EVALUATION OF ABSORPTION CROSS-SECTION FOR THE PHOTOIONIZATION OF ALKALI ATOMS
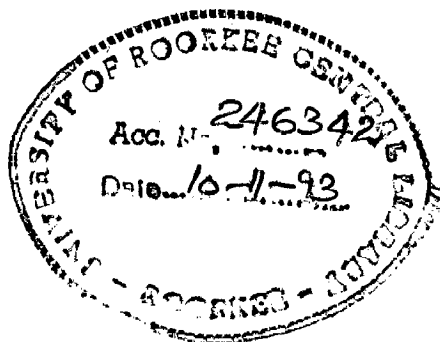
A DISSERTATION

submitted in partial fulfilment of the
requirements for the award of the degree
of
MASTER OF PHILOSOPHY
in
COMPUTER APPLICATIONS

By

ANSUYA CHAUHAN

DEPARTMENT OF MATHEMATICS
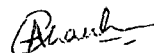UNIVERSITY OF ROORKEE
ROORKEE-247667 (INDIA)

NOVEMBER, 1990

DEDICATED
TO
MY PARENTS
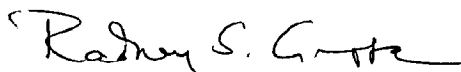
CANDIDATE'S DECLARATION

I hereby certify that the work which is being presented in the dissertation entitled **"EVALUATION OF ABSORPTION CROSS-SECTION FOR THE PHOTOIONIZATION OF ALKALI ATOMS"**, in partial fulfilment of the requirement for the award of the degree of "Master of Philosophy in Computer Applications" submitted in the Department of Mathematics of the University of Roorkee, is an authentic record of my our work carried out during a period from January 1990 to November 1990, under the supervisions of Dr. K.C. Mathur, Professor, Department of Physics and Dr. R.S. Gupta, Professor, Department of Mathematics, University of Roorkee, Roorkee.

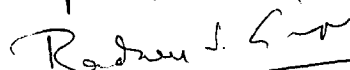The matter embodied in this thesis has not been submitted by me for the award of any other degree.

(ANSUYA CHAUHAN)

This is to certify that the above statement made by the candidate is correct to the best of our knowledge.

(Dr. R.S. Gupta)

(Dr. K.C. Mathur)

forwarded

Professor & Head
Department of Mathematics
University of Roorkee, Roorkee.

ACKNOWLEDGEMENTS

Dated: 17-11-90

(ANSUYA CHAUHAN)

ABSTRACT

The photoionization cross section of lithium atom for the ground (2s) and excited (2p) states have been calculated using the Dipole approximation for the radiation matter interaction. Computer prgramms have been developed and results are presented for the phase shifts, cross sections and the asymmetry parameter. Comparison of the results with other calculation is also presented.

CONTENTS

CHAPTER - I

INTRODUCTION

Atomic collisions is an integral part of quantum mechanics. Quantum mechanics is the mechanics applied to microworld. An atom and its constituents, being relatively quite minute, require more than a microscope for a clear picture. We therefore apply external force to unsettle the atom and thus by observing the consequences of such an action we can predict the behaviour and structure concerning the atom in matter. This external force may be in the form of electron or proton having considerable energy. We thus are considering the collision of microparticle with a microparticle.

Electromagnetic field is also a major contributor towards this external force. A complete picture of interaction of light and microparticle arises only after the consideration of creation and annihilation of electromagnetic fields. But the contribution of Einstein simplifies the matter. Now the behaviour of a quntum system in a given electromagnetic field can be taken as a mechanical problem. Thus the probability of the collision reaction can be evaluated in terms of the theory of quantum transitions.

The external force either makes the atom lose some of its energy or gain some energy. When, this change of energy, only changes the internal quantum state then

<u>inelastic scattering</u> is said to have-occurred. But when the particles themselves are transformed, then <u>reaction</u> is said to have occurred. Also, there are reactions is which there is no change of energy or internal structure and particles are only scattered, these are grouped under the heading of <u>elastic scattering</u>.

Here we have taken <u>lithium</u> for our study. We consider the reaction in which photon strikes the lithium atom and consequently an electron is liberated leaving only lithium ion. Experimentally such a reaction i.e. one to one collision is achieved only after applying suitable conditions. The light beam must be well collimated and nearly monoenergetic. To observe a reasonable number of events, the incident beam should be neither too intense so as to neglect the interaction between the incident particles, nor too weak. Moreover, a single lithium atom is difficult to obtain and always there will be quite many atoms even in a small sample. To overcome such a possibility the de Broglie wavelength of the incident particles is taken quite small with respect to the distances between the lithium atom or scatterers. The enables us to neglect coherence effects between the waves scattered by each of the scattering centers. Also, the target sample is made sufficiently thin so that multiple scattering by several structures can be neglected.

On applying the quantum theory of transitions, we are able to predict the nature of the above reaction. One of the important parameter this theory gives is the absorption cross section which predicts the probability of the reaction. Besides predicting upon the reaction this parameter gives important insights of what is inside the atom. For example total cross-section indirectly gives the value of total angular momentum, J, of the atom. But the matter presented in this dissertation deals only with the calculation of the absorption cross section of the above reaction. Additionally, the asymmetry parameter is also calculated.

This dissertation is divided into four chapters. First chapter is of introductory type. Second chapter explains the theory involved and 3rd chapter explains the numerical methods used. Finally the 4th chapter gives the results. The computer programs are attached in the end in Appendix.

CHAPTER - II

THEORETICAL CONSIDERATIONS

2.1 General Introduction

When the perturbation depends on time, the exact solution of the Schrodinger equation becomes impossible to obtain. To overcome this difficulty, one of the methods is to assume that the time-dependent part of the Hamiltonian is quite small compared to the stationary part. In such a siuation one can apply perturbation techniques[1].

The time-dependent perturbation theory thus concerns with a Hamiltonian which depends on time. We divide the Hamiltonian into stationary part, i.e. H_O and time dependent part, i.e. H', so that

$$H = H_O + H' \qquad \qquad \cdots \ (2.1)$$

and

$$H_O u_n = E_n u_n \qquad \qquad \cdots \ (2.2)$$

Where u_n are the stationary state normalized eigenfunctions and E_n, the energy eigen values:

The time-dependent Schrodinger equation is

$$i\hbar \ \frac{\partial \psi}{\partial t} = H \psi \qquad \qquad \cdots \ (2.3)$$

Expanding ψ as

$$\psi = \sum_n a_n(t) \ u_n \ e^{-i.E_n t/\hbar} \qquad \qquad \cdots \ (2.4)$$

Where $a_n(t)$ are the expansion coefficients, we arrive at the transition probabilities per unit time, ω, for

ionization to a final state,

$$\omega = \frac{2\pi}{\hbar} \rho(k) \left| H'_{Km} \right|^2 \qquad \qquad \ldots (2.5)$$

where $\rho(k)$ is the density of final states and

$$H'_{Km} = \int u_K H'_{um} d\tau \quad , \text{ the matrix element.}$$

2.2   Interaction of radiation with atoms

The Hamiltonian of the atomic electron, having charge (-e) and mass μ, in an electromagnetic field is given as,

$$H = \frac{1}{2\mu} (\vec{p} + \frac{e}{c} \vec{A})^2 - e\phi \qquad \qquad \ldots (2.6)$$

In the coordinate representation this becomes,

$$H = \frac{\vec{p}^2}{2\mu} - e\phi + \frac{e}{\mu c} \vec{A} \frac{\hbar}{i} (\vec{\nabla} . \vec{A}) + \frac{e^2}{2\mu c^2} \vec{A}^2 \qquad ..(2.7)$$

ϕ is the scalar potential and $\vec{A}$ the vector potential.

For a plane electromganetic wave, it is always possible to make the scalar potential zero with a suitable choice of gauge. So we consider only vector potential $\vec{A}$.

We shall apply this Hamiltonian only under the conditions that allow the $\vec{A}^2$ term to be neglected.

Further simplifications are possible with the help of

$$\vec{\nabla}^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = 0 \qquad \qquad \ldots (2.8)$$

$$\phi = 0 \text{ and } \quad \vec{\nabla} . \vec{A} = 0 \qquad \qquad \ldots (2.9)$$

Thus the complete Hamiltonian simplifies to

$$H = \frac{\vec{p}^2}{2\mu} + V_O + \frac{e}{\mu c} \vec{A} . \vec{p} \qquad \qquad ...(2.10)$$

The stationary part H_O and the perturbation part H' make up this Hamiltonian as

$$H = H_O + H' \qquad \qquad ...(2.11)$$

where $\qquad H_O = \dfrac{\vec{p}^2}{2\mu} + V_O \qquad \qquad ...(2.12)$

and $\qquad H' = \dfrac{e}{\mu c} \vec{A} . \vec{p} \qquad \qquad ...(2.13)$

In the electric field gauge the interaction term can be written as

$$H' = e E_O (\hat{\epsilon} . \vec{r}) \qquad \qquad ...(2.14)$$

Where E_O is the amplitude of the electric field and $\hat{\epsilon}$ gives the direction of polarization of light.

Thus the transition matrix is

$$H'_{Km} = \int u_K^* (e E_O \hat{\epsilon} . \vec{r}) u_m d\tau$$

$$= e E_O \int u_K^* (\hat{\epsilon} . \vec{r}) u_m d\tau \qquad \qquad ...(2.15)$$

The differential cross section $\sigma (\theta, \emptyset) \sin \theta d\theta d\emptyset$ for photoionization is equal to ω divided by the incident flux, F, of photons. This flux is obtained by dividing the incident intensity by $w\hbar$.

So $\sigma^-(\theta,\emptyset)\sin\theta d\theta d\emptyset = \dfrac{\omega}{F}$

Using eqn. (2.5) and (2.15) this is obtained as

$$\sigma(\theta,\emptyset)\sin\theta d\theta d\emptyset = \frac{2\pi}{\hbar}\, \rho(k)\, \frac{e^2 E_o^2}{F}|<K|\hat{\epsilon}.\,\vec{r}^>|m>|^2$$

Thus density of final states, $\rho(k)$, is given as

$$\rho(k) = (\frac{\mu L^3}{8\pi^3\hbar^2}\,k)\sin\theta d\theta d\emptyset \qquad\qquad ...(2.16)$$

where L^3 = volume of an arbitrarily large but finite cubical box.

Thus, the differential cross section becomes,

$$\sigma^-(\theta,\emptyset)\sin\theta d\theta d\emptyset = \frac{2\pi}{\hbar}(\frac{\mu L^3 k}{8\pi^3\hbar^2})\,\frac{e^2 E_o^2}{F}|<k|\hat{\epsilon}.\vec{r}^>|m>|^2\sin\theta d\theta d\emptyset$$

$$= \frac{2\pi}{\hbar}(\frac{\mu L^3 k}{8\pi^3\hbar^2})(\frac{e^2\hbar\,2\pi W}{c})|<k|\hat{\epsilon}.\vec{r}^>|m>|^2 ..(2.17)$$

Now we attempt to find out the total cross section for reactions which involve excitation of lithium from initial ground and excited states to continuum state. We therefore study the following process,

$$h\nu + A\ (or\ A^*) \rightarrow e^- + A^+ \qquad\qquad ...(2.18)$$

Where A denotes the lithium atom in initial ground state and A^* in excited state.

2.3   Evaluation of cross section using linearly polarized light

For linearly polarized light, we have

ejected electron lying in continuum.

Also $\psi_K (r_c, r_3) = R_{1s}^{Li^+} (r_c) \, Y_{oo}(\hat{r}_c) \, \psi_K(\vec{r}_3^{>})$ ... (2.21)

$R^{Li^+} (r_c)$ is the radial wave function of lithium ion.

Expanding $\psi_K (\vec{r}_3^{>})$ in partial waves,

$$\psi_K(\vec{r}_3^{>}) = 4\pi \sum_{l=0} \sum_{m} \frac{U_l (kr_3)}{(Kr_3)} \, e^{i(\delta_{l'} + \sigma_{l'})} \, i^{l'}$$

$$x \, Y_{l'm'} (\hat{R}) \, Y_{l'm'} (\hat{r}_3) \qquad \qquad ... (2.22)$$

The wavefunction $U_{l'} (kr_3)$ satisfies the differential equation[21].

$$[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 - 2V(r)] \, U_{l'} (kr) = 0 \qquad ...(2.23)$$

Where l is the orbital angular momentum, k is the momentum vector V(r) is the potential seen by the ejected electron.

$\sigma_{l'}$ is the phase shift due to the pure coulomb potential. $\delta_{l'}$ is phase shift in the modified coulomb field.

The boundary conditions of the above differential equation are given by

$$U_{l'} (kr) \rightarrow 0 \qquad \qquad ... (2.24)$$
$$r \rightarrow 0$$

and $U_{1'}(kr) \rightarrow A_{1'} F_{1'}(kr) + B_{1'} G_{1'}(kr)$ ... (2.25)

$\qquad r \rightarrow \infty$

Where $F_{1'}(kr)$ and $G_{1'}(kr)$ are the regular and irregular solutions of the equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{1(1+1)}{r^2} - \frac{2 \nu k}{r} \right] U_{1'}(kr) = 0 \qquad ... (2.26)$$

$$\text{where} \quad = \frac{m\, z_1 z_2 e^2}{\hbar^2 k}$$

(when we are considering two particles having electric charges $z_1 e$ and $z_2 e$ respectively)

Thus

$$\psi_K = R_{1s}^{Li^+}(r_c)\, Y_{oo}(r_c) \times 4\pi \sum_{1'} \sum_{m'} \frac{U_{1'}(kr_3)}{(kr_3)}$$

$$\times\, e^{i(\delta_{1'} + \sigma_{1'})} \times i^{1'} \times Y_{1'm}^{*}(\hat{k})\, Y_{1'm}(\hat{r}_3) \quad ...(2.27)$$

So eq. (2.20) takes the form

$$\langle k | \hat{e}.\vec{r}_3 | m \rangle = 4\pi \sqrt{\frac{4\pi}{3}} \sum_{1'} \sum_{m'} (-i)^{1'}\, e^{-i(\delta_{1'} + \sigma_{1'})} Y_{1'm'}(\hat{k})$$

$$\times \int R_{1s}^{Li^{+*}}(r_c)\, \frac{U_{1'}^{*}(kr_3)}{(kr_3)} . r_3 . R_{1s}^{Li}(r_c)\, R_{2p}^{Li}(r_3)$$

$$\times\, r_3^2\, dr_c dr_3 \times \int Y_{oo}^{*}(\hat{r}_c)\, Y_{oo}(\hat{r}_c)\, d\hat{r}_c$$

$$\times \int Y_{1'm'}^{*}(\hat{r}_3)\, Y_{10}(\hat{r}_3)\, Y_{oo}(\hat{r}_3)\, dr_3$$

DEPARTMENT OF MATHEMATICS
UNIVERSITY OF ROORKEE
ROORKEE

No.M/SR-6 / 80? /90   Dated: **Nov.17, 1990**

A.R.(EXAMS.)

        Enclosed please find herewith 3 copies of dissertation
entitled" **EVALUATION OF ABSORPTION CROSS-SECTION FOR THE PHOTOIONIZATION**
OF ALKALI ATOMS   " submitted by **Ms. Ansuya Chauhan**
(a student of the session 1989-90) in partial fulfilment of the
requirements for the degree of M.Phil.(Computer Applications).

The Title of the Dissertation has been changed from "Photoionization of
Atms Atoms to "EVALUATION OF ABSORPTION CROSS-SECTION FOR THE PHOTOIONI-
ZATION OF ALKALI ATOMS."

Encl.: As above.

                                Prof. & Head
                                Maths Deptt.

Copy to:

1. Course Coordinator, M.Phil.(C.A.) with a copy of dissertation
   with a request to circulate it amongst other members of Viva-Voce
   Examination Committee, alongwith one copy of dissertation.

2. Supervisor with a request to fix Viva-Voce Examination in
   consultation with Chairman Viva-Voce Examination and Course-
   Coordinator, alongwith one copy of dissertation.

3. Chairman Viva-Voce examination with request to issue notification
   for the Viva-Voce Examination.

                                Prof. & Head
                                Maths Deptt.

No.Maths/SR-~ / 809 /90   Dated: Nov.17, 1990

NOTICE

The Viva-Voce Examination on the dissertation of

Mr./Ms. ANSUYA CHAUHAN a student of M.Phil.(Computer

Application/Maths) for the session 1989-90 will be held as per

detail given below:

    1. TITLE OF DISSERTATION: EVALUATION OF ABSORPTION CROSS-SECTION

                                  FOR THE PHOTOIONIZATION OF ALKALI ATOMS

    2. VENUE   :   Departmental Library

    3. TIME AND DATE   :   3.00 P.M. on Nov.19, 1990

All interested are cordially invited to attend.

Chairman
Viva Committee

CC:
    1. Head of Maths Deptt.
    2. Course Coordinator   Reader Dr.Dani Singh
    3. Member A.P.C.(P & R)   Dr.R.C.Mittal
    4. External Examiner   Dr.R.C.Mittal,Director,CSIC

    5. Supervisor(s)   Dr.R.C.Mathur,Phys.Deptt.
                      Dr.R.S.Gupta,Maths.Deptt.

    6. J.C. Maintenance Library
    7. A.R.Exam.

Chairman
Viva Committee

we know , $Y_{00}(\hat{r}_3) = \dfrac{1}{\sqrt{4\pi}}$

and $\displaystyle\int Y_{1'm'}^{*}(\hat{r}_3)\, Y_{10}(\hat{r}_3)\, d\hat{r}_3 = 1$

$\therefore\quad 1' = 1,\ m' = 0$

$$\langle k|\hat{e}.\vec{r}_3|m\rangle = 4\pi\sqrt{\frac{4\pi}{3}}\,(-i)\,e^{-i(\delta_1 + \sigma_1)}\,Y_{10}(\hat{k})$$

$$\times \frac{1}{\sqrt{4\pi}} \times \int R_{1s}^{Li^{+*}}(r_c)\,\frac{U_1^{*}(kr_3)}{(k)}\,R_{1s}^{Li}(r_c)\,R_{2p}^{Li}(r_3)\,r_3^2 dr_c dr_3$$

$$= \frac{4\pi}{\sqrt{3}}\,(-i)\,e^{-i(\delta_1 + \sigma_1)}\,Y_{10}(\hat{k}) \times I_1$$

where $I_1 = \displaystyle\int R_{1s}^{Li^{+*}}(r_c)\,\frac{U_1^{*}(kr_3)}{k}\,R_{1s}^{Li}(r_c)\,R_{2s}^{Li}(r_3)$

$$\times\ r_3^2\, dr_c\, dr_3$$

we need $|\langle k|\hat{e}.\vec{r}_3|m\rangle|^2$, so

$$|\langle k|\vec{e}.\vec{r}_3|m\rangle|^2 = \frac{16\pi^2}{3}\,Y_{10}(\hat{k})\,Y_{10}^{*}(\hat{k})\,I_1^2$$

Therefore from eqn. (2.17),

$$\sigma(\theta,\emptyset)\sin\theta d\theta d\emptyset = \frac{2\pi}{\hbar}\left(\frac{\mu L^3 k}{8\pi^3\hbar^2}\right) \times \frac{16\pi^2}{3} \times I_1^2 \times \left(\frac{e^2\hbar.2\pi w)}{c}\right)$$

$$x \ Y_{10}(\hat{k}) \ Y^{*}_{10} \ (\hat{k}) \ \sin\theta d\theta d\emptyset$$

On integrating both the sides, we get

$$\sigma \ = \ \sigma \ (\theta,\emptyset)\sin\theta d\theta d\emptyset$$

Also, $\int Y^{*}_{1m} (\hat{k}) \ Y_{1m} (\hat{k}) \ \sin\theta_k d\theta_k d\emptyset_k = 1$

$$\sigma \ = \ \frac{2\pi}{\hbar} \ (\frac{\mu L^3 k}{8 \pi^3 \hbar^2}) \ (\frac{e^2 \hbar w \cdot 2\pi}{c}) \ \times \ \frac{16\pi^2}{3} \ \times \ r^2_1$$

$$= \ \frac{16}{3} \cdot \frac{\pi \mu L^3 k w e^2}{\hbar^2 c} \ \ r^2_1$$

$$= \ \frac{16}{3} \ k \ \alpha \ \pi \ \times \ \frac{1}{2} \ (k^2 + 2I_p) \ (\text{Since } \mu=1, \ \hbar=1,$$
$$= \frac{e^2}{\hbar c} \ , \ L\text{->}1)$$

$$= \ \frac{4}{3} \ \pi \ \alpha \ k \ (k^2 + 2 \ I_p)$$

Where I_p = ionization potential

$$e^{Li+}_{1s} \ - \ e^{Li}_{2s} \qquad\qquad \dots (2.29)$$

2.3.2 Photoionization of the 2p state of lithium

For 2p state, the orbital angular momentum $l=1$ and the magnetic quantum number $m_m=0$, $1,-1$. Let the cross

sections corresponding to m=0,1,-1 be represented by σ_m ($\sigma_0, \sigma_1, \sigma_{-1}$). We evalutate them one by one.

The wavefunction for lithium atom in the $2p_{m_m}$ state

$$\psi_m = U_{1s}^{li} (\vec{r}_c) \, U_{2p_{m_m}}^{Li} (\vec{r}_3)$$

$$= R_{1s}^{Li} (r_c) \, Y_{oo}(\hat{r}_c) \, R_{2p}^{Li} (r_3) \, Y_{m_m}^{'} (\hat{r}_3) \quad \ldots \ (2.30)$$

Where $U_{2p_m}^{Li} (\vec{r}_3)$ and $R_{2p}^{Li} (r_3)$ are the complete and radial wavefunction of the valence electron. $Y_{1m_m} (\hat{r}_3)$ is the spherical harmonics of the valence electron.

For lithium ion-electron, system, the wavefunction is

$$\psi_k = U_{1s}^{Li} (\vec{r}_c) \, \psi_n (\vec{r}_3)$$

$$= R_{1s}^{Li+}(r_c) \, Y_{oo}(\hat{r}_c) \times 4\pi \sum_{l'} \sum_{m'} \frac{U_{l'}(kr_3)}{(kr_3)} e^{i(\delta_{l'} + \sigma_{l'})}$$

$$\times \ i^{l'} \times Y_{l'm'}^{*} (\hat{k}) \, Y_{l'm'}(\hat{r}_3) \qquad \ldots \ (2.31)$$

$$\langle k | \hat{e}.\vec{r}_3 | m \rangle = 4\pi \sqrt{\frac{4\pi}{3}} \sum_{l'} \sum_{m'} (-i)^{l'} e^{-i(\delta_{l'} + \sigma_{l'})}$$

$$\times \ Y_{l'm'} (\hat{k}) \times \int R_{1s}^{Li+*}(r_c) \frac{U_{l'}^{*}(kr_3)}{(kr_3)} r_3$$

$$R_{1s}^{Li} (r_c) \, R_{2p_m} U(r_3) \times r_3^2 \, dr_c dr_3$$

$$x \quad \int Y^*_{00} (\hat{r}_c) \, Y_{00}(\hat{r}_c) \, d\hat{r}_c$$

$$x \quad \int Y_{1'm'}^{*} (\hat{r}_3) \, Y_{10}(\hat{r}_3) \, Y_{1m} (\hat{r}_3) \, d\hat{r}_3 \qquad \dots (2.32)$$

Now $\quad \int Y_{1'm'}^{*} (\hat{r}_3) \, Y_{10}(\hat{r}_3) \, Y_{1m}(\hat{r}_3) \, dr_3 = \sqrt{\dfrac{(3)(3)}{4\pi(21'+1)}}$

$$C^{11\,1'}_{mom'} \quad C^{11\,1'}_{000} \qquad \dots (2.33)$$

Evaluation of σ_0

For σ_0, l' can be either 0 or 2. And $m' = 0$ is possible whether $l' = 0$ or 2. So $l' = 0$, $m' = 0$ and $l' = 2$, $m' = 0$.

And $\quad \int Y^*_{00} (\hat{r}_c) \, Y_{00}(\hat{r}_c) \, dr_c = 1$

$$\langle k | \hat{e} \cdot \vec{r}_3 | m \rangle = 4\pi \sqrt{\frac{4\pi}{3}} \, [\,(-i)^0 e^{-i(\vartheta_0 + \sigma_0)} x \, Y_{00}(\hat{k})$$

$$x \quad \int R^{Li+*}_{1s} (r_c) \, \frac{U^*_0 (kr_3)}{k} \, R^{Li}_{1s} (r_c) R^{Li}_{2p}(r_3) r_3^2 dr_c dr_3$$

$$x \sqrt{\frac{3\times3}{4\pi(1)}} \, C^{110}_{000} \quad C^{110}_{000}$$

$$+ (-i)^2 \, e^{-i(\vartheta_2 + \sigma_2)} \, Y_{20}(\hat{k})$$

$$x \int R_{1s}^{Li*}(r_c) \frac{U_2^*(kr_3)}{k} R_{1s}^{Li}(r_c) R_{2p}^{Li}(r_3) r_3^2 dr_c dr_3$$

$$x \sqrt{\frac{9}{4\pi(5)}} \quad C_{000}^{112} \quad C_{000}^{112}$$

$$\langle k | \hat{e}.\vec{r}_3 | m \rangle =$$

$$= \frac{4\pi}{3} I_0 e^{-i(\delta_0 + \sigma_0)} Y_{00}(\hat{k}) + \frac{8\pi}{\sqrt{3}\sqrt{5}} (-i)^2 I_2$$

$$x \quad e^{-i(\delta_2 + \sigma_2)} Y_{20}(\hat{k})$$

where

$$I_0 = \int R_{1s}^{Li+*}(r_c) \frac{U_0^*(kr_3)}{(k)} R_{1s}^{Li}(r_c) R_{2p}^{Li}(r_3) r_3^2 dr_c dr_3$$

$$= \int R_{1s}^{Li+*}(r_c) R_{1s}^{Li}(r_c) dr_c * \int \frac{U_0^*(kr_3)}{k} R_{2p}^{Li}(r_3)$$

$$r_3^2 dr_3 \qquad \qquad \ldots(2.34)$$

and

$$I_2 = \int R_{1s}^{li+*}(r_c) \frac{U_2^*(kr_3)}{(k)} R_{1s}^{Li}(r_c) R_{2p}^{Li}(r_3) x \, r_3^2 dr_2 dr_3$$

$$= \int R_{1s}^{li+*}(r_c) R_{1s}^{Li}(r_c) dr_c x \int \frac{U_2^*(kr_3)}{k}$$

$$R_{2p}^{li}(r_3) r_3^2 dr_3 \qquad \qquad \ldots(2.35)$$

Now

$$|\langle k | \hat{e}.\vec{r}_3 | m \rangle|^2 =$$

$$= \frac{16\pi^2}{3} I_0^2 Y_{00}^*(\hat{k}) Y_{00}(\hat{k}) + \frac{64\pi^2}{15} I_2^2 Y_{20}^*(\hat{k}) Y_{20}(\hat{k})$$

$$- \left(\frac{4\pi}{\sqrt{3}}\right) \left(\frac{8\pi}{\sqrt{15}}\right) \times 2 \, I_0 I_2 \cos \triangle \eta \quad Y_{00}^*(\hat{k}) \, Y_{20}(\hat{k})$$

where $\cos \triangle \eta = \delta_0 + \sigma_0 - (\delta_2 + \sigma_2)$ ...(2.36)

Therefore from eqn. (2.10), we have

$$\sigma_0(\theta,\emptyset) \sin\theta d\theta d\emptyset = \frac{2\pi}{h} \left(\frac{\mu L^3 k}{8 \pi^3 \hbar^2}\right) \left(\frac{e^2 \hbar w. 2\pi}{c}\right)$$

$$\times \left[\frac{16\pi^2}{3} \, I_0^2 \, Y_{00}^*(\hat{k}) \, Y_{00}(\hat{k})\right.$$

$$+ \frac{64}{15} \pi^2 \, I_2^2 \, Y_{20}^*(\hat{k}) \, Y_{20}(\hat{k})$$

$$\left. - \cos\triangle\eta \, \frac{64\pi^2}{3\sqrt{5}} \, I_0 I_2 \, Y_{00}^*(\hat{k}) \, Y_{20}(\hat{k})\right]$$

$$\times \sin\theta d\theta d\emptyset \qquad\qquad ... (2.37)$$

$$\sigma_0 = \int \sigma_0(\theta,\emptyset) \sin\theta d\theta d\emptyset$$

$$= \frac{2\pi}{\hbar} \left(\frac{\mu L^3 k}{8\pi^3 \hbar^2}\right) \left(\frac{e^2 \hbar w 2\pi}{c}\right) \left[\frac{16\pi^2}{3} I_0^2 \int Y_{00}^*(\hat{k})\right.$$

$$Y_{00}(\hat{k}) \sin\theta_k d\theta_k d\emptyset_k \quad + \quad \frac{64}{15} \pi^2 \, I_2^2 \int Y_{20}^*(\hat{k}) \sin\theta_k d\theta_k d\emptyset_k$$

$$\left. + \left(\frac{-64}{3\sqrt{5}}\right) \pi^2 \, I_0 I_2 \int Y_{00}^*(\hat{k}) \, Y_{20}(\hat{k}) \sin\theta_k d\theta_k d\emptyset_k\right]$$

So $\sigma_0 = \frac{8\pi}{3} \left(\frac{\mu L^3 k w e^2}{\hbar^2 c}\right) \left[I_0^2 + \frac{4}{5} I_2^2\right]$ ... (2.38)

Next, Evaluation of σ_1:

Here, only $l' = 2$, $m' = 1$, is possible

$$\int \psi_k^* \, (\hat{\varepsilon} \cdot \vec{r}_3^>) \, \psi_m d\vec{r}_c^> d\vec{r}_3^> = 4\pi\sqrt{\frac{4\pi}{3}} \, (-i)^2 e^{-i(\delta_2 + \sigma_2)} Y_{21}(\hat{k})$$

$$\times \int R_{1s}^{Li+*} (r_c) \, \frac{U_2^*(kr_3)}{k} \, R_{1s}^{Li} (r_c) \, R_{2p}^{Li} (r_3) r_3^2 dr_c dr_3$$

$$\times \frac{3}{\sqrt{4\pi}\sqrt{5}} \quad C_{101}^{112} \quad C_{000}^{112}$$

so $$\int \psi_k^* \, (\hat{\varepsilon} \cdot \vec{r}_3^>) \, \psi_m d\vec{r}_c^> d\vec{r}_3^> = -\frac{4\pi}{\sqrt{5}} \, I_2 \, e^{-i(\delta_2 + \sigma_2)} Y_{21}^*(\hat{k})$$

$$|<k| \hat{\varepsilon} \cdot \vec{r}_3^> |m>|^2 = \frac{16\pi^2}{5} \, I_2^2 \, Y_{21}^*(\hat{k}) \, Y_{21}(\hat{k}]$$

Again, using eqn. (2.17)

$$\sigma_1 = \sigma_1 (\theta.\emptyset) \, \sin\theta d\theta d\emptyset$$

$$= \frac{2\pi}{\hbar} \left(\frac{\mu L^3 k}{8\pi^3 \hbar^2} \right) \left(\frac{16\pi^2 I_2^2}{5} \right) \left(\frac{e^2 \hbar w.2\pi}{c} \right)$$

$$\int Y_{21}^* (\hat{k}) Y_{21}(\hat{k}) \sin\theta_k \, d\theta_k \, d\emptyset_k$$

$$= \frac{8\pi}{5} \left(\frac{\mu L^3 kwe^2}{\hbar^2 c} \right) I_2^2 \qquad \qquad \dots (2.39)$$

Similarly, evaluation of σ_{-1}:

Here, only $l' = 2$, $m' = 1$, is possible.

So $\qquad \langle k|\hat{e}.\vec{r}_3|m\rangle = -\dfrac{4\pi}{5} e^{-i(\delta_2 + \sigma_2)} Y_{2,-1}(\hat{k}) I_2$

$$\left|\langle k|\hat{e}.\vec{r}_3|m\rangle\right|^2 = \dfrac{16\pi^2}{5} I_2^2 Y_{2,-1}^*(\hat{k}) Y_{2,-1}(\hat{k})$$

Thus, on using eqn. (2.17), we get

$$\sigma_{-1} = \int \sigma_{-1}(\theta,\emptyset)\sin\theta\, d\theta\, d\emptyset$$

$$= \dfrac{8\pi}{5} \left(\dfrac{\mu L^3 kwe^2}{\hbar^2 c}\right) I_2^2 \qquad\qquad \ldots (2.40)$$

So $\qquad \sigma = \dfrac{1}{3}(\sigma_0 + \sigma_1 + \sigma_{-1})$

$$= \dfrac{1}{3} \times \dfrac{8\pi}{3} \left(\dfrac{\mu L^3 kwe^2}{\hbar^2 c}\right)\left[I_0^2 + \dfrac{4}{5} I_2^2 + 3\times\left(\dfrac{I_2^2}{5} + \dfrac{I_2^2}{5}\right)\right]$$

$$= \dfrac{8\pi}{9} \left(\dfrac{\mu L^3 kwe^2}{\hbar^2 c}\right)\left[I_0^2 + \left(\dfrac{4+6}{5}\right) I_2^2\right]$$

$$= \dfrac{8\pi}{9} \left(\dfrac{\mu L^3 kwe^2}{\hbar^2 c}\right)\left[I_0^2 + 2I_2^2\right]$$

And $\qquad \mu = 1$, $\hbar = 1$, $\alpha = \dfrac{e^2}{\hbar c}$, $L = 1$

So $\quad \sigma = \dfrac{8\pi}{9} (\alpha.k) \hbar w (I_o^2 + 2I_2^2)$

$\qquad = \dfrac{8\pi}{9} \alpha k(\dfrac{1}{2}) (k^2 + 2I_p\prime) (I_o^2 + 2I_2^2)$

$\qquad = \dfrac{4\pi}{9} \alpha k(k^2 + 2I_p\prime)(I_o^2 + 2I_2^2) \qquad \ldots (2.41)$

Where Ip' = Ionization potential

$\qquad = e_{1s}^{Li+} - e_{2p}^{Li} \qquad\qquad \ldots (2.42)$

2.3.2.1 <u>Photoelectron angular distribution for Li(2p)</u>

Taking the differential part only, we get, just as from eqn. (2.22)

$$I_p(\theta) = \dfrac{1}{3} x \dfrac{2\pi}{3} (\dfrac{\mu L^3 k}{8\pi^3 \hbar^2}) (\dfrac{e^2 \hbar w.2\pi}{c})$$

$$x \quad [\dfrac{16\pi^2}{3} I_o^2 Y_{oo}^*(\hat{k})Y_{oo}(\hat{k}) + \dfrac{64}{15}\pi^2 I_2^2 Y_{20}^*(\hat{k})Y_{20}(\hat{k})$$

$$- \dfrac{64}{3\sqrt{5}} I_o I_2 \cos\Delta\eta \ x \ Y_{oo}^*(\hat{k}) Y_{20}(\hat{k})$$

$$+ \dfrac{16}{5}\pi^2 I_2^2 Y_{21}^*(\hat{k}) Y_{21}(\hat{k}) + \dfrac{16}{5}\pi^2 I_2^2 Y_{2,-1}^*(\hat{k})Y_{2,-1}(\hat{k})]$$

We know $Y_{oo}(\hat{k}) = \dfrac{1}{\sqrt{4\pi}}$

$\qquad Y_{20}(\hat{k}) = \sqrt{\dfrac{5}{4\pi}} P_2(\cos\theta)$

and
$$\sum_m Y_{lm}^*(\theta,\emptyset)\, Y_{l,m}(\theta,\emptyset) = \frac{2l+1}{4}$$

So
$$I_p(\theta) = \frac{1}{3} \times \frac{2\pi}{\hbar} \left(\frac{\mu\, L^3 k}{8\,\pi^3 \hbar^2}\right) \left(\frac{e^2 \hbar w . 2\pi}{c}\right)$$

$$\times \left[\frac{16\pi^2}{3}\, I_o^2\left(\frac{1}{4\pi}\right) - \frac{64}{3\sqrt{5}}\, I_o I_2 \cos \triangle\eta \times \frac{1}{\sqrt{4\pi}}\sqrt{\frac{5}{4\pi}}\, P_2(\cos\theta)\right.$$

$$+ \frac{16}{3}\pi^2 \left\{\frac{4}{5} Y_{20}^*(\hat{k}) Y_{20}(\hat{k}) + \frac{3}{5} Y_{21}^*(\hat{k}) Y_{21}(\hat{k})\right.$$

$$\left.\left. + \frac{3}{5} Y_{2,-1}^*(\hat{k}) Y_{2,-1}(\hat{k})\right\} I_2^2 \right]$$

we also know,

$$Y_{2,2}(\theta,\emptyset) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\, \sin^2\theta\, e^{2l\emptyset}$$

$$Y_{2,0}(\theta,\emptyset) = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)$$

$$\therefore \quad I_p(\theta) = \frac{1}{3} \times \frac{2\pi}{\hbar}\left(\frac{\mu L^3 k}{8\,\hbar^2}\right)\left(\frac{e^2 \hbar w 2\pi}{c}\right) \times \frac{16\pi^2}{3} \times \frac{1}{4\pi}$$

$$\times \left[I_o^2 - 4\, I_o I_2 \cos\triangle\eta\, P_2(\cos\theta) + 3\, I_2^2\right.$$

$$\left. + \left(\frac{3\cos^2\theta - 1}{4}\right)^2 I_2^2 - \frac{9}{4}\sin^4\theta\, I_2^2 \right.$$

So
$$I_p(\theta) = \frac{32}{9}\pi \left(\frac{\mu L^3 k w e^2}{\hbar c}\right)\left(\frac{1}{4\pi}\right)(I_o^2 + 2I_2^2) \times$$

$$x \quad \left[\frac{I_o^2 + 2I_2^2 + 2P_2(\cos\theta) \, I_2^2 - 4I_o I_2 \cos\Delta\eta \; P_2 \cos\theta)}{(I_o^2 + 2I_2^2)}\right]$$

$$I_p(\theta) = \frac{\sigma(2P)}{4\pi} \left[1 + \frac{2[I_2^2 - 2I_o I_2 \cos\Delta\eta] \, P_2(\cos\theta)}{(I_o^2 + 2I_2^2)}\right]$$

$$= \frac{\sigma(2P)}{4\pi} \left[1 + \beta(2P) \, P_2(\cos\theta)\right] \qquad \ldots (2.27)$$

where $\quad \beta(2P) = \dfrac{2(I_2^2 - 2I_o I_2 \cos\Delta\eta)}{I_o^2 + 2I_2^2} \qquad \ldots (2.43)$

2.3.3 Photoionization for d-state of lithium

For d-state, $l = 2$, and $m = 0, 1, -1, 2, -2$. Analysis shows that the cross sections $\sigma_o, \; \sigma_1, \; \sigma_{-1}, \; \sigma_2, \; \sigma_{-2}$ corresponding to $m = 0, 1, -1, 2, -2$ respectively are given as :

$$\sigma_o = \frac{8\pi}{5} \left(\frac{\mu L^3 kwe^2}{\hbar^2 c}\right) \left[\frac{4I_1^2}{3} + \frac{9}{7} I_3^2\right] \qquad \ldots (2.44)$$

where,

$$I_1 = \int R_{1s}^*(r_c) \; \frac{U_1(kr_3)}{(k)} \; R_{1s}(r_c) R_{2d}(r_3) r_3^2 dr_c dr_3$$

$$\ldots (2.45)$$

and $\quad I_3 = \int R_{1s}^*(r_c) \; \dfrac{U_3(kr)}{k} \; R_{1s}(r_c) R_{2d}(r_3) r_3^2 dr_c dr_3$

$$\ldots (2.46)$$

$R_{2d}(r_3)$ is the valence electron wavefunction.

$$\sigma_1 = \frac{8\pi}{5} \left(\frac{\mu L^3 kw e^2}{\hbar^2 c} \right) \left[I_1^2 + \frac{8}{7} I_3^2 \right]$$

$$\sigma_{-1} = \frac{8\pi}{5} \left(\frac{\mu L^3 kw e^2}{\hbar^2 c} \right) \left[I_1^2 + \frac{8}{7} I_3^2 \right]$$

$$\sigma_2 = \sigma_{-2} = \frac{8\pi}{7} \left(\frac{\mu L^3 kw e^2}{\hbar^2 c} \right) I_3^2$$

So

$$\sigma = \frac{1}{5} \left(\sigma_0 + \sigma_1 + \sigma_{-1} + \sigma_2 + \sigma_{-2} \right)$$

$$= \frac{8}{15} \pi\alpha \, (\hbar w) \, k \, [2I_1^2 + 3I_3^2]$$

$$= \frac{4}{15} \pi\alpha \, k \, (k - \epsilon_d) \, [2I_1^2 + 3I_3^2] \qquad \ldots (2.47)$$

where ϵ_d is the ionization potential

2.3.3.1 Photoelectron angular distribution for d-state

Taking the differential part only, we have

$$I_p(\theta) = \frac{1}{5} \times \frac{2\pi}{\hbar} \left(\frac{\mu L^3 k}{8\pi^3 \hbar^2} \right) \left(\frac{e^2 \hbar w \cdot 2\pi}{c} \right)$$

$$\times \left[\frac{64}{15} \pi^2 I_1^2 Y_{10}^*(\hat{k}) Y_{10}(\hat{k}) + \frac{144}{35}\pi^2 I_3^2 Y_{30}^*(\hat{k}) Y_{30}(\hat{k}) \right.$$

$$\left. - 2 \times \frac{96}{\sqrt{525}} \pi^2 I_1 \cdot I_3 \cos\Delta\eta \; Y_{10}^*(\hat{k}) Y_{30}(\hat{k}) \right.$$

$$+ \frac{16}{5}\pi^2 I_1^2 Y_{11}^*(\hat{k}) Y_{11}(\hat{k}) + \frac{64 \times 2}{35}\pi^2 I_3^2 Y_{31}^*(\hat{k}) Y_{31}(\hat{k})$$

$$- \frac{64}{\sqrt{35}} \frac{\sqrt{2}}{\sqrt{5}}\pi^2 I_1 I_3 \cos \Delta\eta \; Y_{11}^*(\hat{k}) Y_{31}^*(\hat{k})$$

$$+ \frac{16}{5}\pi^2 I_1^2 Y_{1,-1}^*(\hat{k}) Y_{1,-1}(\hat{k}) + \frac{64 \times 2}{35}\pi^2 I_3^2 Y_{3,-1}^*(\hat{k})$$

$$\times Y_{3,-1}(\hat{k}) - \frac{64}{\sqrt{35}} \frac{\sqrt{2}}{\sqrt{5}} I_1 I_2 \pi^2 \cos \Delta\eta \; Y_{1,-1}^*(\hat{k}) Y_{3,-1}(\hat{k})$$

$$+ \frac{16}{7}\pi^2 I_3^2 Y_{3,2}^*(\hat{k}) Y_{3,2}(\hat{k})$$

$$+ \frac{16}{7}\pi^2 I_3^2 Y_{3,-2}^*(\hat{k}) Y_{3,-2}(\hat{k})]$$

which simplifies to

$$I_p(\theta) = \frac{\sigma_2(d)}{4\pi} \left[1 + \frac{\frac{2}{5}(I_1^2 + 6I_3^2 - 18I_1 I_3 \cos\Delta\eta) P_2(\cos\theta)}{(2I_1^2 + 3I_3^2)} \right.$$

$$= \frac{\sigma_2(d)}{4\pi} [1 + \beta(2d) P_2(\cos\theta)] \qquad \dots\,(2.48)$$

where $\quad \beta(2d) = \dfrac{\frac{2}{5}(I_1^2 + 6I_3^2 - 18I_1 I_3 \cos\Delta\eta)}{(2I_1^2 + 3I_3^2)}$ $\qquad \dots\,(2.49)$

Called the asymmetry parameter

and $\cos\Delta\eta = \delta_1 + \sigma_1 - \delta_3 - \sigma_3$

CHAPTER - III

NUMERICAL ANALYSIS AND DETAILS OF

COMPUTER PROGRAM

The evaluation of absorption cross-section requires the evaluation of integrals I_0, I_1 and I_2. For these integrals, wavefunctions of lithium atom in ground and excited states, i.e., 2s, 2p are needed. Also the wavefunctions of the ejected electron for the various values of $l = 0$, 1 and 2 are needed.

The radial wavefunctions of lithium atom for 2s and 2p states i.e. $R_{2s}(r_3)$ and $R_{2p}(r_3)$ are taken from Rapp and Chang[3]. These are given by

$$R_{nl}(r) = Nr^a (r-d)^b (r-e)^c [e^{-fr} + ge^{-hr}] \quad \dots (3.1)$$

Where a,b,c,d,e,f,g,h,N are constants which take on different values for 2s and 2p states.

For the wavefunction of the ejeted electron, we have to solve the following second order differential equation,

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 - 2V(r) \right\} U_l(kr) = 0 \quad \dots (3.2)$$

V(r) is the interaction potential of the ejected electron with the residual Li^+ ion, and is given by[3]

$$V(r) = -\frac{1}{r} - e^{-r/\alpha} \cdot \frac{2}{r} (1 + \frac{r}{2\alpha}) \quad \dots (3.3)$$

with α = 0.301939   ... (3.4)

We have used the Numerov's[4] method to solve the above differential equation (3.2). This method involves the following steps:

The eqn. (3.2) can be written in the general form $y'' = F(r)y + G(r)$ as follows

$$\frac{d^2 U_1(kr)}{dr^2} = \left\{ \frac{l(l+1)}{r^2} - k^2 + 2V(r) \right\} U_1(kr)$$

$$\frac{d^2}{dr^2} U_1(kr) = F(r) U_2(kr) \qquad \ldots \ (3.5)$$

where $\quad F(r) = \dfrac{l(l+1)}{r^2} - k^2 + 2V(r) \qquad \ldots \ (3.6)$

or $\quad U_1''(kr) = F(r) U_1(kr) \qquad \ldots \ (3.7)$

Also, we know that $\quad y'' = F(r) y$

$$\delta^2 y = (\delta r)^2 \left\{ F_j y_j + \frac{1}{12} \delta^2 (Fy)_j \right\}$$

So $\bullet$ $\quad \delta^2 U_1(kr) = h^2 \left\{ F_j U_j + \frac{1}{12} \delta^2 (FU)_j \right\}$

or more fully,

$$U_{j+1} - 2U_j + U_{j-1} = h^2 \left\{ F_j U_j + \frac{1}{12} \{ F_{j+1} U_{j+1} \right.$$

$$- 2F_j U_j + F_{j-1} U_{j-1}])$$

$$[1- \frac{1}{12}h^2 F_{j+1}]U_{j+1} - 2[1-\frac{h^2}{12}F_j]U_j + [1-\frac{1}{12} h^2 F_{j-1}]U_{j-1}$$

$$= h^2 (F_j U_j)$$
.

Let $\qquad [1- \frac{1}{12} h^2 F] U = Y$ $\qquad$ ... (3.8)

Then $\qquad Y^2_j = h^2 [\frac{F_j}{1- \frac{1}{12} h^2 F_j}] Y_j$

This gives

$$Y_{j-1} - 2Y_j + Y_{j-1} = h^2 [\frac{F_j}{1- \frac{1}{12}h^2 F_j}] Y_j$$

or $\qquad Y_{j+1} - \{2 + \frac{h^2 F_j}{1- \frac{1}{12} h^2 F_j} \} Y_j + Y_{j-1} = 0$

$$Y_{j+1} = \{2+ \frac{h^2 F_j}{1- \frac{1}{12}h^2 F_j} \} Y_j - Y_{j-1} \qquad ... (3.())$$

We thus have a simple logic to follow. Using this equation computer program is made resulting in the calculation of the wavefunction $U_1(kr)$. We took the initial value of the wavefunction to be

$$U_1(kr) = Ar^{1+1} \qquad\qquad ... (3.10)$$

Where A is a constant.

Starting the solution from two points using eqn. (3.10), the solution for other values of r is continued through equation (3.9). We have taken the two initial points as $0.0001 a_0$ and $0.0002 a_0$, where a_0 is the Bohr's radius. With each shift of the decimal to right hand side, the value of discretization, i.e., H is made twice as large. Initial value of H was 0.0001. This increasing of H is carried on untill we reach a large value of r, say $50 a_0$, where we compare the solution $U_1(kr)$ with eqn. (2.25).

The integral

$$I = \int_0^\infty \frac{U_1(kr)}{(k)} R_{nl}(r)\, r^2 dr \qquad \cdots (3.11)$$

is now evaluated using the trapezoidal rule,

$$\int_a^b f(x)dx = (\frac{b-a}{2})\, [f(a) + f(b)] \qquad \cdots (3.12)$$

CHAPTER - IV

RESULTS AND DISCUSSION

4.1 RESULTS

The absorption cross-section for lithium in 2s state is

$$\sigma(2s) = \frac{4\pi}{3} \alpha \ k(k^2 + 2I_p)I_1^2 \qquad \ldots (4.1)$$

where α is the fine structure constant having value $(\frac{1}{137})$ and I_p is the ionization potential of lithium in ground state i.e. 2s state, which is equal to 5.39 eV.

Also, the absorption cross section for lithium in 2p state is

$$\sigma(2p) = \frac{4\pi}{9} \alpha \ k(k^2 + 2I_p')(I_o^2 + 2I_2^2) \qquad \ldots (4.2)$$

where I_p' is the ionization potential of lithium in 2p state which is equal to 3.5427429 eV.

We have evaluated these cross-sections for different values of k. These are then plotted against the values of k.

Also, phase-shifts for s-ware, p-wave and d-ware are plotted against different values of k. The solid lines indicate our results while the dashed lines indicate results of Ritchie, Pindzola and Garrett[5].

Table I gives our results for phase shifts of s-wave, p-wave & d-wave. Table II gives the results of absorption cross section of lithium in 2s and 2p states. Table III gives the values of β (2p) for different values of k.

TABLE I :   PHASE SHIFTS   IN   ELECTRON   LITHIUM   ION   SCATTERING

k	s-wave	p-wave	d-wave
0.1	1.2648	0.1490	0.0030
0.2	1.2627	0.1519	0.0034
0.3	1.2593	0.1565	0.0041
0.4	1.2545	0.1626	0.0051
0.5	1.2483	0.1701	0.0064
0.6	1.2407	0.1786	0.0081
0.7	1.2318	0.1879	0.0102
0.8	1.2214	0.1976	0.0126
0.9	1.2097	0.2076	0.0154
1.0	1.1969	0.2176	0.0186
1.1	1.1829	0.2274	0.0222
1.2	1.1682	0.2369	0.0261
1.3	1.1529	0.2460	0.0302
1.4	1.1369	0.2546	0.0346
1.5	1.1208	0.2628	0.0393
1.6	1.1044	0.2703	0.0441
1.7	1.0879	0.2774	0.0489
1.8	1.0715	0.2838	0.0539
1.9	1.0552	0.2897	0.0591

TABLE II :   PHOTOIONISATION   CROSS-SECTIONS

k	$\sigma(2s) \times 10^{-18}$	$\sigma(2p) \times 10^{-18}$
0.1	1.6506	14.1164
0.2	1.8476	10.3622
0.3	2.0329	6.5457
0.4	2.0839	3.7671
0.5	1.9599	2.0738
0.6	1.7049	1.1311
0.7	1.3952	0.6252
0.8	1.0933	0.3549
0.9	0.8335	0.2083
1.0	0.6260	0.1283
1.1	0.4679	0.0799
1.2	0.3507	0.0522
1.3	0.2649	0.0351
1.4	0.2024	0.0243
1.5	0.1567	0.0172
1.6	0.1231	0.0124
1.7	0.0980	0.0090
1.8	0.0791	0.0067
1.9	0.0646	0.0050

TABLE III   ASSYMETRY PARAMETER

k	$\beta(2p)$
0.1	1.3426
0.2	1.5044
0.3	1.6272
0.4	1.7112
0.5	1.7595
0.6	1.7759
0.7	1.7648
0.8	1.7313
0.9	1.6806
1.0	1.6181
1.1	1.5484
1.2	1.4755
1.3	1.4023
1.4	1.3308
1.5	1.2623
1.6	1.1974
1.7	1.1363
1.8	1.0788
1.9	1.0247
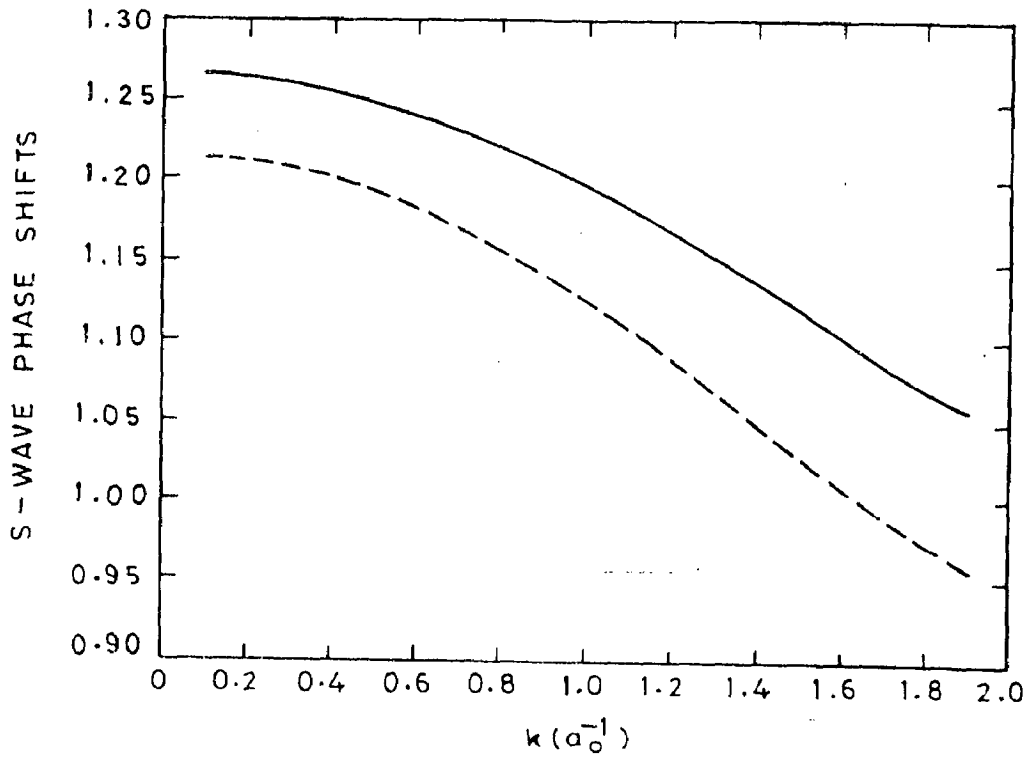
Figure 1

Figure 2

Figure 3

Figure 4

4.2   DISCUSSION

Figure 1 illustrates the variation of s-wave phase shifts for different values of k. From the figure we notice that for lower values of k, there is not much difference in the present results (solid curves) and the calculation of Ritchie et al . As the energy incrases we notice that there are differences in the two calculations. The possible reason for different results in the two calculations may be due to the fact that the wavefunctions used in our calculatons are different from those considered by the other authors. Since the wavefunctions differ, the potential V(r) also differs.

Similarly, figure 2 and 3, which illustrate the variation of p-wave and d-wave phase shifts with different values of k, show small difference between the two curves at lower energies while the difference grows larger as the energy increases.

Figure 4 shows the variation of absorption cross section σ (2s) for different values of k. Again the two calculations show some difference.

Figure 5 shows the variation of absorption cross-section σ (2p) for different values of k. Figure 6 shows the variation of asymmetry parameter σ (2p) for different values of k. The curves differ slightly.
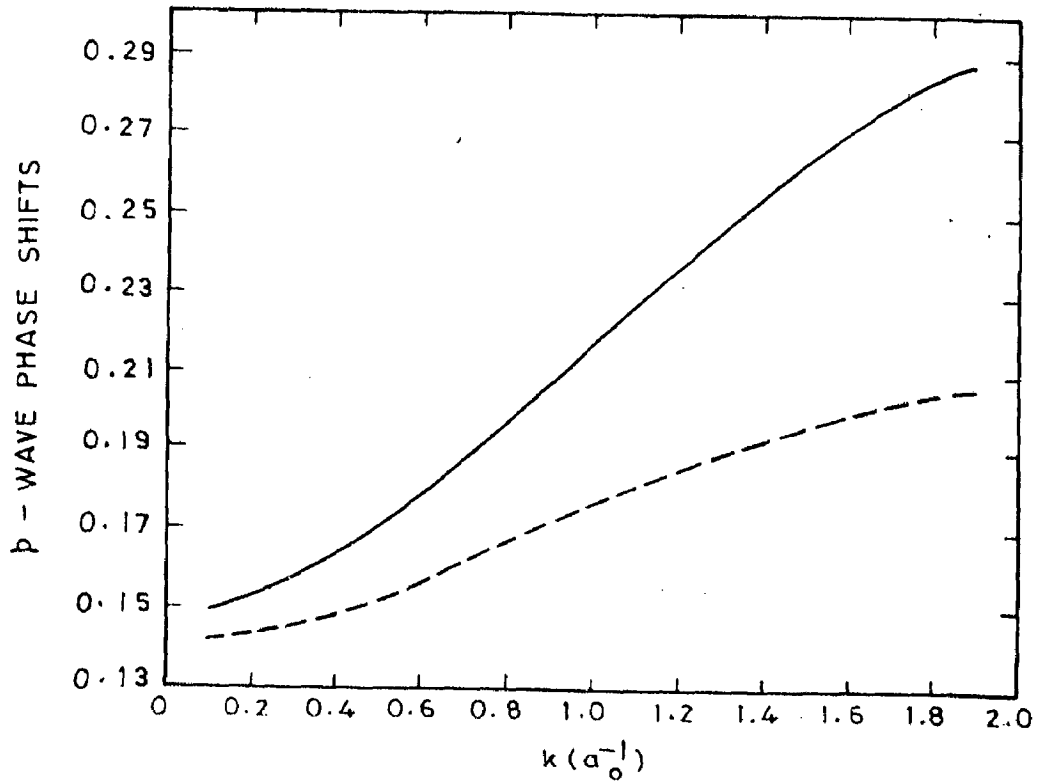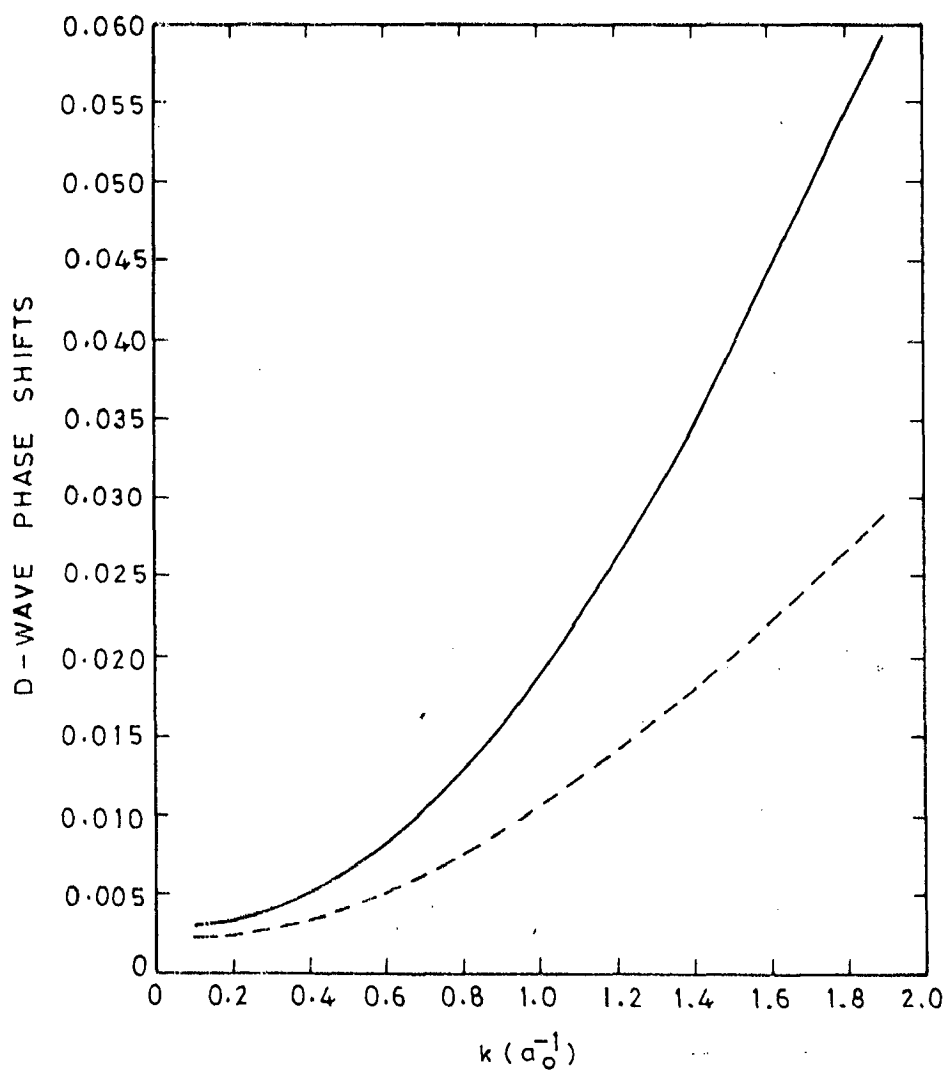
Figure 5
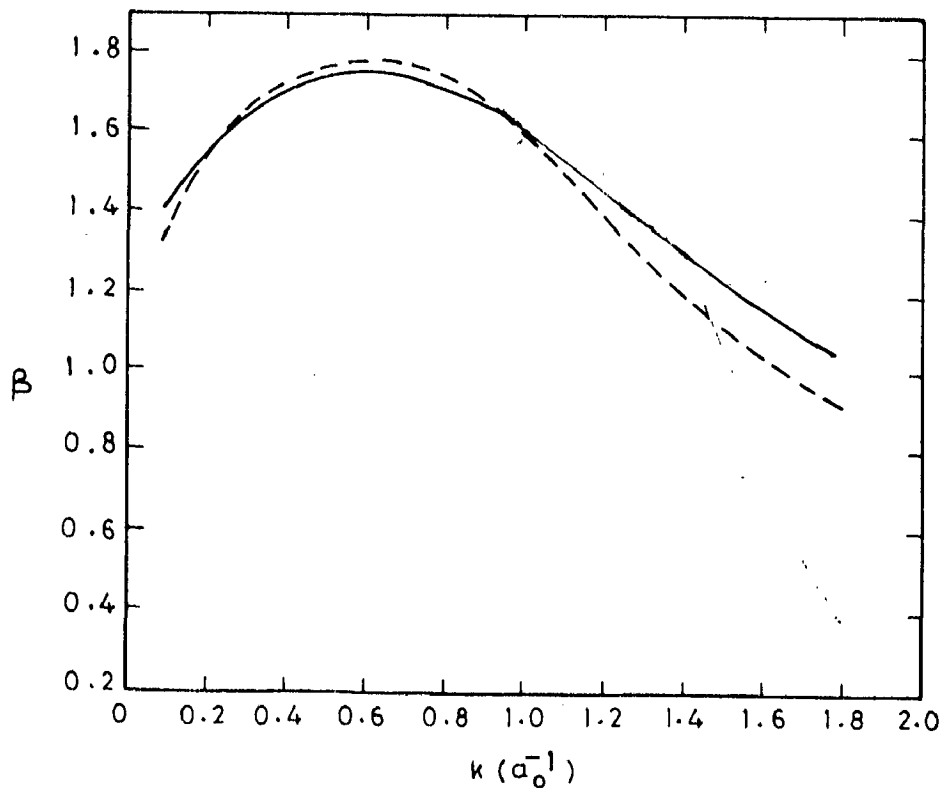
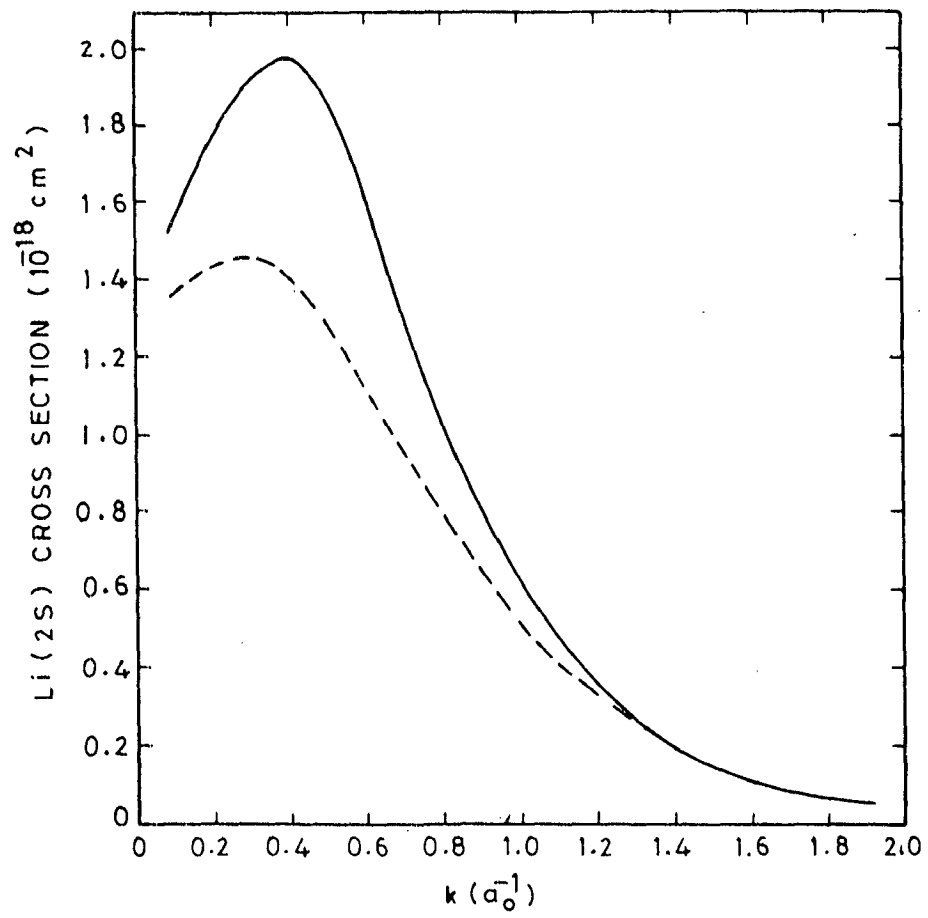Figure 6

4.2   DISCUSSION

Figure 1 illustrates the variation of s-wave phase shifts for different values of k. From the figure we notice that for lower values of k, there is not much difference in the present results (solid curves) and the calculation of Ritchie et al . As the energy incrases we notice that there are differences in the two calculations. The possible reason for different results in the two calculations may be due to the fact that the wavefunctions used in our calculatons are different from those considered by the other authors. Since the wavefunctions differ, the potential $V(r)$ also differs.

Similarly, figure 2 and 3, which illustrate the variation of p-wave and d-wave phase shifts with different values of k, show small difference between the two curves at lower energies while the difference grows larger as the energy increases.

Figure 4 shows the variation of absorption cross section σ (2s) for different values of k. Again the two calculations show some difference.

Figure 5 shows the variation of absorption cross-section σ (2p) for different values of k. Figure 6 shows the variation of asymmetry parameter σ^{*} (2p) for different values of k. The curves differ slightly.
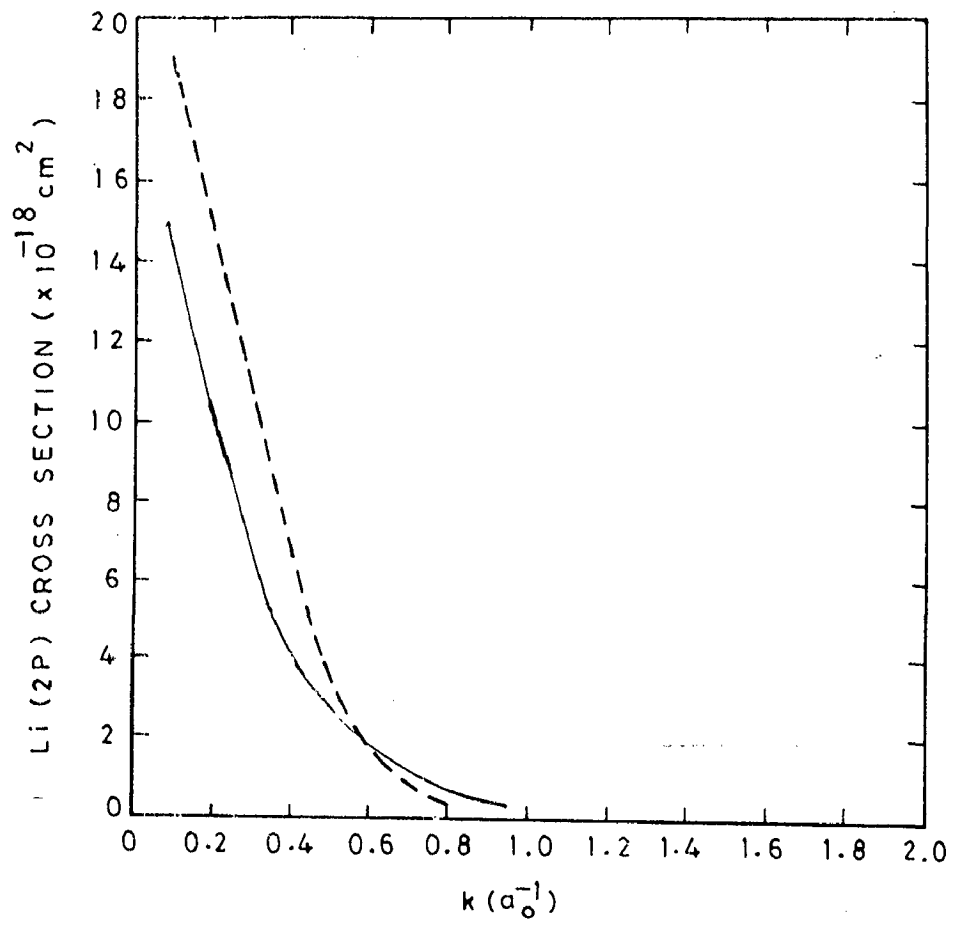
APPENDIX

```fortran
C          EVALUATION OF PHOTOIONISATION  CROSS-SECTION AND ASSYMETRY
C          PARAMETER OF LITHIUM IN GROUND AND EXCITED STATES
           IMPLICIT REAL *8(A-H,O-Z)
           COMMON/CHAR/ION,CHARG,CHINP,CHTAR,IEXNG,XKF
           DIMENSION U(0:40000),R(0:40000),Y(0:40000),V(0:40000),F(0:40000)
           DIMENSION RV(0:40000),SIGMA(20,20)
           DIMENSION PHI1(10),RSIG1(10),BETA(20,20)
           WRITE(*,125)
110        OPEN(UNIT=4,STATUS='UNKNOWN',FILE='F.DAT')
           READ(4,*)L,A,AKI,AL
           WRITE(*,125)
           WRITE(*,50)'L=',L,'A=',A,'AKI=',AKI,'AL=',AL
50         FORMAT(1X,A2,I2,2X,2(2X,A4,2X,F4.2),2X,A3,F10.8)
           WRITE(*,125)
125        FORMAT('********************************************')
           ION=1
           CHARG=1.0D0
           CHINP=-1.0D0
           CHTAR=1.0D0
           IEXNG=0
           XKF=AKI
           XKO=AKI
           NI=2
           DO 2 LI=0,1
           TYPE*,'NI=',NI,'  ','LI=',LI
           R(0)=0.0001D0
           R(1)=0.0002D0
           H=0.0001D0
           V(0)=-1.0D0/R(0)-2.0D0*DEXP(-R(0)/AL)*(1.0D0+R(0)/(2.0D0*AL))/R(0)
           V(1)=-1.0D0/R(1)-2.0D0*DEXP(-R(1)/AL)*(1.0D0+R(1)/(2.0D0*AL))/R(1)
           F(0)=L*(L+1)/(R(0)**2)-AKI**2+2.0D0*V(0)
           F(1)=L*(L+1)/(R(1)**2)-AKI**2+2.0D0*V(1)
           U(0)=A*R(0)**(L+1)
           U(1)=A*R(1)**(L+1)
           Y(0)=(1.0D0-((H**2)*F(0))/12.0D0)*U(0)
           Y(1)=(1.0D0-((H**2)*F(1))/12.0D0)*U(1)
           I=1
           NN=0
           J=8
           RA=80.0D0
           NA=21875
           SUM=0
10         Y(I+1)=(2.0D0+((H**2)*F(I))/(1.0D0-(H**2)*F(I)/12.0D0))*Y(I)-Y(I-1)
11         R(I+1)=R(I)+H
           V(I+1)=-1.0D0/R(I+1)-2.0D0*DEXP(-R(I+1)/AL)*
1          (1.0D0+R(I+1)/(2.0D0*AL))/R(I+1)
           F(I+1)=L*(L+1)/(R(I+1)**2)-AKI**2+2.0D0*V(I+1)
           U(I+1)=Y(I+1)/(1.0D0-((H**2)*F(I+1))/12.0D0)
```

```
RV(I+1)=R(I+1)*V(I+1)
TM1=U(I)*RLI(NI,LI,R(I))*(R(I)**2)/AKI
TM2=U(I+1)*RLI(NI,LI,R(I+1))*(R(I+1)**2)/AKI
SUM=SUM+0.5D0*(TM1+TM2)*(R(I+1)-R(I))
I=I+1
NN=NN+1
IF(NN.EQ.J)THEN
        NN=0
        H=2.0D0*H
        J=K
        K=45
ENDIF
IF(NN.EQ.K)THEN
        NN=0
        H=2.0D0*H
        K=5*K
ENDIF
IF(NN.EQ.NA+2)THEN
        UA=Y(I-2)/(1.0D0-((H**2)*F(I-2))/12.0D0)
        TYPE*,'NN= ',NN-2,'   ','RA= ',R(I)-2*H,'UA=',UA
ENDIF
RB=RA+313*H
RAK=XKO*RA
RBK=XKO*RB
IF(NN.EQ.(NA+313))THEN
        UB=Y(I)/(1.0D0-((H**2)*F(I))/12.0D0)
        TYPE*,'NN=',NN,'   ','R3=',RB,'   ','UB=',UB
ENDIF
IF(R(I).LT.RB)THEN
IF(NN.EQ.0)THEN
        Y(I+1)=(2.0D0+((H**2)*F(I))/(1.0D0-(H**2)*
1               F(I)/12.0D0))*Y(I)-Y(I-2)
        GO TO 11
     ELSE
        GO TO 10
     ENDIF
    ELSE
        TYPE*,'RAK=',RAK,'   ','RBK=',RBK
        GO TO 20
ENDIF
20      CALL COUL(L,XKO,RAK,RZF,RZG,RZFP,RZGP,RSIG)
AJ=RZF
AN=RZG
CALL COUL(L,XKO,RBK,RZF,RZG,RZFP,RZGP,RSIG)
BJ=RZF
BN=RZG
TYPE*,'RSIG=',RSIG
D1=BN*UA-AN*UB
```

```
        D2=AJ*UB-BJ*UA
        D3=AJ*BN-BJ*AN
        ALK=D1/D3
        BLK=D2/D3
        TH=BLK/ALK
        TYPE*,'TH IS=',TH
        PHI=DATAN2(BLK,ALK)
        TYPE*,'PHI IS=',PHI
        U1=ALK*AJ+BLK*AN
        U2=ALK*BJ+BLK*BN
        IF(RA.GT.79)THEN
                RA=RA+313*H
                NA=NA+313
                IF(RA.GT.81)THEN
                        GO TO 30
                   ELSE
                        GO TO 10
                ENDIF
             ELSE
                RA=RA+3000*H
                NA=NA+3000
                GO TO 10
        ENDIF
30      TYPE*,'SUM=',SUM
        ALK1=ALK/DCOS(PHI)
        TYPE*,'ALK1=',ALK1
        TRANM=SUM/ALK1
        TYPE*,'TRANM=',TRANM
        WRITE(*,120)
120     FORMAT(5X,'********************************************'/)
        IF(L.EQ.1)THEN
                IF(LI.EQ.0)THEN
                        TYPE*,'L=',L,'   ','NI=',NI,'   ','LI=',LI
                        PI=3.14159270D0
                        ALPHA=(1.0D0)/(137.0D0)
                        ENIP1=(5.39D0)/(27.2D0)
                        A0=5.29E-9
                        SIGMA(2,0)=4.0D0*PI*ALPHA*AKI*((AKI**2)+
     1                          (2.0D0*ENIP1))*(TRANM**2)*
     2                          (A0**2)/3.0D0
                        TYPE*,'SIGMA(2,0)=',SIGMA(2,0)
                ENDIF
        ENDIF
        IF(L.EQ.0)THEN
                IF(LI.EQ.1)THEN
                        TYPE*,'L=',L,'   ','NI=',NI,'   ','LI=',LI
                        XINO=TRANM
                        TYPE*,'XINO=',XINO
```

```fortran
                ENDIF
                PHI1(0)=PHI
                TYPE*,'PHI1(0)=',PHI1(0)
                RSIG1(0)=RSIG
                TYPE*,'RSIG1(0)=',RSIG1(0)
          ENDIF
          IF(L.EQ.2)THEN
                PHI1(2)=PHI
                TYPE*,'PHI1(2)=',PHI1(2)
                RSIG1(2)=RSIG
                TYPE*,'RSIG1(2)=',RSIG1(2)
                IF(LI.EQ.1)THEN
                      TYPE*,'L=',L,'   ','NI=',NI,'   ','LI=',LI
                      XIN2=TRANM
                      TYPE*,'XIN2=',XIN2,'XINO=',XINO
                      PI=3.1415927D0
                      ALPHA=(1.0D0)/(137.0D0)
                      ENIP2=(5.39D0-1.847257 1D0)/(27.2D0)
                      AO=5.29E-9
                      SIGMA(2,1)=4.0D0*PI*ALPHA*AKI*((AKI**2)+
     1                      2.0D0*ENIP2)*((XINO**2)+2.0D0*
     2                      (XIN2**2))*(AO**2)/9.0D0
                      TYPE*,'SIGMA(2,1)=',SIGMA(2,1)
                      DELTA=RSIG1(0)+PHI1(0)-RSIG1(2)-PHI1(2)
                      BETA(2,1)=2.0D0*((XIN2**2)-2.0D0*XINO*XIN2*
     1                      DCOS(DELTA))/((XINO**2)+2.0D0*XIN2**2)
                      TYPE*,'BETA(2,1)=',BETA(2,1)
                ENDIF
          ENDIF
          WRITE(*,120)
2         CONTINUE
C         *************************************************************
          IF(AKI.LT.2)THEN
                GO TO 110
          ENDIF
          STOP
          END
C*****************************************************************************
C*****************************************************************************
          FUNCTION RLI(NI,LI,R)
          LL=LI+1
          GO TO (200,250)LL
200       IF(NI.EQ.2)THEN
                RLI=(0.6719289D0)*((R-0.869875D0)**1)*
     1            (DEXP(-0.713054D0*R)+1.602850D0*DEXP(-2.05067D0*R))
          ENDIF
          IF(NI.EQ.3)THEN
                RLI=(0.0563759D0)*((R-4.64853D0)**1)*((R-0.921797D0)
     1            **1)*(DEXP(-0.432737D0*R)+2.897910D0*DEXP(-1.36761D0*R))
```

```
        ENDIF
        RETURN
250     IF(NI.EQ.2)THEN
            RLI=(0.219217D0)*(R**1)*
     1          (DEXP(-0.518D0*R)+0.834D0*DEXP(-1.75D0*R))

        ENDIF
        IF(NI.EQ.3)THEN
            RLI=(0.0223536D0)*(R**1)*((R-5.7073D0)**1)*
     1          (DEXP(-0.345D0*R)+0.76D0*DEXP(-1.34318D0*R))
        ENDIF
        RETURN
        END
```

REFERENCES

[1]   L.I. Schiff, 'Quantum Mechanics', McGraw-Hill Book Company, Singapore (1968).

[2]   Charles J. Joachain, 'Quantum Collision Theory', North Holland, Netherland (1975).

[3]   D. Rapp, C.M. Chang, J. Chem. Phy. 57 (1972) 4283-4286.

[4]   D.R. Hartree, 'Numerical Analysis', Oxford University Press, Amen House, London (1958).

[5]   B. Ritchie, M.S. Pindzola, W.R. Garrett, Physical Review A, 23 (1981) 2905-2913.