        p1=1.d0
        p2=0.d0
        do 11 j=1,n
            p3=p2
            p2=p1
            p1=((2.d0*j-1.d0)*z*p2-(j-1.d0)*p3)/j
11      continue
        pp=n*(z*p1-p2)/(z*z-1.d0)
        z1=z
        z=z1-p1/pp
        if(abs(z-z1).gt.EPS)goto 1
        x(i)=xm-x1*z
        x(n+1-i)=xm+x1*z
        w(i)=2.d0*x1/((1.d0-z*z)*pp*pp)
        w(n+1-i)=w(i)
12      continue
        return
        END
-----
        SUBROUTINE SIMPS(F,A,B,RTOL,RESULT)
        REAL F,A,B,RTOL,RESULT,WX,
+OSUMX,HX,SUMX
        INTEGER I,M
        EXTERNAL F
        M=0
        OSUMX=-1.E30
77      M=M+1
        HX=(B-A)/REAL(2**M*20)
        SUMX=0.0
        DO 22 I=0,2**M*20
            WX=4.0
            IF (MOD(I,2).EQ.0) WX=2.0
            IF (I.EQ.0.OR.I.EQ.2**M*20) WX=1.0
            SUMX=SUMX+HX*WX*F(A+HX*I)
22      CONTINUE
        SUMX=SUMX/3.0
        IF ((ABS(SUMX-OSUMX).LT.RTOL*ABS(OSUMX))) GOTO 40
        IF (I.GT.20) GOTO 50
        OSUMX=SUMX
        PRINT*, 'SUM-P', SUMX
        GOTO 77
50      PRINT*, 'WARNING :'
        PRINT*, 'FAIL TO REACH THE REQUIRED EPSX '
        PRINT*, 'ERROR FOR P-INT.', ABS(SUMX-OSUMX)
40      RESULT=SUMX
        RETURN
        END
-----

```

```

SUBROUTINE SIMPS3(F,A,B,M,RESULT)
REAL F,A,B,RESULT,WX,
+HX,SUMX
INTEGER I,M
HX=(B-A)/REAL(M)
SUMX=0.0
DO 22 I=0,M
  WX=4.0
  IF (MOD(I,2).EQ.0) WX=2.0
  IF (I.EQ.0.OR.I.EQ.M) WX=1.0
  SUMX=SUMX+HX*WX*F(A+HX*I)
22 CONTINUE
RESULT=SUMX/3.0
RETURN
END

*-----
REAL*8 FUNCTION U(P)
REAL*8 P,D1,FF,AY,BY,RESULT,RESULT1,RESULT2
EXTERNAL FF
COMMON /PP1/D1
COMMON /YLIMIT/AY,BY
D1=P
CALL DGAUSS(FF,-1.0D0,1.0D0,AY,5.0D0,0.00001D0,0.0001D0,RESULT1)
CALL DGAUSS(FF,-1.0D0,1.0D0,5.0D0,BY,0.00001D0,0.0001D0,RESULT2)
RESULT=RESULT1+RESULT2
U=RESULT
PRINT*, 'FF RESULT=',RESULT
RETURN
END

*-----
REAL*8 FUNCTION U2(P)
REAL*8 P,D2,FF2,AY,BY,RESULT,RESULT1,RESULT2
EXTERNAL FF2
COMMON /PP2/D2
COMMON /YLIMIT/AY,BY
D2=P
CALL DGAUSS(FF2,-1.0D0,1.0D0,AY,5.0D0,0.0001D0,0.001D0,RESULT1)
CALL DGAUSS(FF2,-1.0D0,1.0D0,5.0D0,BY,0.0001D0,0.001D0,RESULT2)
RESULT=RESULT1+RESULT2
U2=RESULT
PRINT*, 'FF2 RESULT=',RESULT
RETURN
END

*-----
REAL FUNCTION RIJ(PM)
REAL*8 P,U,U2
REAL PM
EXTERNAL U,U2

```

```
P=PM
RIJ=(U(P)**2+U2(P)**2)*P
PRINT*, 'P=', PM, ' RIJ=', RIJ
PRINT*, '-----'
RETURN
END
```

Program 4  
(Mathematica Notebook)

In[1]:=

T1[U\_]:=F1[U] F2[U] F3[U]^(I V)

In[2]:=

T2[U\_]:=1/U D[T1[U],U];

In[3]:=

T3[U\_]:=1/U D[T2[U],U];

In[4]:=

T3[U]/.F1[U]->F1/.F2[U]->F2/.F3[U]->F3/.  
 Derivative[1][F1][U]->DF1/.  
 Derivative[1][F2][U]->DF2/.  
 Derivative[1][F3][U]->DF3/.  
 Derivative[2][F1][U]->DDF1/.  
 Derivative[2][F2][U]->DDF2/.  
 Derivative[2][F3][U]->DDF3

Out[4]=

$$\left( - \frac{DF2 F1 F3^{I V} + DF1 F2 F3^{I V} + I DF3 F1 F2 F3^{-1 + I V}}{U^2} + \right. \\
 \left. (2 DF1 DF2 F3^{I V} + DDF2 F1 F3^{I V} + DDF1 F2 F3^{I V} + \right. \\
 \left. 2 I DF2 DF3 F1 F3^{-1 + I V} V + 2 I DF1 DF3 F2 F3^{-1 + I V} V + \right. \\
 \left. I DDF3 F1 F2 F3^{-1 + I V} V + I DF3^2 F1 F2 F3^{-2 + I V} V + (-1 + I V) V \right) / U / U$$

In[5]:=

```
FortranForm[T3[U]/.F1[U]->F1/.F2[U]->F2/.F3[U]->F3/.
Derivative[1][F1][U]->DF1/.
Derivative[1][F2][U]->DF2/.
Derivative[1][F3][U]->DF3/.
Derivative[2][F1][U]->DDF1/.
Derivative[2][F2][U]->DDF2/.
Derivative[2][F3][U]->DDF3]
```

Out[5]//FortranForm=

```
(-((DF2*F1*F3**((0,1)*V) + DF1*F2*F3**((0,1)*V) +
- (0,1)*DF3*F1*F2*F3**(-1 + (0,1)*V)*V)/U**2) +
- (2*DF1*DF2*F3**((0,1)*V) + DDF2*F1*F3**((0,1)*V) +
- DDF1*F2*F3**((0,1)*V) +
- (0,2)*DF2*DF3*F1*F3**(-1 + (0,1)*V)*V +
- (0,2)*DF1*DF3*F2*F3**(-1 + (0,1)*V)*V +
- (0,1)*DDF3*F1*F2*F3**(-1 + (0,1)*V)*V +
- (0,1)*DF3**2*F1*F2*F3**(-2 + (0,1)*V)*(-1 + (0,1)*V)*V)/U
- )/U
```

In[6]:=

```
F1[U_] := (Z2 (1.0-X)/U-1.0)
```

In[7]:=

```
FortranForm[F1[U]]
```

Out[7]//FortranForm=

```
-1. + (1. - X)*Z2/U
```

In[8]:=

```
F2[U_] := (U^2+W2)^-1
```

In[9]:=

```
FortranForm[F2[U]]
```

Out[9]//FortranForm=

```
1/(U**2 + W2)
```

In[10]:=

```
F3[U_] := (C[U]-J 2.0 U KI)/(U^2+W2)
```

In[11]:=

```
FortranForm[F3[U]]
```

Out[11]//FortranForm=

```
(-2.*J*KI*U + C(U))/(U**2 + W2)
```

In[12]:=

Derivative[1][F1][U]

Out[12]=

$$-\left(\frac{(1. - X) Z^2}{U^2}\right)$$

In[13]:=

FortranForm[Derivative[1][F1][U]]

Out[13]//FortranForm=

$$-((1. - X)*Z^2/U**2)$$

In[14]:=

Derivative[1][F2][U]

Out[14]=

$$\frac{-2 U}{(U^2 + W^2)}$$

In[15]:=

FortranForm[Derivative[1][F2][U]]

Out[15]//FortranForm=

$$-2*U/(U**2 + W^2)**2$$

In[16]:=

Derivative[1][F3][U]/.  
Derivative[1][C][U]->DC/.  
C[U]->C

Out[16]=

$$\frac{-2 U (C - 2. J K I U)}{(U^2 + W^2)} + \frac{DC - 2. J K I}{U^2 + W^2}$$

In[17]:=

FortranForm[Derivative[1][F3][U]/.  
Derivative[1][C][U]->DC/.  
C[U]->C]

Out[17]//FortranForm=

$$-2*U*(C - 2.*J*KI*U)/(U**2 + W^2)**2 + (DC - 2.*J*KI)/(U**2 + W^2)$$

In[18]:=

Derivative[2][F1][U]

Out[18]=

$$\frac{2 (1. - X) Z^2}{U^3}$$

In[19]:=

FortranForm[Derivative[2][F1][U]]

Out[19]//FortranForm=

2\*(1. - X)\*Z2/U\*\*3

In[20]:=

Derivative[2][F2][U]

Out[20]=

$$\frac{8 U^2}{(U^2 + W^2)^3} - \frac{2}{(U^2 + W^2)^2}$$

In[21]:=

FortranForm[Derivative[2][F2][U]]

Out[21]//FortranForm=

8\*U\*\*2/(U\*\*2 + W2)\*\*3 - 2/(U\*\*2 + W2)\*\*2

In[22]:=

Derivative[2][F3][U]/.

Derivative[1][C][U]->DC/.

C[U]->C/.Derivative[2][C][U]->DDC

Out[22]=

$$\frac{8 U^2 (C - 2. J K I U)}{(U^2 + W^2)^3} - \frac{4 (DC - 2. J K I) U}{(U^2 + W^2)^2} - \frac{2 (C - 2. J K I U)}{(U^2 + W^2)^2} + \frac{DDC}{U^2 + W^2}$$

In[23]:=

```
FortranForm[Derivative[2][F3][U]/.
Derivative[1][C][U]->DC/.
C[U]->C/.Derivative[2][C][U]->DDC]
```

Out[23]//FortranForm=

```
8*U**2*(C - 2.*J*KI*U)/(U**2 + W2)**3 -
- 4*(DC - 2.*J*KI)*U/(U**2 + W2)**2 -
- 2*(C - 2.*J*KI*U)/(U**2 + W2)**2 + DDC/(U**2 + W2)
```

In[24]:=

```
T1[U_]:= (Z2 (1.0-X)/U-1.0) ((C[U]-J 2.0 U KI)/
(U^2+W2))^(I V) (U^2+W2)^-1;
```

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