THE DETERMINATION OF THE IONIZATION PROBABILITY OF NICKEL

by
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ABSTRACT

An ionisation probability P_k measurement was done across the 3.152 MeV resonance in ^{58}Ni. A program was written to calculate P_k and this was used to make a mathematical model of P_k by comparing the experimental values of P_k with the calculated ones. Actual values were calculated for the atomic amplitudes and values for the final energy of the electron ϵ_f and the width of the resonance were obtained by the comparison procedure.

I declare that this thesis is my own work and has not previously been submitted for a degree at any university.

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CONTENTS

Chapter 1

INTRODUCTION

K-shell ionisation takes place in an atom when an energetic projectile, such as a proton, incident on a target nucleus, ionises the K-shell electron before or after hitting the nucleus. This ionisation event may be identified by a coincidence between an X-ray of the inonised atom and the elastically scattered particle.

In 1962 Gugelot (1) came up with the idea for an experiment in which it would be possible to determine the lower limit of the lifetime of the compound nucleus.

According to him the width of a nuclear reaction can be estimated from an equation that describes the decay of a compound nucleus. In order to use this formula an approximation has to be made for the level densities of the compound nucleus as well as the residual nucleus. This value for the width of the reaction is of the same order of magnitude as the width of the K-X-radiation of the heavy atom.

The X-radiation has to be measured before the compound nucleus has had a chance to emit a proton ie before the compound nucleus has had a chance to decay.

Therefore, by determining the width or the lifetime of the X-radiation one can obtain the width or lifetime of the compound nucleus. When the compound nucleus emits a proton and this is established too, then the compound nuclear lifetime can be determined accurately. This leads to the coincident measurement of the proton and the X-ray.

Very short nuclear lifetimes can be measured by this technique since the standard of time is set by the lifetime of the K vacancy and this is generally greater than 10^{-18} seconds. (Mersbacher (2)).

In 1963 Ciochetti and Molinari (3) suggested that the shape elastic and compound elastic scattering may be determined seperately by a time delay measurement between the incoming and outgoing elastically scattered particles.

They reasoned that since the atomic electrons are so close to the nucleus, any nuclear phenomenon such as a resonance, would cause a perturbation in the electron states.

According to them, ionisation of the K-shell electrons occurs because of the elelctro-magnetic interaction between the K-shell electron and the charged incident or outgoing particle, as well as the nuclear recoil during the reaction.

Therefore the nuclear time delay associated with a resonance formed in a nuclear reaction would be able to influence the probability for ionisation of the K-shell electrons. (Trail (23)).

To understand this more clearly one can look at the quantum mechanical expression for the ionisation probability P_k

$$P_k(\theta, E) \simeq \int_0^\infty d\epsilon_f \sum_{\lambda\mu} |D^\lambda_{\mu 0}(\theta) b_\lambda + (-1)^\lambda \delta_{\mu 0} (f(\theta, E - \Delta E)/f(\theta, E)) b^*_\lambda|^2$$

where

$D^\lambda_{\mu 0}(\theta)$ is the rotational matrix, b^*_λ, b_λ are the atomic amplitudes, $f(\theta, E)$ is the elastic scattering amplitude for the scattering angle θ and the centre of mass energy E.

ϵ_f is the final energy of the evicted electron.

If an atomic K-shell vacancy is created on the way into a collision, the projectile has only an energy

$$E - \hbar\omega = E - \Delta E$$

left to initiate the nuclear reaction. If the K-shell vacancy is produced on the way out, the full energy E will have been available to the nuclear reaction. Therefore the elastic scattering amplitude f will have a resonant behaviour as the nuclear resonance, due to compound nuclear formation, is traversed. When there is no collision between the particle and the electron then

$$f(\theta, E - \Delta E) = f(\theta, E)$$

and P_k reduces to

$$P_k(\theta, E) \simeq \int_0^\infty d\epsilon_f \sum_{\lambda\mu} |D^\lambda_{\mu 0}(\theta) b_\lambda + (-1)^\lambda \delta_{\mu 0} b^*_\lambda|^2$$

which is just the semiclassical prediction for a 'fast' nuclear reaction. No interference will be detected in the probability P_k.

The time delay is known from the width Γ of the resonance. The magnitude of the variation of P_k across a nuclear resonance depends on the ratio U_k/Γ. U_k is the K-shell electron binding energy and the variation in P_k is expected to be the largest for $U_k = \Gamma$.

$$\begin{aligned} U_k &= \Delta E - \epsilon_f \\ &= \hbar\omega - \epsilon_f \\ &\simeq \Delta E \end{aligned}$$

Since the K-shell electron orbiting period can be expressed as $\hbar/U_k$ and the width of the resonance is $\Gamma\,\hbar/\tau$, with τ the time delay of the compound nucleus. Then, if

$$\begin{aligned} U_k &= \Gamma \\ U_k/\hbar &= \Gamma/\hbar \\ U_k/\hbar &= \hbar/\tau\hbar \qquad \text{so that} \\ \hbar/U_k &= \tau \end{aligned}$$

The orbiting period of the electron 'matches' the time delay.

In 1979, Chemin (21) suggested that although the principle of coincidence measurements are relatively straightforward, the actual experiment is rather more complicated. The reason for this is the large number of random coincidences between X-rays and protons and the small number of true coincidences between the X-rays and protons from the same atom.

In order to get an acceptable ratio for true to rand[illegible]s a very closed detection geometry is necessary (Chemin (22)) ie large solid a[illegible] required for both the X-ray and particle detectors. (Chemin (24)).

Various experiments were done where the U_k/Γ parameter was investigated in order to try and determine the variation in P_k as well as the contributions made to P_k by the atomic amplitudes b_λ.

In 1982 Anholt (4), and in 1983 Chemin (5) were able to display the original Ciochetti and Molinari idea by incorporating the compound elastic scattering and the direct elastic scattering into the expression for P_k. Thus, by first looking at the interference of the ionisation probability the amount of compound elastic scattering can be determined for any element provided one looks at a doorway state such as an isobaric analogue resonance at backward scattering angles.

They also found that the atomic amplitudes were in phase for the direct elastic scattering but as soon as the compound elastic scattering occured the atomic amplitudes were no longer in phase due to the longer lifetime of the compound nucleus formation.

In this work P_k was measured across the 3.15 MeV resonance in ^{58}Ni. This experiment was originally done by Blair (9) before too much was known about the theory.

Earlier it was thought that P_k should be measured across a resonance previously found in cobalt by Erlandsson (15). This resonance was detected by a $^{59}Co(p,p_0)$ reaction but proved too small to ensure a dramatic effect in P_k.

Chapter 2

THEORY AND A REVIEW OF THE LITERATURE
CALCULATION OF THE IONIZATION PROBABILITY IN THE D W B A

The ionisation probability is defined by

$$P_k(\theta, E) = d\sigma_k/d\Omega \; / \; |f(\theta, E)|^2$$

where $f(\theta, E)$ is the nuclear scattering amplitude evaluated at energy E at a scattering angle θ. According to the Distorted Wave Born Approximation the differential cross section for the ionisation of a K-shell electron is given by

$$d\sigma_k/d\Omega = \sum_{\lambda\mu} \int_0^\infty d\epsilon_f |A_{\epsilon_f \lambda\mu}(\theta, E)|^2$$

where ϵ_f, λ, μ, are the energy and orbital quantum numbers, E is the centre of mass energy and θ is the scattering angle of the proton.

According to the formula of Blair (6) partial wave expansions are made of the incoming and outgoing projectile waves, while also taking into account the coupling between the electronic and projectile angular momenta.

The nuclear scattering is described by a spherically symmetric potential $V_N(R)$ which consists of the sum of the Coulomb and nuclear terms. The wave function of the nuclear scattering is assumed to be a function of the internuclear coordinate $\vec{R}$ only, so that one can observe the contribution made by the ionisation when the projectile and target nuclei overlap.

There is a three body system under consideration: the incident nuclear projectile with charge $Z_1 e$, a spin zero target nucleus with charge Z_2 and a mass M_2 from which the projectile is scattered elastically, and the electron that gets ionised. This system is described by

$$A_{\epsilon_f \lambda\mu} = \frac{\sqrt{KK'}}{2\pi\hbar v} \langle \chi^-(\vec{K}', \vec{R}) \varphi_{\epsilon_f \lambda\mu}(\vec{r}) | H' | \chi^+(\vec{K}, \vec{R}) \varphi_{1s}(\vec{r}) \rangle$$

where the perturbation Hamiltonian is given by

$$H' = \frac{-Z_1 e^2}{|\vec{r} - \vec{R}|} + \frac{mM\omega^2}{M_2}(\vec{R} \cdot \vec{r})$$

The first term is the Coulomb potential between the projectile nucleus and the electron whereas the second term is the recoil term.

The $\vec{K}', \vec{K}$ are the final and initial centre-of-mass momenta

v is the velocity of the projectile

$\vec{r}$ is the electron coordinate

φ is the electronic wave function

M is the reduced mass of the projectile and target nucleus

m is the reduced mass of the electron and target nucleus

The energy transferred to the electron is

$$\Delta E = \hbar\omega = U_k + \epsilon_f$$

where U_k is the binding energy of the K-shell electron.

The matrix elements of the electronic wave functions are

$$1/\hbar v \langle \varphi_{\epsilon_f \lambda\mu} | H' | \varphi_{1s} \rangle$$

$$= (1/\hbar v) \left| \left\langle \varphi_{\epsilon_f \lambda\mu} \left| \frac{-Z_1 e^2}{|\vec{r} - \vec{R}|} + \frac{mM\omega^2}{M_2}(\vec{R} \cdot \vec{r}) \right| \varphi_{1s} \right\rangle \right|$$

$$= \frac{-Z_1 e^2}{\hbar v} \int_0^\infty r^2 R_{\epsilon_f \lambda}(r) R_{1s}(r) / |\vec{r} - \vec{R}| dr$$

$$\int_0^\infty Y^*_{\lambda\mu}(\hat{r}) Y_{00}(\hat{r}) d\Omega$$

$$+ \frac{mM\omega^2}{\hbar v M_2} \int_0^\infty r^2 R_{\epsilon_f \lambda}(r) R_{1s}(r) dr \int Y^*_{\lambda\mu}(\hat{r}) Y_{00}(\hat{r}) d\Omega$$

with $Y_{00}(\hat{r}) = 1/\sqrt{4\pi}$

$$1/|\vec{r} - \vec{R}| = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (2l+1) \frac{r_<^l}{r_>^{l+1}} Y_{lm}^*(\hat{R}) Y_{lm}(\hat{r})$$

from Jackson (7)

$$\vec{r} \cdot \vec{R} = r R \cos\gamma$$

and

$$\cos\gamma = P_1(\cos\gamma) = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \delta_{l1} \sum_{m=-l}^{\infty} Y_{lm}^*(\hat{R}) Y_{lm}(\hat{r})$$

Substituting this into the above equation and taking orthogonality into account one finds

$$1/(\hbar v) \langle \varphi_{\epsilon_f \lambda\mu} | H' | \varphi_{1s} \rangle = \frac{-Z_1 e^2}{\hbar v} \frac{1}{2\lambda+1}$$

$$\int r^2 dr \mathcal{R}_{\epsilon_f \lambda} R_{1s} \frac{r_<^\lambda}{r_>^{\lambda+1}} \frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}} Y_{\lambda\mu}^*(\hat{R})$$

$$+ \frac{mM\omega^2}{\hbar v M_2} \frac{\delta_{\lambda 1} R}{2\lambda+1} \int r^3 dr \mathcal{R}_{\epsilon_f \lambda} R_{1s} \frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}} Y_{\lambda\mu}^*(\hat{R})$$

$$= (C\lambda + W_\lambda) \frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}} Y_{\lambda\mu}^*(\hat{R}) = G_\lambda \frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}} Y_{\lambda\mu}^*(\hat{R}) \quad (1)$$

where W_λ is the recoil term and C_λ is the term originating from the Coulomb potential part of the Hamiltonian. The nuclear distorted wave χ^+ can be written as the partial wave expansion

$$\chi^+(\vec{K}, \vec{R}) = 4\pi \sum_{lm} i^l Y_{lm}^*(\hat{K}) Y_{lm}(\hat{R}) (1/(KR)) \exp(i\delta_l) F_l(K, R) \quad (2)$$

$$\chi^-(\vec{K}', \vec{R})^* = 4\pi \sum_{lm} (-1)^l Y_{lm}(\hat{K}') Y_{lm}^*(\hat{R}) (1/(K'R)) \exp(i\delta_l') F_l(K', R)$$

which is the final state distorted wave function corresponding to the energy $E' = E - \Delta E$.

The F_l are the exact radial wave functions for the nuclear Hamiltonian $H_N = T_N + V_N$. Also

$$\lim_{R\to 0} F_l(K',R) \simeq R^{l+1} \qquad \text{and} \qquad \lim_{R\to\infty} F_l(K,R) = \sin\left(KR - l\pi/2 - \eta\ln(2KR) + \delta_l(E)\right)$$

where

$$\eta = \frac{Z_1 Z_2 e^2}{\hbar v} \qquad \text{and}$$

$\delta_l(E)$ is the sum of the Coulomb and nuclear phase shifts. We now have $A_{\epsilon_f \lambda\mu}$.

$$= \frac{\sqrt{KK'}}{4\pi} 4\pi \sum_{lm} (-i^l) Y_{lm}(\hat{K}') Y^*_{lm}(\hat{R}) \left(1/(K'R)\right) \exp\left(i\delta_l\right) F_l(K',R)$$

$$G_\lambda(R) \frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}} Y^*_{\lambda\mu}(\hat{R}) 4\pi \sum_{lm} (i^l) Y^*_{lm}(\hat{K}) Y_{lm}(\hat{R}) (1/(KR)) \exp\left(i\delta_l\right) F_l(K,R) \int d\hat{R}$$

Clearly

$$i^{-l} = -i^l$$

and from Rose (8)

$$Y_{l_1 m_1}(\theta,\varphi) Y_{l_2 m_2}(\theta,\varphi)$$

$$= \sum_l \frac{\sqrt{(2l_1+1)(2l_2+1)}}{\sqrt{4(2l+1)}} C(l_1\, l_2\, l; m_1\, m_2) C(l_1\, l_2\, l; 0\,0) Y_{l,m_1+m_2}(\theta,\varphi)$$

This important coupling rule can only be applied when θ and φ are in the same plane. It is important to note that the Y^*_{lm} refers to the nuclear part (equation 1) and the $Y_{\lambda\mu}$ the electronic part (equation 2). The axis chosen to apply quantum mechanics to is the $\hat{K}$ axis (Blair (6)), so that

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$$Y(\hat{K}) = \delta_{m0}\frac{\sqrt{2l+1}}{\sqrt{4\pi}}$$

We now have

$$\frac{\sqrt{4\pi}}{\sqrt{2\lambda+1}}\frac{\sqrt{2l+1}}{\sqrt{4\pi}}\delta_{m0}Y^*_{lm}(\hat{R})Y^*_{\lambda\mu}(\hat{R})$$

$$= \frac{\sqrt{4\pi(2l+1)}}{\sqrt{(2\lambda+1)4\pi}}Y^*_{l0}(\hat{R})Y^*_{\lambda\mu}(\hat{R})$$

$$= \sum_{ll'}\frac{\sqrt{(2\lambda+1)(2l+1)4\pi}}{\sqrt{(4\pi)^2(2l'+1)}}C(l\,\lambda\,l';000)C(l\,\lambda\,l;0\,\mu\,\mu)Y^*_{l'\mu}(\hat{R})\frac{\sqrt{4\pi(2l+1}}{\sqrt{(2\lambda+1)4\pi}}$$

This is the coupling between the outgoing particle and the electron. Since R is the internuclear coordinate, the above may only couple when lying in the same plane.

Further

$$\sum_{ll'}\frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}}C(l\,\lambda\,l';000)C(l\,\lambda\,l;0\,\mu\,\mu)Y^*_{l'\mu}(\hat{R})Y_{lm}(\hat{R})$$

$$= \sum ll'\frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}}C(l\,\lambda\,l';0\,\mu\,\mu)\delta_{l'l}\delta_{\mu m}$$

and

$$Y_{lm}(\hat{K}')\delta_{l'l}\delta_{\mu m} = Y_{l'\mu}(\hat{K}')$$

so that after integrating over $\hat{l}$ one finds $A_{\epsilon,\lambda\mu}$

$$= \frac{8\pi}{\sqrt{KK'}}\sum_{ll'}(i)^{l-l'}\exp i(\delta_l+\delta'_{l'})\frac{\sqrt{(2l+1)}}{\sqrt{4\pi(2l'+1)}}$$

$$Y^*_{l'\mu}(\hat{K}')C(l\,\lambda\,l';000)C(l\,\lambda\,l';0\,\mu\,\mu)$$

$$\int dRF_l(K'R)F_l(KR)G_\lambda(R)$$

Lengths of this electronic nuclear system that are of interest are

(i) The K-shell radius for the target

$$a(z_2) = \frac{(\hbar)^2}{Z_2 e^2 m}$$

(ii) The distance of closest approach

$$D = \frac{Z_1 Z_2 e^2}{E}$$

(iii) The radius of the nuclear potential R_N

(iv) The nuclear Coulomb distortion

$$\xi = \frac{D/2}{1/q} \qquad \text{where } 1/q = 1(K - K') \simeq v/\omega$$

(v) The radius R_m is between the electronic and nuclear distances so th-

$$1/q, a(Z_2) >> R_m >> D, (1/K), R_N$$

By looking at R_m the radial integral will now be split into two parts. One part will reflect the distance between R_m and the nuclear part while the other will be the ditance outside R_m. The reason for this procedure is to make it possible to evaluate the radial integral asymptotically. (Blair (6))

$$\int_{R_m}^{\infty} F_l'(K'R) F_l(KR) G_\lambda \, dR$$

$$= -\int_{R_m}^{\infty} (2i)^{-2} (\exp -i(KR - \eta \ln(2KR) - l\pi/2 + \delta_l(E)) - \exp i(KR - \eta \ln(2KR)$$

$$-l\pi/2 + \delta_l(E)))$$

$$(\exp(-i(K'R - \eta \ln(2K'R) - l\pi/2 + \delta_l'(E)))$$

$$-(\exp i(K'R - \eta \ln(2K'R) - l\pi/2 + \delta^{l}l'(E)))\, G_\lambda\, dR$$

The integrals containing the rapidly oscillating terms

$$\exp \pm i(K + K')R$$

were neglected so that only the following terms are left. (Blair (6))

$$\int_{R_m}^{\infty} F_{l'}'(K'R) F_l(KR) G_\lambda dR$$

$$\simeq (1/4) \int_{R_m}^{\infty} \exp(i(K' - K)R + i\eta \ln(2KR) - i\eta \ln(2K'R)) G_\lambda (\exp(i(\delta_{l'}' - \delta_l)) i^{l-l'} +$$

$$\int_{R_m}^{\infty} \exp i(K - K')R + i\eta \ln(2K'R)$$

$$G_\lambda\, dR (\exp i(\delta_l - \delta_{l'}') i^{l-l'} \simeq (1/4)(b_\lambda^* \exp i(\delta_{l'}' - \delta_l) i^{l-l'} + b_\lambda \exp i(\delta_l - \delta_{l'}') i^{l'-l})$$

with

$$(K - K')R - \eta \ln(2KR) + \eta \ln(2K'R) = qR - \eta \ln(2KR) + \eta \ln(2K'R) \simeq qR - \xi \ln(2KR)$$

so that

$$b_\lambda = \int_{R_m}^{\infty} dR\, G_\lambda(R) \exp(i(qR - \xi \ln(2KR))$$

and

$$A_{\epsilon_f \lambda \mu} = \frac{4\pi}{\sqrt{KK'}} \sum_{ll'} \frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}} Y_{l'\mu}^*(\hat{K'})\, C(l\lambda l'; 000)$$

$$-(\exp i(K'R - \eta \ln(2K'R) - l\pi/2 + \delta' l'(E))) G_\lambda \, dR$$

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$$\int_{R_m}^{\infty} F_l'(K'R) F_l(KR) G_\lambda dR$$

$$\simeq (1/4) \int_{R_m}^{\infty} \exp(i(K' - K)R + i\eta \ln(2KR) - i\eta \ln(2K'R)) G_\lambda (\exp(i(\delta_{l'}' - \delta_l)) i^{l-l'} +$$

$$\int_{R_m}^{\infty} \exp i(K - K')R + i\eta \ln(2K'R)$$

$$G_\lambda \, dR (\exp i(\delta_l - \delta_{l'}') i^{l-l'} \simeq (1/4)(b_\lambda^* \exp i(\delta_{l'}' - \delta_l) i^{l-l'} + b_\lambda \exp i(\delta_l - \delta_{l'}') i^{l'-l})$$

with

$$(K - K')R - \eta \ln(2KR) + \eta \ln(2K'R) = qR - \eta \ln(2KR) + \eta \ln(2K'R) \simeq qR - \xi \ln(2KR)$$

so that

$$b_\lambda = \int_{R_m}^{\infty} dR \, G_\lambda(R) \exp(i(qR - \xi \ln(2KR))$$

and

$$A_{\epsilon,\lambda\mu} = \frac{4\pi}{\sqrt{KK'}} \sum_{ll'} \frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}} Y_{l'\mu}^*(\hat{K}') \, C(l\,\lambda\,l'; 0\,0\,0)$$

$$C(l\,\lambda\,l';0\,\mu\,\mu)(\exp(i2\delta_l)b_\lambda + \exp(2i\delta_{l'})b^*_\lambda(-1)^{l-l'}) = A_1 + A_2$$

where

$$A_1 = \frac{4\pi}{2K}\sum_{ll'}\exp(2i\delta_l)\frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}}Y^*_{l'\mu}(\hat{K}')C(l\,\lambda\,l';000)C(l\,\lambda\,l';0\,\mu\,\mu)b_\lambda\frac{\sqrt{4\pi(2\lambda+1)}}{\sqrt{(2\lambda+1)4\pi}}$$

From previous considerations:

$$Y^*_{l0}(\hat{K}')Y^*_{\lambda\mu}(\hat{K}') = \frac{\sqrt{(2l+1)(2\lambda+1)}}{\sqrt{(2l'+1)4\pi}}C(l\,\lambda\,l';000)C(l\,\lambda\,l';0\,\mu\,\mu)Y^*_{l'\mu}(\hat{K}')$$

and

$$Y^*_{l0}(\hat{K}') = \frac{\sqrt{(2l+1)}}{\sqrt{4\pi}}P_l(\cos\theta)$$

$$D^\lambda_{\mu 0}(0,\theta,0) = \frac{\sqrt{4}}{\sqrt{(2\lambda+1)}}Y^*_{\lambda\mu}(\hat{K}')$$

one finds that

$$A_1 = i(2Ki)^{-1}D^\lambda_{\mu 0}(\hat{K}')\sum_l(2l+1)P_l(\cos\theta)\exp(2i\delta_l)b_\lambda = if(\theta,E)D^\lambda_{\mu 0}(\hat{K}')b_\lambda$$

so that the nuclear scattering amplitude is given by

$$f(\theta,E) = (2iK)^{-1}\sum_l(2l+1)P_l(\cos\theta)\exp(2i\delta_l(E))$$

By using the symmetry relation for the addition of angular momenta as given by Rose (8)

$$C(j_1\,j_2\,j_3\,;\,m_1\,m_2\,m_3) = (-1)^{j_2+m_2}\frac{\sqrt{(2j_3+1)}}{\sqrt{(2j_1+1)}}C(j_3\,j_2\,j_1\,;\,-m_3\,m_2\,-m_1)$$

one finds that

$$C(l\,\lambda\,l';000)C(l\,\lambda\,l';0\,\mu\,\mu)$$

$$= (-1)^{\lambda+0}(-1)^{\lambda-\mu-0}C(l'\,\lambda\,l;000)C(l'\,\lambda\,l;-\mu\,\mu\,0)\frac{\sqrt{(2l'+1)(2l'+1)}}{\sqrt{(2l+1)(2l+1)}}$$

Therefore

$$A_2 = (-1)^{l-l'}\frac{4\pi}{2K}\sum_{ll'}\exp(2i\delta_l^l)\frac{\sqrt{(2l+1)^2}}{\sqrt{4\pi(2l'+1)}}Y^*_{l'\mu}(\hat{K}')b^*_\lambda\frac{(2l'+1)}{(2l+1)}(-1)^{2\lambda-\mu}$$

$$C(l'\,\lambda\,l;000)C(l'\,\lambda\,l;-\mu\,\mu\,0)$$

with

$$l+\lambda = l'$$

so that

$$(-1)^{l-l'}(-1)^{2\lambda-\mu} = (-1)^{-\lambda}(-1)^{2\lambda-\mu} = (-1)^{\lambda}(-1)^{-\mu}$$

According to the orthogonality relation of the Clebsch-Gordon coefficients :

$$\sum_l C(l'\,\lambda\,l;000)C(l'\,\lambda\,l;-\mu\,\mu\,0) = \delta_{-\mu 0}$$

Since

$$Y^*_{l'\mu}(\hat{K}') = P_{l'}(\cos\theta)\frac{\sqrt{(2l'+1)}}{\sqrt{4\pi}}$$

A_2 becomes

$$A_2 = \delta_{-\mu 0}(01)^{\lambda}(-1)^{-\mu}(2K)^{-1}b^*_\lambda\sum_{l'}\exp(2i\delta_{l'}^l(E'))P_{l'}(\cos\theta)(2l'+1)$$

$$= \delta_{\mu 0}(-1)^{\lambda} i b_{\lambda}^{*} f(\theta, E')$$

with

$$f(\theta, E') = f(\theta, E - \Delta E) = \frac{(-1)^{-\mu}}{2iK} \sum_{l'} \exp(2i\delta_{l'}^{l}) P_{l'}(\cos\theta)(2l+1)$$

so that $A_{\epsilon_f \lambda \mu}$

$$= i(f(\theta, E) D_{\mu 0}^{\lambda}(0, \theta, 0) b_{\lambda} + i(-1)\delta_{\mu 0} f(\theta, E') b_{\lambda}^{*})$$

If ionisation occurs on the way into the nuclear collision with an atomic amplitude b_{λ}^{*} only $\mu = 0$ electronic states can be populated and the projectile loses an energy ΔE before reaching the nuclear potential and therefore the nuclear scattering amplitude will be reduced by $E - \Delta E$.

Should ionisation occur on the way out with an amplitude b_{λ}, f will be evaluated at the energy E. The rotation matrix will predict the direction of the projectile on its way out.

From the definition P_k becomes

$$P_k(\theta, E) = \frac{\int_0^{\infty} d\epsilon_f \sum_{\lambda\mu} |f(\theta, E) D_{\mu 0}^{\lambda} b_{\lambda} + (-1)^{\lambda} f(\theta, E - \Delta E) \delta_{\mu 0} b_{\lambda}^{*}|^2}{|f(\theta, E)|^2}$$

$$\simeq \int_0^{\infty} d\epsilon_f \sum_{\lambda\mu} |D_{\mu 0}^{\lambda}(\theta) b_{\lambda} + (-1)^{\lambda} \delta_{\mu 0} (f(\theta, E - \Delta E)/f(\theta, E) b_{\lambda}^{*}|^2$$

The scattering amplitude f consists of a Coulomb scattering amplitude f_c and a nuclear (resonant) amplitude f_n.

$$f = f_c + f_n$$

The variation in P_k is expected to be the largest for $f_n << f_c$ ie. at backward scattered angles.

It must be noted that the atomnic amplitudes

$$b_\lambda = \int_{R_m}^{\infty} dR\, G_\lambda(R) \exp i(qR - \xi \ln(2KR))$$

is independent of the l-value of the nuclear resonance and is generally only important for $\lambda = 0$ and $\lambda = 1$.

Due to the importance of the U_K/Γ parameter referred to in Chapter 1, a detailed analysis of this parameter now follows:

$$U_k/\Gamma = 1$$

The probability for the production of K-shell X-rays by protons elastically scattered from ^{58}Ni was observed to change as the proton energy was varied over the $s_{1/2}$ nuclear resonance at $E_p = 3.151$ MeV by Blair (9) in 1978 . The energy spread of the incident beam was small compared to the width of the nuclear resonance. In this situation the nuclear amplitudes of the $s_{1/2}$ isobaric analogue resonance were well understood so that it gave them the opportunity to study the atomic amplitudes at a laboratory scattering angle of $\theta = 90^0$. By choosing certain laboratory angles, significant contributions of neighbouring p or d wave resonances can be eliminated because

$$f_n(\theta, E) = (2iK)^{-1} \int_l (2l + 1)\, P_l(\cos\theta) \exp(2i\delta_l(E))$$

with

$$P_0(\cos\theta) = 1 \qquad l = 0$$

$$P_1(\cos,\theta) = \cos\theta \qquad l = 1$$

$$P_2(\cos\theta)(1/2)(3\cos^2\theta - 1) \qquad l = 2$$

They found P_k to be very sensitive to the phase of δ_λ. The choice of solid angle resulted in a large yield for the surface barrier detector at $\theta \simeq 95^0$ and for the NaI(Tl)

scintillator 0.8 cm from the target at $\theta = -90^0$. U_k was 8.3 keV and Γ_p was 5.6 keV which resulted in a $U_k/\Gamma = 1.5$ which in turn le.. an interference of about 50%.

In 1981 Chemin (10) measured the depen.nce of the ^{88}Sr K-shell ionisation probability on the projectile energy in the vicinity of the d wave (J = 5+/2) isobaric analogue resonance at 5060 keV in the reaction: $^{88}Sr(p,p_0)$. Γ_p was 19 keV and U_k = 16.1 keV so that this ratio was equal to 0.8. The protons were elastically scattered at a lab angle of 90^0. The surface barrier detectors as well as the NaI scintillators were placed at 90^0 to the beam direction. The angular aperture of the particle detectors was approximately 15 degrees. The solid angles for the two scintillators were 3.45 sr. P_k was insensitive to the phase of b_λ and gave a variation of about 20%. The ^{88}Sr isobaric analogue resonance is made up of many narrow resonances in order to see the effect on P_k.

$$U_k/\Gamma < 1$$

In 1982 Chemin (11) measured P_K across the 6.06 MeV s wave elastic scattering resonance in $H^+ + ^{88}Sr$ for which $U_k/\Gamma = 0.24$. The variation in P_k in the vicinity of the resonance energy was of the order of 10%. They found that a comparison between the values of the maximum excursions of $P_k(\theta, E)$ and the values of U_k/Γ does not lead to any simple relation. They also showed that the P_k at the resonance energy did not only depend on the resonance width but also on the Coulomb scattering.

$$U_k/\Gamma << 1$$

In 1980 Duinker (12) made coincident measures on ^{12}C between KLL Auger electrons and elastically backscattered protons at 125^0. P_k was measured across the 0.46 MeV (l = 0) resonance in the $^{12}C(p,p_0)$ reaction. Γ was 35 keV and U_k = 0.28 keV which gave a ratio of 0.008. They then succeeded in obtaining a 70% variation in P_k which was not in accordance with the theory. In 1982 Meyerhof (14) also measured P_k for the same resonance. Instead of using a carbon target they used a methane gas jet target which the proton beam had to traverse. They concluded that they did not see any time delay effect at all. The spurious results from Duinker were most likely due to proton scattering

external to the target accompanied by secondary electrons.

$$U_k/\Gamma >> 1$$

In 1983, Chemin (5) presented a new experimental method to extract the compound elastic (CE) scattering cross section. This method can be used where the nucleur excitation takes place through a doorway state such as an isobaric analogue state. This state has the property that the total width is the sum of the partial width Γ_p corresponding to the decay through the continuum and a width Γ_{CN} which corresponds to decay through the complicated compound nuclear states. When the elastic scattering takes place the CE fraction would be delayed with respect to the direct elastic (DE) scattering. Therefore the measurement of P_k across an IAR would reflect quantitively the amount of CE scattering.

The nuclear reaction amplitude can be written as

$$f(\theta, E) = \bar{f} + f^{fl}$$

where $\bar{f}$ consists of f_c and the part of f_n which varies slowly with energy, whereas f^{fl} is the part of f which fluctuates rapidly with energy due to the influence of compound nuclear levels in the IAR.

The parameter under consideration is thus the compound nuclear level width Γ_{CN} which is very much smaller than U_k. The slowly varying part of f has a resonance shape with a width Γ_{IAR}. The spread of the beam energy is assumed to be very much larger than the spacing between the CN levels so that the average is over hundreds of compound nuclear levels. Since f^{fl} depends on the energy, one finds

$$\langle f_{fl} \rangle_e = 0$$

The averaged scattering cross section is defined as

$$
\begin{aligned}
(d\sigma/d\Omega) &= \langle |f^2| \rangle \\
&= |\bar{f}(E)|^2 + \left\langle |f^{fl}(E)|^2 \right\rangle \\
&= (d\sigma/d\Omega)_{DE+IAR} + (d\sigma/d\Omega)_{CE} \\
&= \sigma_{DE} + \sigma_{CE}
\end{aligned}
$$

The direct elastic differential cross section σ_{DE} contains the Coulomb scattering, the potential scattering as well as the decay of the isobaric analogue resonace through the continuum.

By finding an expression for the scattering matrix

$$\left\langle S^{fl}_{cc'}(E)\, S^{*fl}_{cc'}(E) \right\rangle$$

one can find the expression for $\left\langle |f^{fl}(E)|^2 \right\rangle$ which is the compound nuclear contribution to the scattering cross section.

According to King (13) the expresson for the scattering matrix is:

$$\left\langle S^{*fl}_{cc'}, S^{fl}_{c'_1 c_1} \right\rangle = \exp i(\delta_c + \delta_{c'}) \exp -i(\delta_{c_1} + \delta_{c'_1}) \left(\frac{p_1 \beta}{p_1 + \sum_{\bar{c}} p_{\bar{c}}}\right)$$

$$\frac{\Gamma_c{}^{1/2} \Gamma_{c'}{}^{1/2} \Gamma_{c_1}{}^{1/2} \Gamma_{c'_1}{}^{1/2}}{(E - E_R)^2 + (1/4)\Gamma^2}$$

for scattering between channels coupled to the IAR, with

$$p_1 = \frac{\Gamma' \Gamma''}{(E - E_R) + (1/4)\Gamma^2}$$

the eigenvalue obtained form the resonant part of (S).

δ_c is the real optical model phase shift.

For resonances below the (p,n) threshold one can assume $\beta \simeq 1$ and for those 600 keV above this threshold β increases approximately to 1.2. The c, c', c_1, c'_1 are the physical channels coupled to the IAR. The channels not coupled to the resonance are denoted by $\bar{c}$.

According to Anholt (4):

$$\sigma_{CE} \simeq \frac{p_1}{p_1 - \sum_e p_e(E_R - E)^2 + (\Gamma/2)^2}$$

when $E = E_R$, $p_1 >> \sum_e p_e, \sigma_{CE}$ becomes

$$\sigma_{CE} = \frac{\sigma_0(\theta)(1/4)\Gamma^2}{(E - E_R)^2 + (1/4)\Gamma^2}$$

with $\sigma_0(\theta)$ a constant, ie the peak cross section at the scattering angle. It is well known that for scattering angles less than 90^0 the CE contribution in the ionization probability one should look at backward scattering angles.

P_k becomes, from Chemin(5)

$$= \sum_{\lambda\mu} \int_0^\infty d\epsilon_f |f(\vartheta, E) b_\lambda D^\lambda_{\mu 0}(\theta) + f(\theta, E - \Delta E) b^*_\lambda (-1)^\lambda \delta_{\mu 0}|^2 / (d\sigma/d\Omega)$$

$$\simeq \sum_{\lambda\mu} \int_0^\infty d\epsilon_f (|\bar{f}(E) b_\lambda D^\lambda_{\mu 0} + (-1)^\lambda \delta_{\mu 0} \bar{f}(E - \Delta E)|^2 +$$

$$\langle |f'^{\prime}(E) b_\lambda D^\lambda_{\lambda\mu} + f'^{\prime}(E - \Delta E) b_\lambda (-1)^\lambda \delta_{\mu 0}|^2 \rangle)(1/(\sigma_{DE} + \sigma_{CE}))$$

$$\simeq \sum_{\lambda\mu} \int_0^\infty d\epsilon_f \, (|\bar{f}(E) b_\lambda D^\lambda_{\mu 0} \bar{f}(E - \Delta E) b^*_\lambda|^2) +$$

$$\sum_{\lambda\mu} \int_0^\infty d\epsilon_f |b_\lambda|^2 (\langle |f'^{\prime}(E)|^2 + |f'^{\prime}(E - \Delta E)|^2 \rangle)(1/(\sigma_{DE} + \sigma_{CE}))$$

The first term refers to the elastic cross section of Blair (9) with b_λ and b^*_λ in phase. The second term

$$\sum_{\lambda\mu} \int_0^\infty d\epsilon_f |b_\lambda|^2 (\sigma_{CE}(E) + \sigma_{CE}(E - \Delta E))$$

is the creation of a K-vacancy by a particle that has been scattered by the compound nucleus. The time delay due to this reaction is therefore long and the ionization amplitudes b_λ are no longer necessarily in phase, ie no longer add coherently. Also the imaginary part

of b_λ falls away completely. For $\sigma_0 = 0$, P_k reduces to the usual Blair-Anholt formula. Anholt (4) found that, when compound elastic scattering only is considered, at large scattering angles, the dip normally associated with P_k was filled in, so that P_k is almost independent of the projectile energy at these angles.

Chemin (5) measured the 5.06 MeV $^{88}Sr(p,p_0)$ resonance at 160^0 by using an annular detector with a mean angle of 155 - 160 degrees. By using a value

$$\sigma_0(160^0) = 40 \pm 10\, mb/sr$$

their theoretical curve fits their experimental data very well, unlike the $\sigma_0 = 0$ value. They therefore concluded that for a $d_{5/2}$ resonance there is an important elastic contribution to P_k at large scattering angles.

The usual way of measuring compound elastic scattering is by looking at the interference of partial waves in the entrance channel, ie by looking at polarized and unpolarized beams. Therefore s wave resonances cannot be detected by this method. According to Chemin (5) this restriction need not apply to this new experimental method. They measured the P_k across the 6.02 MeV s wave resonance of $^{88}Sr(p,p_0)$ at 155^0. For this reaction the total width Γ was 34 keV and Γ_p was 11.5 keV. The best fit to their experimental data was when they used the value $\sigma_0 = 0$ and not $\sigma_0 = 40$, thereby indicating that compound elastic scattering is not an important factor for s wave resonances at any angle. In conclusion, it can be said that the ionization probability P_k is affected by the compound nuclear structure of the IAR.

In 1985 M Dost (19) et al extended the parameter range to Z = 56 and l = 3 by observing P_k for the $f_{7/2}$ isobaric analogue resonance seen in the H^+ ^{33} Ba collision at 10.003 MeV.

P_k was measured at two different scattering angles, approximately at 60^0 and 113^0. An annular particle detector was placed at 170^0 which served to locate the nuclear resonance in the elastic cross section. The solid angle for the particles were 2.8 sr and for the X-rays, 4.2 sr. These large solid angles resulted in a good yield. The detector geometry was optimized for maximum solid angles and all the detectors were placed in the same plane.

The value for U_k is 32.9 keV and Γ_{TOTAL} is 69 keV, which resulted in a P_k variation of 50% at backward scattered angles and 10% for the $45^0 \leq \theta \leq 80^0$ interval.

In 1987 Spooner (26) detected a large resonance effect in P_k whilst measuring it very accurately. They cooled down their surface barrier detectors and ensured reproducibility of their data by measuring each point for 30 hours. By using this method they got a coincidence peak with a very short rise time even though their beam current was relatively high. A high beam current usually results in a more noisy spectrum. They fitted their data with a least squares fitting routine and by using values for the cross section instead of P_k. They did not gain any information about the imaginary parts of the atomic amplitudes, and gave the atomic amplitudes the values of mostly 1.00. An interesting conclusion they reached was that the value $\sigma_0 = 40\,mb$ represented an upper limit to the CE cross section.

THE RATIO R

Ever since Blair (9) defined the coincidence to singles ratio R, ie

$$R = (Im\, b_0 / Re\, b_0)$$

others have also looked at similar ratios. R is treated as a parameter and by fitting R to the experimental curve they obtain a value for R and thus the b_λ content. This leads to information about the incoming and outgoing atomic ionisation amplitudes in P_k.

Blair (9) found that there was a large difference when R was varied from -0.6 to 0.6. Chemin(10) found variations of only 10% when they changed from -6 to 6.

Chemin (11) defined R as the following:

$$R = P_k(\theta, E - E_R)/P_k(\theta, /E >> E_R)$$

and found that there was no simple dependence between R and the parameter

$$y = 2\,U_k/\Gamma$$

Later Chemin (5) defined the relative excursion

$$R(\theta) = (P_k(\theta)(\text{on resonance}))/(P_k(\theta)(\text{off resonance}) - 1)$$

and looked at $\theta = 90^0$ and $\theta = 155, 160$ degrees.

They found that the values of $R(\theta)$ were $0.09 \pm 0.14\,(\theta = 90^0)$ for the s wave resonance and $-0.24 \pm 0.14\,(\theta = 155^0 - 160^0)$ which is in accordance with the general Blair-Anholt formula. Their $R(\theta)$ value for the d wave resonance was in accordance with the compound elastic theory and differed from the general Blair-Anholt formula. The values were:

$$-0.34 \pm 0.17 \qquad \theta = 90^0$$

$$0.05 \pm 0.14 \qquad \theta = 155^0 - 160^0$$

Dost (19) defined

$$R_\lambda = Im\, b_\lambda / Re\, b_\lambda$$

and calculated a value

$$R_0 = -0.30 \pm 0.30$$

by choosing $Im\, b_0$ from on resonance data and $Re\, b_0$, $Re\, b_1$ from off resonance data. R_0 was treated as the fitting parameter. The value for R_0 obtained were at the angles of $45^0 - 135^0$. A lot of approximations were made in order to calculate $b_\lambda\, f$.

Chapter 3

Computation of the Ionization Probability

This program was written in order to make a comparison between the theory and the experimental results. In previous publications (Chemin (10), Dost (20)) various methods of calculation were done in order to determine P_k. In this work P_k was calculated very accurately using different functions for $R_{\epsilon_f \lambda}$ and calculating R_λ instead of using it as a parameter and then trying to fit it with the data (Blair (9)), thereby assuming the data is the reality in the first place.

What was done in this work was a completely theoretical calculation of P_k independent of the experimental results. Actual values of the atomic amplitudes b_λ were obtained as well as values for the scattering amplitude f, and also P_k. By using this program it was possible to calculate a value for the Ratio R, for both $\lambda = 0$ and $\lambda = 1$. It also shows what P_k actually looks like. By inserting values for the partial widths Γ_p and the total width Γ the amount of elastic scattering can be determined. A value for Γ_p was given as 5.6 keV by Browne (27) for the nickel resonance. According to Browne (27), the Γ_p/Γ ratio should be close to one for the $^{58}Ni(p, p_0)$ reaction. For example: the values chosen for Γ_p and for Γ, that resulted in the best model for P_k, were 7.0 keV and 9.0 keV respectively, so that the ratio is approximately one thereby indicating that only elastic scattering took place.

What now follows is the mathematical description of the different functions that were used in order to calculate P_k.

The Ionization Probability P_k

$$P_k(\theta, E) = \frac{\int_0^\infty d\epsilon_f \sum_{\lambda\mu} |D^\lambda_{\mu 0} f(\theta, E) b_\lambda + (-1)^\lambda \delta_{\mu 0} f(\theta, E - \Delta E) b^*_\lambda|^2}{|f(\theta, E)|^2}$$

consists of the scattering amplitude given by Blair (6):

$$f(\theta, E) = -\frac{D}{4} (1/\sin)^2 (\frac{\theta}{2}) \exp(i\eta \ln((1/\sin)^2(\frac{\theta}{2})) + 2i\sigma_l)$$

$$+(2K)^{-1}\exp(2i\sigma_l)\left[\frac{\Gamma_p}{(E_R - E) - i\Gamma/2}\right]$$

as well as the rotation matrix $D^{\lambda}_{\mu 0}$ and the ionization amplitudes b_λ, b^*_λ with

$$\Delta E = U_k + \epsilon_f$$

THE FUNCTION $\sigma = \arg\Gamma(\lambda + 1 + i\eta)$

The σ_λ can be rewritten as (Abramowitz (18))

$$\arg\Gamma(\lambda+1+i\eta) = \eta\frac{\Gamma'(\lambda+1)}{\Gamma(\lambda+1)} + \sum_{n=0}^{\infty}\left(\frac{\eta}{\lambda+1+n} - \arctan\frac{\eta}{\lambda+1+n}\right)$$

$$= \eta\frac{\Gamma(\lambda+1)}{\Gamma(\lambda+1)}\left(-C + \sum_{m=0}^{\infty}\left(\frac{1}{m+1} - \frac{1}{\lambda+1+m}\right)\right)$$

$$+ \sum_{n=0}^{\infty}\left(\frac{\eta}{\lambda+1+n} - \arctan\frac{\eta}{\lambda+1+n}\right)$$

with

$$\Gamma'(\lambda+1) = \int_0^\infty x^{\lambda+1-1}\exp^{-x}\ln x\,dx$$
$$= \Gamma(\lambda+1)[\psi(\lambda+1)]$$

and

$$\psi(\lambda+1) = -C + \sum_{m=0}^{\infty}\left(\frac{1}{m+1} - \frac{1}{\lambda+1+m}\right)$$

from Gradshteyn (17).

THE FUNCTION $D^{\lambda}_{\mu 0}(0,\theta,0)$

From Rose (8) we have

with

$$d^j_{m'm}(\beta) = \frac{\sqrt{(j-m)!\,(j+m')!}}{\sqrt{(j+m)!\,(j-m')!}} \frac{(\cos\frac{\beta}{2})^{2j+m-m'}(-\sin\frac{\beta}{2})^{m'-m}}{(m'-m)!}$$

$$_2F_1(m'-j, -m-j;\, m'-m+1;\, -\tan^2\frac{\beta}{2})$$

so that

$$D^\lambda_{\mu 0} = d^\lambda_{\mu 0}(\theta) = \frac{\sqrt{(\lambda)!\,(\lambda+\mu)!}}{\sqrt{(\lambda)!\,(\lambda-\mu)!}} \frac{(\cos\frac{\theta}{2})^{2\lambda-\mu}(-\sin\frac{\theta}{2})^{\mu}}{\mu!}$$

$$_2F_1\,(\mu-\lambda, -\lambda;\, \mu+1;\, -\tan^2\frac{\theta}{2})$$

λ is assumed to be important for $\lambda = 0$ and $\lambda = 1$ only and was calculated for both these values. The program subsequently showed that this is a valid assumption since the equation for $\lambda = 1$ is a few orders smaller than that for $\lambda = 0$.

THE IONIZATION AMPLITUDE

b_λ is assumed to be independent of the proton energy E_p and is evaluated for eight different ionisation energies ϵ_f, at the resonance energy E_R.

The Coulomb part of b_λ is given by Blair (6).

$$b^C_\lambda = \int_{Rm}^{\infty} \exp(-iq(\epsilon_f)R)\, C_\lambda(R)\, dR$$

with

$$q = (\frac{U_k + \epsilon_f}{\hbar v})$$

and

$$C_\lambda(R) = \frac{-Z_1 c}{137\, v(E_R)}(2\lambda+1)^{-1/2}$$

$$C_\lambda(R) = \frac{-Z_1 c}{137\, v(E_R)}(2\lambda+1)^{-1/2}$$

$$\left(\int_R^\infty r^2\, \mathcal{R}_{\epsilon_f \lambda} \mathcal{R}_{1s} \frac{R^\lambda}{r^{\lambda+1}}\, dr + \int_0^R r^2\, \mathcal{R}_{\epsilon_f \lambda} \mathcal{R}_{1s} \frac{r^\lambda}{R^{\lambda+1}}\right) \qquad (1)$$

and

$$\mathcal{R}_{1s} = \left(\frac{Z_2}{a_0}\right)^{3/2} 2 \exp\left(\frac{-Z_2}{a_0}\right)$$

is the radial wave function for the bound electron.

THE FUNCTION $\mathcal{R}_{\epsilon_f \lambda}$

This function represents the unbounded electron and several functions can actually be chosen to describe this unbounded state. The function for $\mathcal{R}_{\epsilon_f \lambda}$ was chosen for the computation by observing the following:

The Coulomb potential acts in the exterior region of the atom for which the Schrödinger equation is:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right)\psi(\vec{r}) = E\psi(\vec{r})$$

with the wave function given by

$$\psi(\vec{r}) = \sum_\lambda R_\lambda(r) P_\lambda(\cos\theta)$$

This can be rewritten as

$$\left(\nabla^2 + k^2 - \frac{2\eta k}{r}\right)\psi = 0$$

with

$$\eta = \frac{Z_1 Z_2 e^2}{\hbar v(\epsilon_f)}$$

and $k = 2\mu E/\hbar^2$ is the wavenumber.

The radial equation is given by Jackson (7) as

$$\frac{1}{r}\frac{d}{dr}(r^2\frac{d}{dr})R_\lambda(r) +$$

$$[k^2 - \frac{2\eta k}{r} - \frac{\lambda(\lambda+1)}{r^2}]R_\lambda(r) = 0$$

with the asymptotic form of the radial wave function for a large r given by Jackson (7) as:

$$R_\lambda(r) \simeq \frac{v^{-1/2}(2ik)^\lambda \exp(-\eta\pi/2)\Gamma(\lambda+1+i\eta)}{(2\lambda)!}$$

$$\frac{\exp(\eta\pi/2)\exp(i\sigma_\lambda)\Gamma(2\lambda+2)}{(2k)^\lambda\Gamma(\lambda+1+i\eta)(kr)}(\sin(kr-\lambda\pi/2-\eta\ln(2kr)+\sigma_\lambda)$$

$$= \frac{v^{-1/2}\exp(i\sigma_\lambda)i^\lambda(2\lambda+1)}{(kr)}(\sin(kr-\lambda\pi/2-\eta\ln(2kr)+\sigma_\lambda)$$

The asymptotic form of the confluent hypergeometric function $F_\lambda(\eta(\epsilon_f), k(\epsilon_f)r)$ is given by Jackson (7) as

$$F_\lambda(\eta, kr) \simeq \sin(kr - \lambda\pi/2 - \eta\ln(2kr) + \sigma_\lambda)$$

so that $R_\lambda(r)$ can be written as

$$R_\lambda(r) = \frac{v^{-1/2}\exp(i\sigma_\lambda)i^\lambda(2\lambda+1)}{(kr)} F_\lambda(\eta, kr)$$

The function $F_\lambda(\eta, kr)$ is also the regular Coulomb function. Putting $kr = \rho$ one finds from Abramowitz (17):

$$F_\lambda(\eta,\rho) = C_\lambda(\eta)\rho^{\lambda+1}e^{i\rho}M(\lambda+1-i\eta, 2\lambda+2, 2i\rho)$$

with

$$C_\lambda(\eta) = \frac{2^\lambda\exp(-\eta\pi/2)|\Gamma(\lambda+1+i\eta)|}{\Gamma(2\lambda+2)}$$

The radial equation is given by Jackson (7) as

$$\frac{1}{r}\frac{d}{dr}(r^2\frac{d}{dr})R_\lambda(r) +$$

$$[k^2 - \frac{2\eta k}{r} - \frac{\lambda(\lambda+1)}{r^2}]R_\lambda(r) = 0$$

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$$= \frac{v^{-1/2}\exp(i\sigma_\lambda)i^\lambda(2\lambda+1)}{(kr)}(\sin(kr-\lambda\pi/2-\eta\ln(2kr)+\sigma_\lambda)$$

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$$F_\lambda(\eta,\rho) = C_\lambda(\eta)\rho^{\lambda+1}e^{i\rho}M(\lambda+1-i\eta, 2\lambda+2, 2i\rho)$$

with

$$C_\lambda(\eta) = \frac{2^\lambda\exp(-\eta\pi/2)|\Gamma(\lambda+1+i\eta)|}{\Gamma(2\lambda+2)}$$

$$F_\lambda(\eta,\rho) = \frac{\exp(\frac{-\eta\pi}{2})|\Gamma(\lambda+1+i\eta)|(2\rho)^{\lambda+1}M(\lambda+1+i\eta,2\lambda+2,-2i\rho)}{(2\lambda+1)!}$$

which is the form given by Jackson (7)

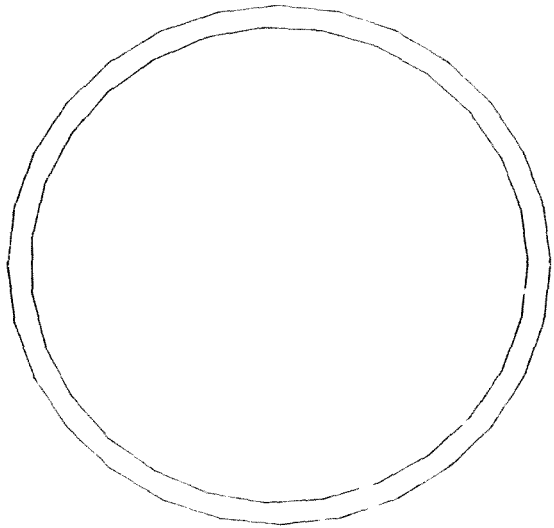
The evaluation of the regular Coulomb wave function $F_\lambda(\eta,\rho)$ is accomplished by using the subroutine RCWFF. (Barnett (19)).

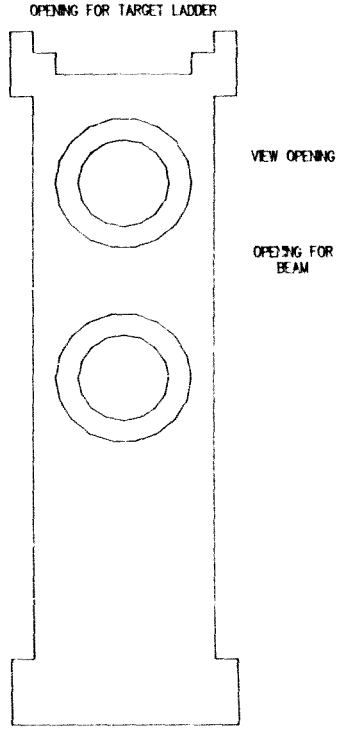
The subroutine used for the integration is called QTFE. (IBM System/360 Scientific Subroutine Package) This subroutine evaluates the trapesoid rule. By using this subroutine it was easy to manipulate R to go from $R \rightarrow \infty$ in the first integral in equation 1, and then from $0 \rightarrow R$ in the second integral , as well as taking other functions of R into account. It was important that the same R be calculated at the same time for the different functions of R.

This program is accurate for values of $Z_2 \geq 25$ and for $\epsilon_f \leq 290$ eV. In order to increase the accuracy for other values of Z_2 the dimensions will have to be increased in the CLAMBDA subroutine.

The program assumes that the projectile is a proton since the theory was developed for this situation.

FIG 1 THE TARGET CHAMBER





Chapter 4

THE EXPERIMENTAL EQUIPMENT

A. THE COINCIDENCE EXPERIMENT

The research obtained in this work was done by using the Wits Tandem Van De Graaff Accelerator. The proton beam obtained from the ion source of the accelerator were deviated to the 30^0 West beam line in the target room. The "pancake" target chamber which is of a design to optimise the solid angles of the detectors involved, is situated on this beam line.

The experiments performed on this beam line includes the coincidence experiments as well as the 3.151 MeV nickel resonance determinations. A cobalt resonance determination was also done on this line as well as the 30^0 East line.

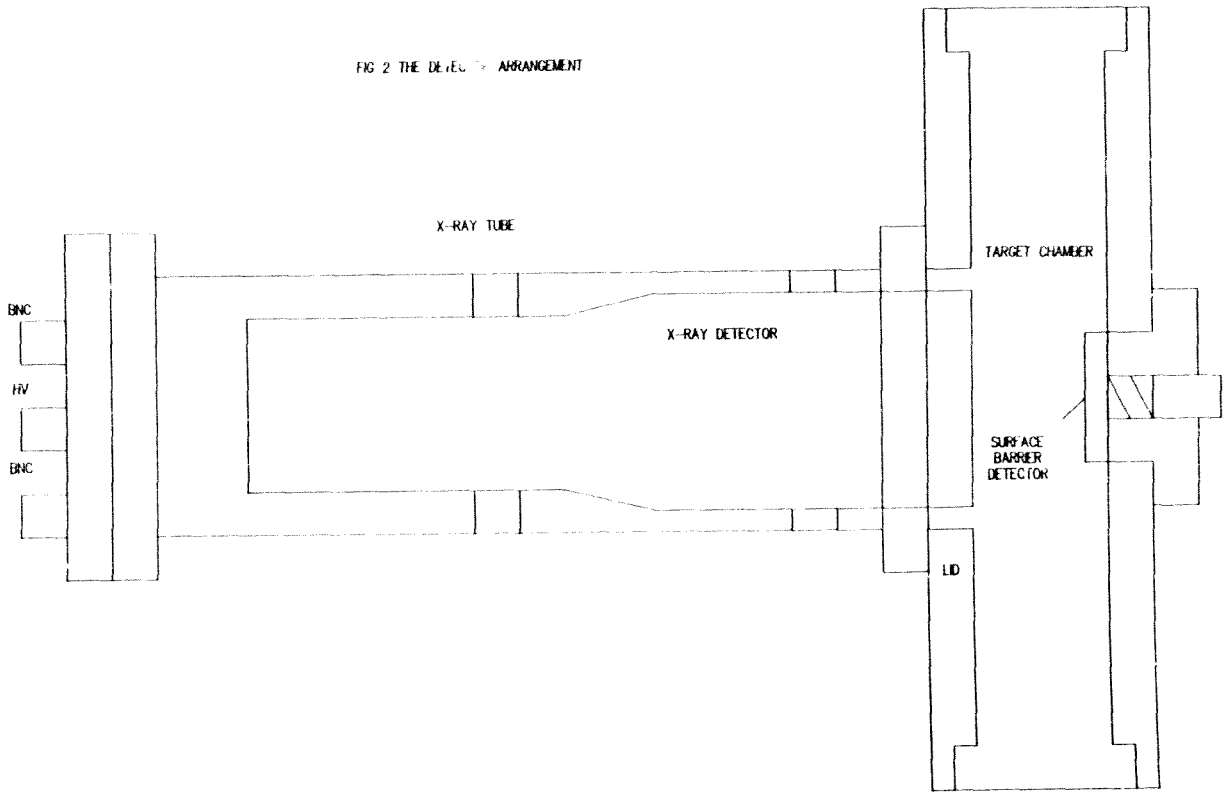
1. The Target Chamber and Detector Arrangement.

The target chamber consisted of a steel 5 cm wide cylinder with a diameter of 26 cm. (FIG 1) The lids were made of aluminium in order to reduce the X-rays that might scatter off iron if steel were used. The target holder was lowered into this "pancake" chamber from an aperture at the top of the tube. The target ladder consisted of a thin aluminium rod which was fastened onto the target holder and then tilted at 45^0 with respect to the beam direction.

The protons elastically scattered from the target were detected by a surface barrier detector. This detector was fastened onto one of the aluminium lids of the chamber so that it was situated at 90^0 with respect to the beam direction in the horizontal plane.

The X-rays resulting from the ionisation of the K-shell, were detected by a 7.62 cm diameter x 0.6 cm thick sodium iodide scintillation detector with a 0.025 cm thick Be window, placed at 90^0 to the beam direction. The X-ray detector was mounted in an aluminium tube which fastened onto the other aluminium lid of the chamber so that both the detectors were housed inside the vacuum of the target chamber. (FIG 2)

FIG 2 THE DETECTOR ARRANGEMENT



This resulted in the two detectors being very close to the target and in the same horizontal plane. The solid angles were 2.23 sr for the particle detector and 3.81 sr for the X-ray detector.

2.Target Thickness and preparation.

The cobalt and nickel metal targets were vacuum deposited onto $10\mu g/cm^2$ carbon films. The cobalt metal was spectrographically pure. The nickel was enriched ^{58}Ni. The cobalt/nickel was placed into an electron bombardment crucible inside a glass vessel which was kept at a pressure of around 5 x 10^{-6} torr. The filament was set at a temperature of about 1800^0 C and then a high voltage supply was adjusted to the crucible, until all the nickel/cobalt was evaporated onto the carbon films. (Rose (16)).

The cobalt evaporated onto the carbon had a thickness of $15\mu g/cm^2$, whilst that of the nickel was $10\mu g/cm^2$. These thicknesses were found to be sufficient to determine the resonances in both the cobalt and the nickel.

3.The Electronics Circuit.

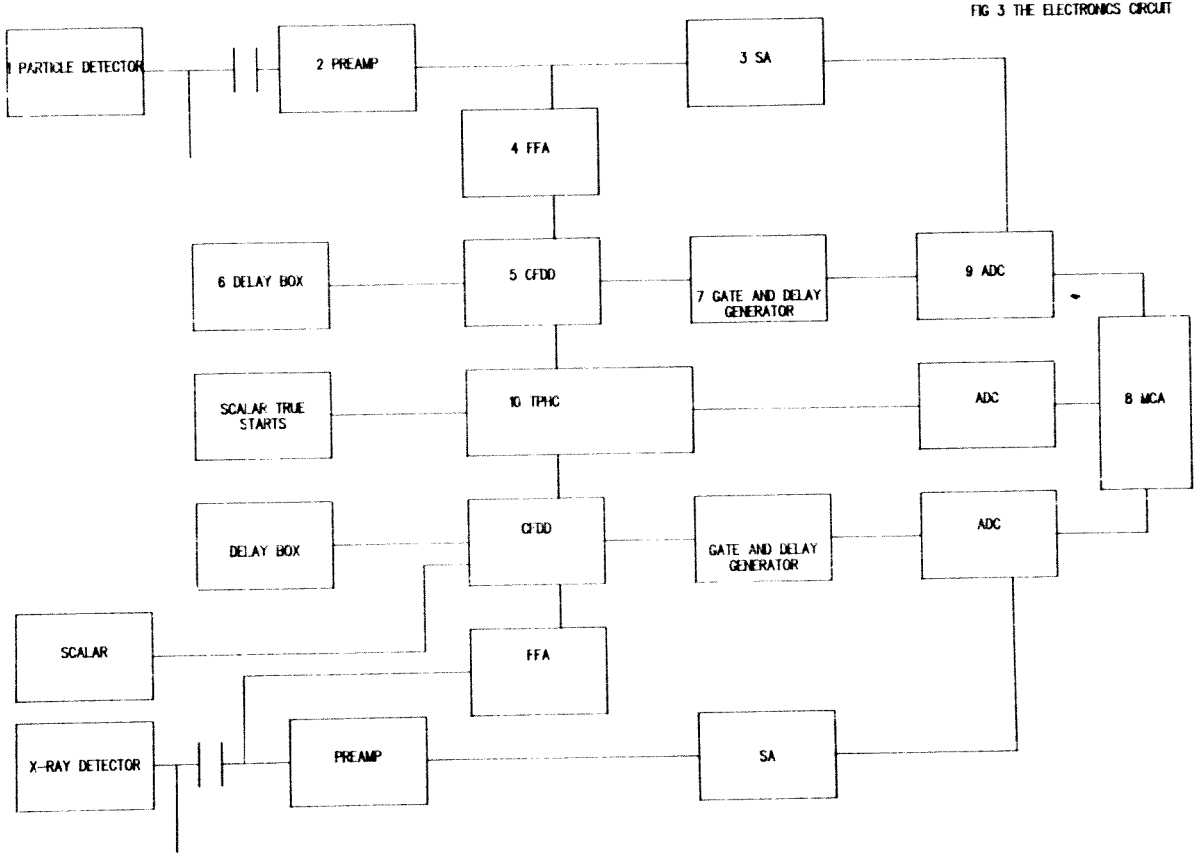
The nickel and cobalt K-shell ionization probabilities were measured by a fast coincidence timing circuit. The actual circuit used is shown in Figure 3.

The energy signals of both the particle as well as the X-ray detectors were fed into preamplifiers. The energy signals were then amplified (SA) and sent through to the multichannel analyzer (MCA) to interpret the spectra.

It was found that, by not sending the timing signal from the X-ray detector through a preamplifier, better timing resolution was obtained. The timing signal from the particle detector went through the same preamplifier as the energy signal. The timing signals were amplified (FFA) and then sent through constant fraction discriminators (CFDD). The timing signals still contain energy information so that the CFDD enables one to discriminate between different energy peaks from inspection by the oscilloscope. By adjusting the FFA, the rise time of the timing signals can be varied. This leads to optimization of the coincidence rate between the particle and the X-ray signals, since all the signals then have similar rise times.

The pulses coming from the output of the CFDD were fast logic pulses and had to be delayed by a gate and delay generator in order to coincide with the slow pulses coming

FIG 3 THE ELECTRONICS CIRCUIT



1. Surface Barrier Detector. ORTEC/EG and G. BA 25-450-100

2. Preamplifier. Canberra 970D: Surface Barrier Detector. ORTEC 113: X-ray Detector

3. Spectroscopy Amplifier. Canberra 1413.

4. Fast Filter Amplifier. ORTEC 579.

5. Constant Fraction Differential Discriminator. ORTEC 583.

6. Delay Box. ORTEC 425A.

7. Gate and Delay Generator. ORTEC 416A.

8. Multichannel Analyzer. Nuclear Data.

9. Analogue to Digital Converter. Nuclear Data.

10. Time to Pulse Height Converter ORTEC 467.

1. Surface Barrier Detector. ORTEC/EG and G. BA 25-450-100

2. Preamplifier. Canberra 970D: Surface Barrier Detector. ORTEC 113: X-ray Detector

3. Spectroscopy Amplifier. Canberra 1413.

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7. Gate and Delay Generator. ORTEC 416A.

8. Multichannel Analyzer. Nuclear Data.

9. Analogue to Digital Converter. Nuclear Data.

10. Time to Pulse Height Converter. ORTEC 467.

from the energy signal from the SA. After adjusting the CFDD one could clearly observe the effect in the various peaks on the MCA by switching the gate on or off on the ADC.

The start signal to the time-to-pulse-height converter (TAC) was assigned to the particle pulses because they come at a lower rate than the X-ray pulses; the latter were assigned as stop signals. The TAC display on the MCA is a time scale distribution unlike the SA display which is an energy scale. The TAC displays the coincidences between the signals coming from the X-rays and those coming from the particles within a pre-selected coincidence resolving time.

The nickel resonance was determined by counting the number of particles in the proton energy peaks as the resonance was traversed. The beam energy was changed each time by adjusting the magnet on the accelerator.

There are many random coincidences. Consider the following approximations for the count rates

The count rates for the particles were calculated using the formula

$$N_p = n_i x(\delta\Omega)(d\sigma/d\Omega).$$

The differential cross section for Nickel is almost the same as the Rutherford cross section so that

$$\frac{d\sigma}{d\Omega} = \frac{b^2}{16} \frac{1}{\sin^4(\theta/2)}$$

with

$$b = \frac{Z_1 Z_2 e^2}{E_p}$$

n_i is the number of ions in the beam per second and is given by

$$n_i = \frac{\text{beam current}}{e}$$

$\delta\Omega$ is the solid angle

x is the target thickness in atoms per area:

$$x = \frac{\text{target thickness x Avogadros number}}{\text{Mass of the Nickel}}$$

This leads to a value of 58 particles per second for Np. The countrate in the X-ray detector is given by

$$N_x = N_p P(b) \frac{\Omega_x}{4\pi} \omega_k$$

with ω_k the fluoressence and Ω_x the solid angle.

$P(b)$ is an approximation for the ionisation probability

$$P(b) = P(0)(1 + 1.96x' + (7/16)\pi x'^2)e^{-2x'}$$

$P(0)$ represents the ionization probability at zero impact parameter

$$P(0) = Ad(1 + 0.062\,\xi + 1.238(\xi)^2)^{-4}$$

Ad is the adiabatic limit

$$Ad = \frac{2^7 e^2 Z_1^2 \xi^6}{7 a_0 \,(\text{K-shell binding energy})}$$

and

$$\xi = \frac{\hbar v(Z_2 - 0.3)}{(\text{K-shell binding energy})a_0}$$

$$x' = \frac{b_1(\text{K-shell binding energy})}{\hbar v}$$

with b_1 taken from

$$\tan\frac{\theta}{2} = \frac{b}{2b_1}$$

The value for N_x was calculated to be 0.021153 particles per second.

The total X-ray countrate

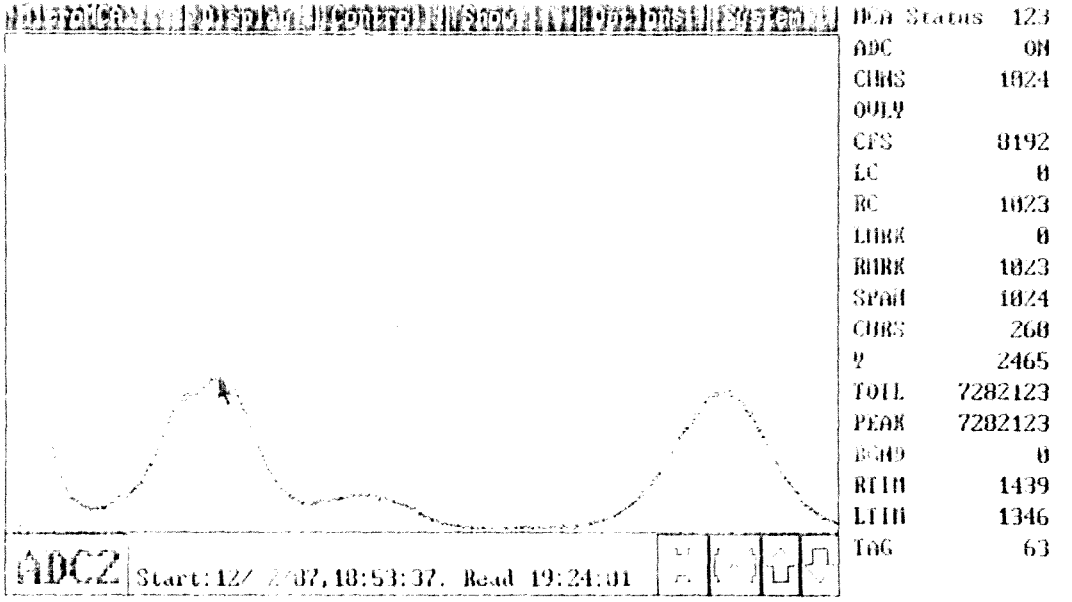
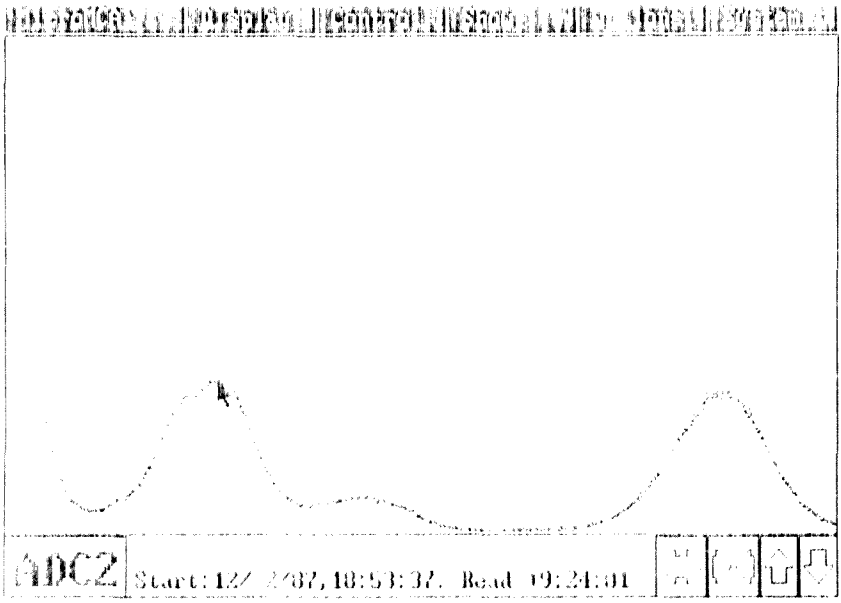

MCA Status 123
ADC ON
CHNS 1024
OVLV
CFS 8192
LC 0
RC 1023
LMRK 0
RMRK 1023
SPAN 1024
CHRS 268
Y 2465
TOTL 7282123
PEAK 7282123
BGND 0
RTIM 1439
LTIM 1346
TAG 63
ADC2
Start: 12/ /87, 18:53:37. Read 19:24:01

FIG 4



Hist Status	123
ADC	ON
CHNS	1024
ONLY	
CPS	8192
LC	0
RC	1023
LHRX	0
RHRX	1023
SPad	1024
CHRS	268
Y	2465
TOTL	7282123
PEAK	7282123
BGND	0
RTIM	1439
LTIM	1346
TAG	63

FIG 4

$$N_{TOT\,x} = n_i\, x\, \sigma_x \frac{\Omega_x}{4\pi} = 348415 \text{ particles per second}$$

with

$$\sigma_x = 2\pi \int P(b)\, b\, db$$

which is the summation of the ıtion probability over all impact parameters . Therefore the total X-ray count: rate leads to random as well as true coincidences

The true coincidences will, due to the geometry, (Chemin (2)) be in the majority and happen at the same time which will be visible on the time scale and therefore produce a peak.

The efficiency of the X-ray detector as well as the particle detector were determined by using a ^{241}Am 0.114321 μCi alpha, gamma and X-ray radiating source. oincidence spectra were obtained for the 59 keV gamma and alpha coincidences, the L-shell X-ray and alpha coincidences as well as the M-shell X-ray and alpha coincidences.

The energy spectra for the various gamma and X-rays were also used for calibration purposes. Since the energy of the K-shell X-ray ı 7.7 keV for the cobalt and 8.3 keV for the nickel, it was very useful to optimize conditions for the 6.12 keV M-shell - alpha coincidence peak of ^{241}Am. The L_1-shell and L_2-shell peaks of ^{241}Am are located at 23.7 and 22.9 keV. (FIG 4)

B.THE COBALT RESONANCE DETERMINATION EXPERIMENT

The proton beam from the accelerator was deviated to the 30^0 East beam line which was more suitable for cnarged particle resonance detection work. The target chamber consisted of a 75 cm diameter aluminium drum with a perspex lid. This chamber housed several surface barrier detectors located at various angles.

The energy signals coming from the particle detectors were fed through preamplifiers to the spectroscopy amplifiers so that the energy peaks were clearly visible on the MCA.

The number of elastically scattered particles in each detector was determined as the resonance was traversed.

A resonance suggested by Demeter (21) situated at 2.448 MeV in the reaction $^{59}Co(p,\gamma)^{60}Ni$ was looked for but not located.

Chapter 5

Results and Discussion

The results for the nickel conicidence experiment are given in Table 1. The time taken for each point ranged from five to six hours. This accumulation time resulted in errors ranging from 11% to 15%. The beam current was kept steady at 0.1×10^{-9} Amperes. In order to determine the size of P_k, $P_k/P_{k\,off}$ was calculated for every energy. A variation of about 50% was obtained just like Blair (9) and according to the theory this was to be expected.

The results of the nickel resonance determination experiments are given in Table 2. In order to obtain a high accuracy measurement of the resonance the beam current was kept at 40 - 50 nA. Run # 1 was measured during the coincidence run while Run # 2 was measured later. The resonance occured at 3.152 MeV. (FIG 6 & 7)

The results of the cobalt resonance determinations are given in Table 3. This resonance was originally measured by Erlandsson (15) at 2.100 MeV in the reaction $^{59}Co(p,\gamma)^{60}Ni$. This cobalt resonance determination was a $^{59}Co(p,p_0)$ reaction and since the energy of is so low the maximum beam cur ent obtained was only 30 - 40 nA. In order to determine where the resonance occured the machine was calibrated by measuring a well known carbon resonance at 4.8 MeV. I concluded that the cobalt resonance occured at 2.090 Mev. (FIG 8 & 9)

The results of the program that calculated the ionization probability P_k are given in Table 4. Eight values of ϵ_f were calculated. At around 10 eV the b_λ, b_λ^* were at their largest so that it might not be necessary to calculate ϵ_f for values close to U_k. (Spooner (26))

The ratio R_0 is equal to 0.9 for $l = 0$ and R_1 is equal to - 3.5 for $l = 0$. The first value seems to indicate that there are equal amounts of real and imaginary ionization amplitude contributions to P_k at 90^0. At backward scattering angles a value for R_0 was calculated to be -0.3. (Dost (20)). Blair (9) tried to fit his four points of the nickel coincidence by using the following values for R_0:

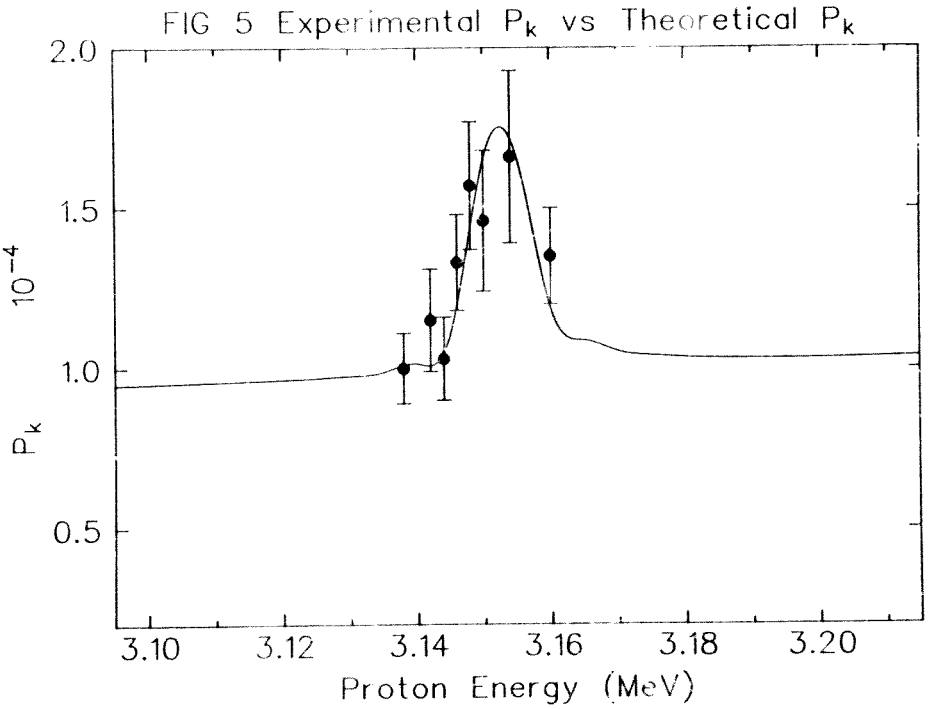


FIG 5 Experimental P_k vs Theoretical P_k
2.0
1.5
1.0
0.5
P_k 10^{-4}
3.10
3.12
3.14
3.16
3.18
3.20
Proton Energy (MeV)

FIG 5 Experimental P_k vs Theoretical P_k

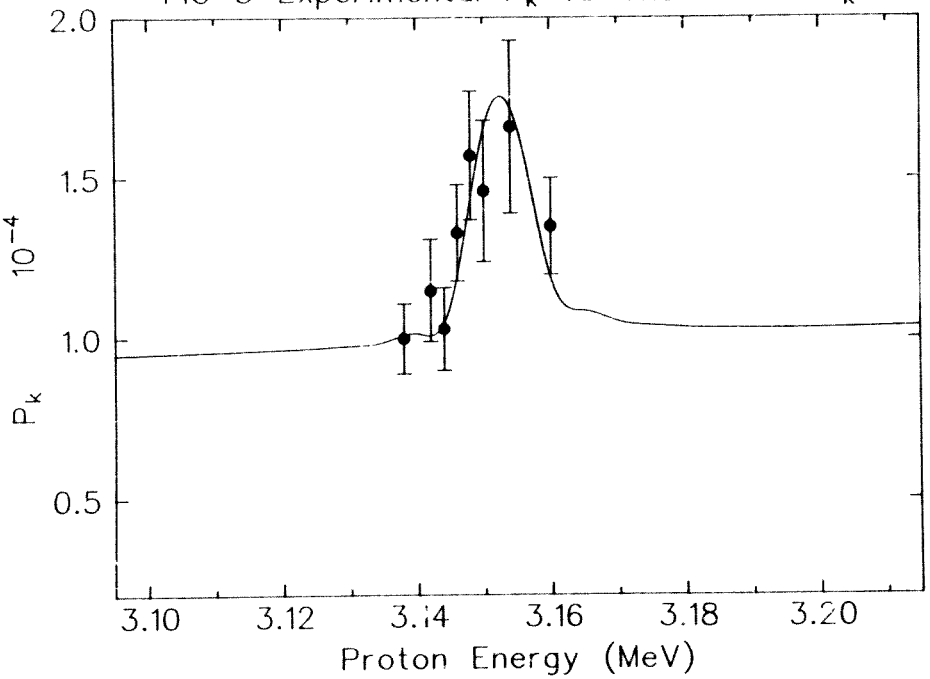


TABLE 1 THE COINCIDENCE EXPERIMENT

ENERGY (MEV)	PARTICLES FROM CFDD	TRUE STARTS	COINCID ENCES	PARTICLES AFTER SPASM	COINC AFTER SPASM	ERRORS %	PK X10 −4	PK/PK OFF
3.138	2202777	2207701	492	2003489	393	11.3	1.96	1.00
3.142	1728496	1733257	448	1558449	350	13.5	2.25	1.15
3.144	2058974	2063130	367	1790842	362	13.4	2.02	1.03
3.146	2209544	2217436	1111	2198555	573	11.5	2.61	1.33
3.148	2339490	2345337	720	1652571	508	14.3	3.07	1.57
3.150	2199650	2209774	785	1774925	510	15.4	2.87	1.46
3.154	2090355	2096451	997	1765118	576	18.2	3.12	1.66
3.160	1509029	1512379	453	1377054	364	11.2	2.64	1.35

FIG 6 Nickel Resonance Run #1

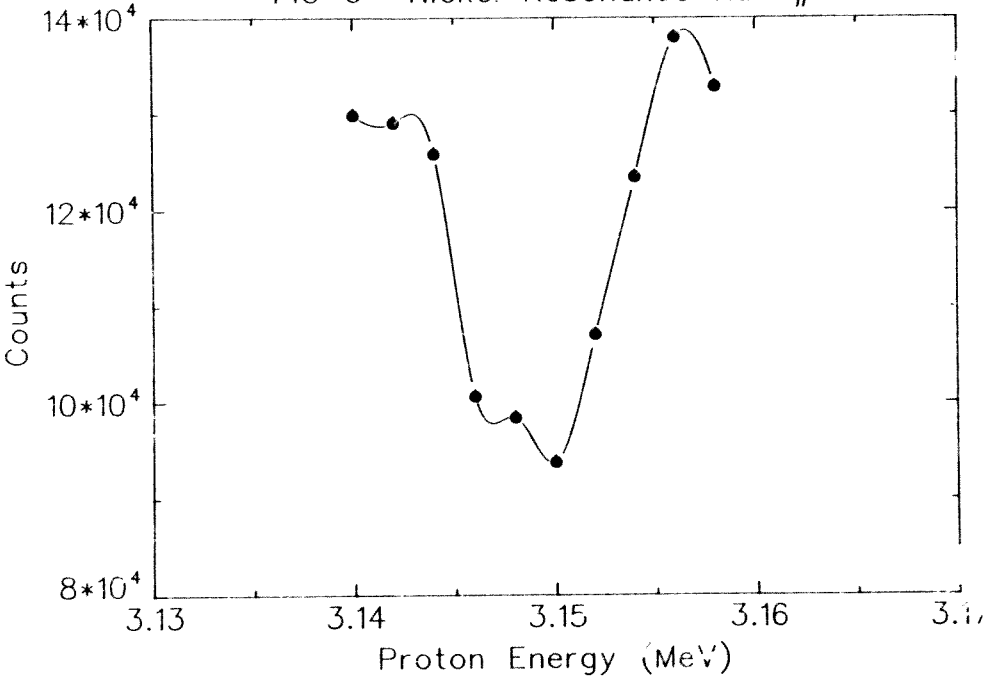


FIG 7 Nickel Resonance Run #2

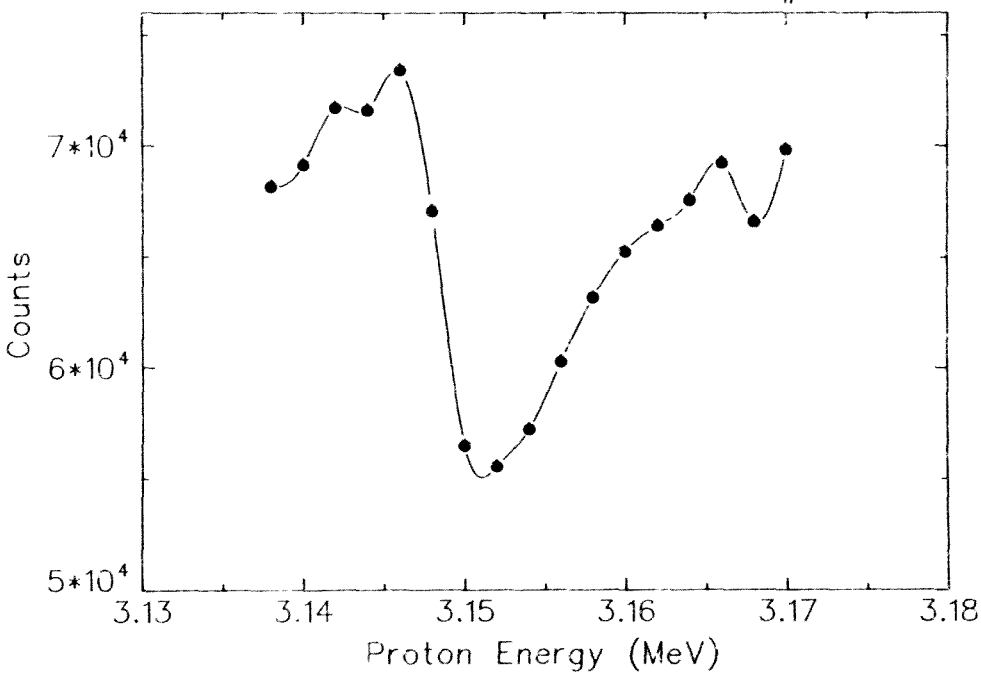


TABLE 2 THE NICKEL RESONANCE

RUN #1		RUN #2	
ENERGY (MEV)	TRUE STARTS	ENERGY (MEV)	PARTICLES FROM CFUD
3.140	129878	3.138	68163
3.142	129071	3.140	69122
3.144	125835	3.142	71714
3.146	100627	3.144	71599
3.148	98441	3.146	73407
3.150	93763	3.148	67066
3.152	107076	3.150	56492
3.154	123481	3.152	55551
3.156	137964	3.154	57244
3.158	132842	3.156	60282
		3.158	63199
		3.160	65251
		3.162	66407
		3.164	67572
		3.166	69219
		3.168	66591
		3.170	69822

TABLE 2 THE NICKEL RESONANCE

RUN #1		RUN #2	
ENERGY (MEV)	TRUE STARTS	ENERGY (MEV)	PARTICLES FROM CFDD
3.140	129878	3.138	68183
3.142	129071	3.140	69122
3.144	125835	3.142	71714
3.146	100627	3.144	71599
3.148	98441	3.146	73407
3.150	93783	3.148	67066
3.152	107076	3.150	56492
3.154	123481	3.152	55551
3.156	137964	3.154	57244
3.158	132842	3.156	60282
		3.158	63199
		3.160	65251
		3.162	66407
		3.164	67572
		3.166	69219
		3.168	66591
		3.170	69822

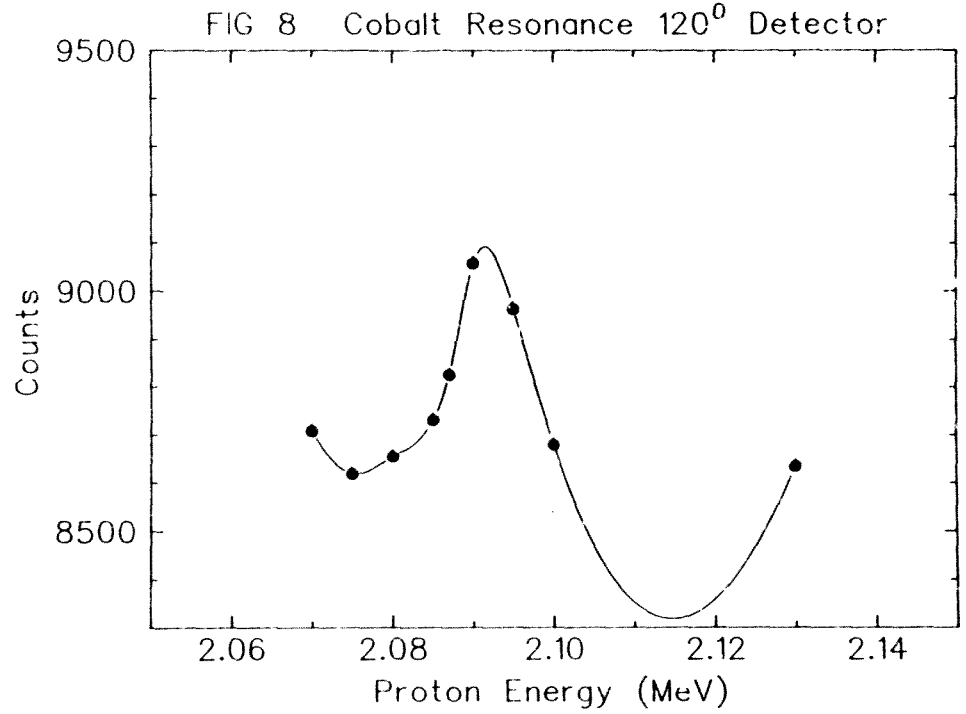


FIG 8 Cobalt Resonance 120° Detector
9500
9000
8500
Counts
2.06
2.08
2.10
2.12
2.14
Proton Energy (MeV)

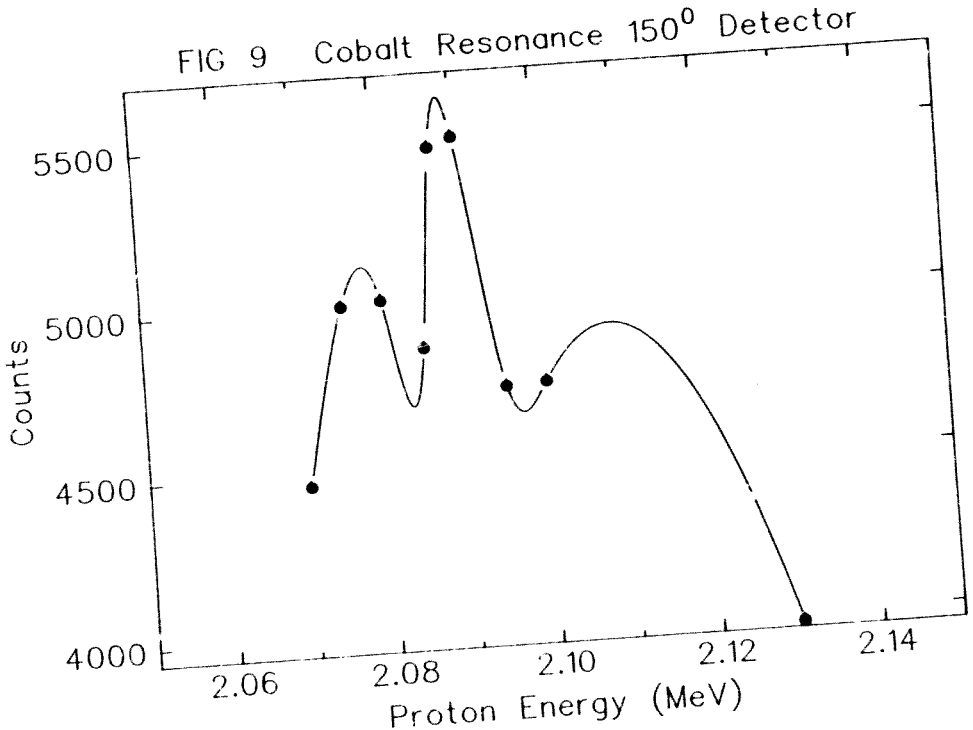


FIG 9 Cobalt Resonance 150° Detector
5500
5000
4500
4000
Counts
2.06
2.08
2.10
2.12
2.14
Proton Energy (MeV)

TABLE 3 THE COBALT RESONANCE

ENERGY (MEV)	PARTICLES FROM CFDD				
	COUNTS FROM DETECTORS SITUATED AT				
	150 DEGREES	130 DEGREES	120 DEGREES	110 DEGREES	100 DEGREES
2.070	4467	5653	8708	3682	12052
2.075	5007	5911	8619	7611	12217
2.080	5019	5896	8655	3275	12219
2.085	4868	6176	8731	4329	12658
2.087	5474	6246	8826	3729	———
2.090	5502	6180	9057	5216	12082
2.095	4737	6074	8963	5375	12090
2.100	4745	6233	8680	4505	12050
2.130	3968	6010	8635	4633	———

TABLE 4 RESULTS FROM THE PROGRAM OF PK

INPUT: GAMMA = 9 KEV, GAMMA P = 7 KEV, ER = 3.152 MEV, BIGM = 922.2629 MEV, SMALLM = 0.511 MEV, Z? = 28

THETA = 1.57 RAD, INCREMENT = 0.005, NUMBER OF VALUES = 25, FIRST ENERGY VALUE = 3.09

ENERGY (MEV)	PK X10 −4	PK/PK OF ? X10 −4	EF (EV)	B0 X 10 −9	B1 X 10 −14
3.095	0.193838	0.94731	10	−0.3119 − I 0.1968	+0.3603 − I 1.5660
3.100	0.194459	0.95034			
3.105	0.195096	0.95348	50	−0.0382 − I 0.0417	+0.2948 − I 0.1266
3.110	0.195761	0.95671			
3.115	0.196473	0.96019	90	+0.0272 : I 0.0312	+0.1368 − I 0.1839
3.120	0.197277	0.96411			
3.125	0.198265	0.96894	130	+0.0746 − I 0.0213	+0.0129 + I 0.1211
3.130	0.199651	0.97572			
3.135	0.202037	0.98738	170	+0.0764 + I 0.0197	−0.1069 + I 0.0409
3.140	0.207483	1.01399			
3.145	0.226215	1.10554	210	−0.0115 + I 0.0384	−0.0616 − I 0.0317
3.150	0.337985	1.65182			
3.155	0.339669	1.66000	250	−0.0104 − I 0.0109	−0.0429 − I 0.0710
3.160	0.242881	1.18699			
3.165	0.222202	1.08593	290	+0.0127 − I 0.0114	−0.0089 − I 0.0623
3.170	0.215389	1.05265			
3.175	0.212533	1.03867			
3.180	0.211227	1.03229			
3.185	0.210657	1.02950			
3.190	0.210485	1.02866			
3.195	0.210550	1.02898			
3.200	0.210766	1.03004			
3.205	0.211083	1.03159		R0 = IM B0/RE B0 = 0.918	R1 = IM B1/RE B1 = − 3.49
3.210	0.211471	1.03348			
3.215	0.211911	1.03563		R0* = IM B0*/RE B0* = − 0.918	R1* = IM B1*/RE B1* = 3.49

$$R_0 = -0.6; 0; 0.6$$

The shape of the calculated P_k is shown in figure 5. It is similar to Spooners (26) experimental one. The calculated P_k is compared to the experimental values of P_k obtained in the coincidence run. The best model was obtained when Γ_p was taken to be 7 keV rather than 5.6 keV. Γ was chosen to be 9 keV so that $\Gamma_p/\Gamma \simeq 1$ which is an indication of elastic scattering.

Blair (9) concluded that the best fit to his four points was with $R_0 = 0$. The coincidence run in this work was done across the same resonance as Blairs (9). Since twice the amount of data points were obtained and my theoretical curve fits my experimental data so well I conclude that the value of R_0 is closer to one.

The value $R_1 = -3.49$ indicates a lot of imaginary ionization amplitude contributing to P_k for $\lambda = 1$, although the contribution to P_k is the largest for $\lambda = 0$. This is the first calculation of R_1.

A better comparison with the data was obtained than Chemin (10) did with theirs when they measured P_k across the 5060 keV resonance in ^{88}Sr.

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      C
      C   CALCULATION OF A(EPSILON F,LAMBDA,ML)
            COMPLEX XX,A,B,FF1,FF2,C,D,E,F,G,H,C,P,B00,E21,E11,F1,F2
            COMPLEX FF3,R,S
            DIMENSION A(8),B(8),FF1(25),FF2(25),C(25,8),D(8)
            DIMENSION E(8),F(25,8),G(25,8),H(25,8),C(25,8),F(25,8),S(8)
            DIMENSION EF(290),ECNN(25),B00(1),E21(1),E11(1)
            DIMENSION FR(8,25),FFF(8)
            DIMENSION PR(25),S(25),A(25),FFF(25)
            REAL M,LL
            WRITE(5,1)
            READ(5,*) EINC
      1     FORMAT(' ENTER ENERGY INCREMENT EINC IN MEV ')
            WRITE(5,2)
            READ(5,*) EN
      2     FORMAT(' ENTER  FIRST ENERGY VALUE EN IN MEV ')
            WRITE(5,3)
            READ(5,*) K
      3     FORMAT(' ENTER NUMBER OF ENERGY VALUES K ')
            WRITE(5,4)
            READ(5,*) THETA
      4     FORMAT(' ENTER THETA IN RADIANS ')
            WRITE(5,5)
            READ(5,*) Z2
      5     FORMAT(' ENTER Z2 ')
            WRITE(5,6)
            READ(5,*) SMALLM
      6     FORMAT(' ENTER SMALLM IN MEV  ')
            WRITE(5,7)
            READ(5,*) M
      7     FORMAT(' ENTER M IN MEV ')
            WRITE(5,8)
            READ(5,*) UK
      8     FORMAT(' ENTER UK IN MEV ')
            WRITE(5,9)
            READ(5,*) ER
      9     FORMAT(' ENTER ER IN MEV ')
            WRITE(5,10)
            READ(5,*) GAMMAP
      10    FORMAT(' ENTER GAMMAP IN MEV ')
            WRITE(5,11)
            READ(5,*) GAMMAT
      11    FORMAT(' ENTER GAMMAT IN MEV ')
            WRITE(5,12)
            READ(5,*) LL
      12    FORMAT(' ENTER L-VALUE LL ')
      C
      C
            DO 16 J   = 1,29,4
            EF(J)     = 10.0 + J
            EFF       = EF(J)
            CALL BLAMBDA(B00,E01,B11,EFF,ER,UK,SMALLM,M,Z2,0)
            DO 13 L = 1,K,1
            M1        = (J + 3)/4
            ECMM(L)   = (L * EINC) + EN
            ECM       = ECMM(L)
```

```
C LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0202-2096-0  ***, SEE DOCUMENT
      CALL FF(F1,F2,ECM,GAMMAP,GAMMAT,ES,ZZ,M,THETA,EFF,UK,LL)
      FF1(L)  = F1
      FF2(L)  = F2
      A(M1)   = B00(1)
      B(M1)   = CONJG(B00(1))
      D000    = 1.0
      XX      = (0,1)
      C(L,M1) = XX * FF1(L) * D000 * A(M1) + (XX * FF2(L) *
     +            B(M1))
   13 CONTINUE
      CALL BLAMBDA(B00,E01,B11,EFF,ER,UK,SMALLM,M,ZZ,1)
      DO 14 L   = 1,K,1
      M1        = (J + 3)/4
      ECMM(L)   = (L * EINC) + EN
      ECM       = ECMM(L)
      CALL FF(F1,F2,ECM,GAMMAP,GAMMAT,ER,ZZ,M,THETA,EFF,UK,LL)
      FF1(L)    = F1
      FF2(L)    = F2
      XX = (0,1)
      D001      = (-2.0 * (SIN(THETA/2.0) + SIN(THETA/2.0)))
      D(M1)     = B01(1) + B11(1)
      E(M1)     = CONJG(D(M1))
      F(L,M1)   = XX * FF1(L) * D001 * D(M1) - (FF2(L) * XX *
     +            E(M1))
      D101      = SQRT(2.0) * (SIN(THETA/2.0) * SIN(THETA/2.0))
     +            * TAN(THETA/2.0)
      G(L,M1)   = XX * FF1(L) * D101 * D(M1)
   14 CONTINUE
      DO 15 L   = 1,K,1
      M1        = (J + 3)/4
      H(L,M1)   = C(L,M1) + F(L,M1) + G(L,M1)
      Q(L,M1)   = CONJG(H(L,M1))
      P(L,M1)   = H(L,M1) * C(L,M1)
   15 CONTINUE
   16 CONTINUE
      DO 18 L   = 1,K,1
      DO 17 M1  = 1,8,1
      FFF(M1,L) = P(L,M1)
      FFF(M1)   = FFF(M1,L)
      CALL QTFE(8,31,FFF,G,8)
   17 CONTINUE
   18 CONTINUE
C   CALCULATION OF PK
      DO 19 L   = 1,K,1
      ECMM(L)   = (L * EINC) + EN
      ECM       = ECMM(L)
      CALL FF(F1,F2,ECM,GAMMAP,GAMMAT,ES,ZZ,M,THETA,EFF,UK,LL)
      FF3(L)    = F1
      R(L)      = FF3(L)
      S(L)      = CONJG(FF3(L))
      PK(L)     = G(8)/(S(L) * R(L))
   19 CONTINUE
C
C
      WRITE(6,20)
   20 FORMAT(' 00 ')
      WRITE(6,21) (A(M1),M1=1,8,1)
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-8888-2896-8  ***, SEE DOCUMENTA
  21 21 FORMAT(2E14.6)
        WRITE(8,22)
  22 22 FORMAT(' B0* ')
        WRITE(8,23) (B0(M1),M1 = 1,8,1)
  23 23 FORMAT(2E14.6)
        WRITE(8,24)
  24 24 FORMAT(' B1 ')
        WRITE(8,25) (D(M1),M1 = 1,8,1)
  25 25 FORMAT(2E14.6)
        WRITE(8,26)
  26 26 FORMAT(' B1* ')
        WRITE(8,27)(E(M1),M1 = 1,8,1)
  27 27 FORMAT(2E14.6)
        WRITE(8,28)
  28 28 FORMAT(' EF ')
        WRITE(8,29) (EF(J),J = 1,29,4)
  29 29 FORMAT(E14.6)
        WRITE(8,30)
  30 30 FORMAT(' ECM ')
        WRITE(8,31) (ECM(L),L = 1,25,1)
  31 31 FORMAT(E14.6)
        WRITE(8,32)
  32 32 FORMAT(' PK ')
        WRITE(8,33) (PK(L),L = 1,25,1)
  33 33 FORMAT(E14.6)
        STOP
        END

D  R84-00     MAINPROG     MAIN     14/02/87  15:43:39  TABLE SPACE:   6 KB
SER:    20 LINES/1321 BYTES    STACK SPACE: 165 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2002-2096-0  ***, SEE DOCUMENTA
  C
  C
  C
  C
  C
  C   CALCULATION OF THE IONIZATION AMPLITUDE BLAMEDA
        SUBROUTINE BLAMEDA(B00,B01,B11,EFF,ER,UK,SMALLM,M,Z2 LAMEDA)
        COMPLEX XX,PG,PER,GE,EG,CC,EX,EXX,WCR,STH,CRNE,B00,B01,B11
        COMPLEX B1,B2,B3,C0,C1
        DIMENSION B1(1),B2(1),B3(1),C0(1),C1(1),GRI(200),WCR(1),
       +          STH(1),CRNE(1),PPP(1),B00(1),B01(1),B11(1)
        REAL M
        A0    = 0.5291771
        H     = 6.582173E-22
        CC    = 2.9979E+10
        ETA   = EE(EFF,Z2)
        VELL  = V(ER,M,CC)
        GLE   = G(UK,EFF,M,VELL)
        W     = WN(EFF,SMALLM)
        CALL CLAMEDA(Z2,EFF,ETA,A0,C0,C1,GLE,W,GRI)
        B1(1)    = C0(1)
        B2(1)    = C1(1)
        B3(1)    = GRI(200)
        VVEL     = VV(EFF,CC)
        EXX      = EX(YY,ETA,LAMEDA)
        PER      = PG(EXX)
        EG       = GE(ER,M,EXX,SMALLM)
        RINE     = F(CC,Z2,A0,VELL,VVEL,W)
        WCR(1)   = PER
        STH(1)   = EG
        CRNE(1)  = EXX
        PPP(1)   = RINE
        B00(1)   = B1(1) * CRNE(1) * PPP(1)
        B01(1)   = B2(1) * WCR(1)  * PPP(1)
        B11(1)   = B3(1) * STH(1)  * PPP(1)
        RETURN
        END

D  R04-00     SUBROUTINE  BLAMEDA   14/22/87  15:43:41  TABLE SPACE:   3 KB
FER:   20 LINES/1321 BYTES    STACK SPACE: 113 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
C   CALCULATION OF GLAMEDA, AND THE INTEGRATION
C   OVER R
      SUBROUTINE CLAMEDA(Z2,EFF,ETA,A0,C0,C1,GLE,X,GRI)
      COMPLEX XX,CII,CCII,C2A,C2E
      COMPLEX CCI,CJI,CL,CM,C0,C1
      DIMENSION FC(2),GC(1),FCF(1),GCF(1)
      DIMENSION RR(2000),RHI(200),RI(200),RK(200),Z(200),ZZ(200)
     +         ,C0I(200),C02(200),C03(200),C04(200),C0A(1),C2E
     +         (1),CR(200),CI(200),RGI(200),CRR(1),CII(1)
     +          ,CCR(200),CCI(200),CCRR(1),CCII(1)
      DIMENSION HR(2200),GR(2000),HRI(220),GRI(200),
     +          C05(220),C06(200),C07(220),C08(220),CG(220),
     +         CJ(200),CK(200),CGR(1),CGI(1),CJR(1),CJI(1),
     +          CM(1),HH(200),CH(202),CL(1),C0(1),C1(1)
      DIMENSION RG(2000),HE(2000),PL(2000)
      DIMENSION FGW(200),FER(200),ERG(220),RINE(220)
      REAL M
      DO 60 J = 1,2000,10
      RR  = 0.001 * J
      RRC = RR * X
C   CALCULATION OF THE COULOMB FUNCTION, LAMBDA = 0
      CALL RCWFF(RRO,ETA,0.0,FC,GC,FCF,GCF,1.0E-5,102.2,1)
      PL(J) = FC(1)
      RI(J) = E(RR,A0,Z2) * PL(J)
      RG(J) = CWH(RR,A0,Z2) * PL(J)
C   CALCULATION OF THE COULOMB FUNCTION, LAMBDA = 1
      CALL RCWFF(RRO,ETA,0,1,FC,GC,FCF,GCF,1.0E-5,102.2,1)
      HE(J) = FC(2)
      HR(J) = D(RR,A0,Z2) * HE(J)
      GR(J) = AA(RR,A0,Z2) * HE(J)
60 CONTINUE
C   MAKING ARRAY SMALLER SO THAT PROGRAM RUNS FASTER
C   WITHOUT LOSING ACCURACY
      DO 70 NN = 1,200,1
      J = (NN * 10) - 9
      FGW(NN)  = RHI(J)
      FER(NN)  = RG(J)
      ERG(NN)  = HRI(J)
      RINE(NN) = GR(J)
70 CONTINUE
      DO 80 I = 2,200
      N = 1 + I
C   MODIFIED GTFE SUBROUTINE TO THAT R GOES FROM R
C   TO INFINITY
      CALL QTFEM(0.001,FGW,RHI,200,N)
      CALL QTFEM(0.001,ERG,HRI,220,N)
      K = N - 1
      RI(K) = RHI(200)
      HR(K) = HRI(220)
80 CONTINUE
C   INTEGRATION SUBROUTINE FOR R THAT GOES FROM
C   0 TO R
      CALL QTFE(0.001,FER,RGI,200)
      CALL QTFE(0.001,RINE,GRI,200)
      DO 90 L = 1,200,1
```

```
      K = L
      RK(L)   = 0.021 * L
      Z(L)    = COS(RK(L))/SIZE)
      ZZ(L)   = SIN(RK(L))/SIZE)
      CB1(L) = Z(L)  * FI(L)
      CB2(L) = ZZ(L) * FI(L)
      CB3(L) = Z(L)  * FGI(L)  * (1.0/(RK(L)))
      CB4(L) = ZZ(L) * FGI(L) * (1.0/(RK(L)))
      CB5(L) = Z(L)  * FH(L)  * RK(L)
      CB6(L) = ZZ(L) * FH(L) * RK(L)
      CB7(L) = Z(L)  * GRI(L) * (1.0/(RK(L) * RK(L)))
      CB8(L) = ZZ(L) * GRI(L) * (1.0/(RK(L) * RK(L)))
   90 CONTINUE
      CALL QTFE(0.001,CB1,CR,200)
      CALL QTFE(0.001,CB2,CI,200)
      CALL QTFE(0.001,CB3,CGR,200)
      CALL QTFE(0.001,CB4,CGI,200)
      CALL QTFE(0.001,CB5,CG,200)
      CALL QTFE(0.001,CB6,CH,200)
      CALL QTFE(0.001,CB7,CJ,200)
      CALL QTFE(0.001,CB8,CK,200)
      XX  = (0,1)
      CRR(1)  = CR(200)
      CGRR(1) = CGR(200)
      CII(1)  = XX * CI(200)
      CGII(1) = XX * CGI(200)
      CBR(1)  = CRR(1) + CII(1)
      CBE(1)  = CGRR(1) + CGII(1)
      CGR(1)  = CG(200)
      CGI(1)  = XX * CH(200)
      CJR(1)  = CJ(200)
      CJI(1)  = XX * CK(   )
      CL(1)   = CGR(1) +   JI(1)
      CM(1)   = CJR(1) -    I(1)
      CB(1)   = CBA(1) + CJBE(1)
      C1(1)   = CL(1)  * CM(1)
      RETURN
      END
```

```
D  R84-00     SUBROUTINE  CL4MECA   14/02/87  15:43:  TABLE SPACE:   5 KB
FER:    28 LINES/1321 BYTES     STACK SPACE: 202 WORD
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
C
C     CALCULATION OF THE SCATTERING AMPLITUDE F(THETA,E)
C     F1 IS A FUNCTION OF THETA,E
C     F2 IS A FUNCTION OF THETA,E - DELTA E
      SUBROUTINE FF(F1,F2,ECM,GAMMAP,GAMMAT,ER,Z2,M,THETA,EFF,UK,LL)
      COMPLEX XX,SCATT,GAMMATT,SS,GG,GER,S,OWE,FUNC,F1
      COMPLEX SCATD,GERD,FUNCD,F2,ARD
      REAL M,MOMEN,MOMEND
      REAL LL
      CD = 2.9979E+23
      H  = 6.582173E-22
      DELTAE = UK + (EFF * 1.0E-06)
      EDASH  = ECM - DELTAE
      VEL    = V(ECM,M,CD)
      ETAA   = EEE(ECM,Z2,VEL,CD)
      SCATT  = SS(GAMMAP,GAMMAT,ER,ECM)
      GER    = ARD(YY,ETAA,LL)
      MOMEN  = HK(M,ECM)
      DIST   = DD(Z2,ECM)
      ANGLE  = ST(THETA)
      FUNC   = OWE(ETAA,ANGLE)
      VELD   = V(EDASH,M,CD)
      ETAAD  = EEE(EDASH,Z2,VELD,CD)
      SCATD  = SS(GAMMAP,GAMMAT,ER,EDASH)
      GERD   = ARD(YY,ETAAD,LL)
      MOMEND = HK(M,EDASH)
      DISTD  = DD(Z2,EDASH)
      FUNCD  = OWE(ETAAD,ANGLE)
      F1     = (DIST * ANGLE * GER * FUNC) + (
     -            MOMEN * GER * SCATT)
      F2     = (DISTD * ANGLE * GERD * FUNCD) +
     +         (MOMEND * GERD * SCATD)
      RETURN
      END
```

C FE4-00   SUBROUTINE FF   14/02/87 15:43:18 TABLE SPACE: 2 KB
PER.   28 LINES/1321 BYTES   STACK SPACE: 92 WORDS
ICN FLOATING PT SUPPORT REQUIRED FOR EXECUTION

```
 (LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0000-0000-2  ***) SEE DOCUMENTA
  C
  C
        FUNCTION SS(GAMMAF,GAMMAT,ER,E)
        COMPLEX XX,SS,GAMMATT
        XX = (E,1)
        GAMMATT = XX * GAMMAT
        SS = GAMMAF*((ER - E) - (GAMMATT/2.0))
        RETURN
        END

D  R04-00     FUNCTION    SS          14-02-87  15:43:48  TABLE SPACE:   1 KB
PER     26 LINES/1321 BYTES     STACK SPACE: 121 WORDS
ICATING FI SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
C
C
      FUNCTION ARD(YY,AS,NU)
      COMPLEX XX,GG,ARD
      XX   = (0,1)
      CALL SIGMA(YY,AS,NU)
      GG   = XX * YY * 2.0
      ARD = EXP(GG)
      RETURN
      END
```

D R04-00 FUNCTION ARD 14/02/87 15:43:49 TABLE SPACE: 1 KB
FER: 20 LINES/1321 BYTES STACK SPACE: 65 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION

```
C
C
C
      FUNCTION EX(YY,AS,NU)
      COMPLEX XX,GO,EX
      XX = (0,1)
      CALL SIGMA(YY,AS,NU)
      GO = XX * YY
      EX = EXP(GO)
      RETURN
      END
```

```
0  R04-00     FUNCTION    EX        14/02/87  15:43:49  TABLE SPACE    1 KE
PER:    28 LINES/1321 BYTES    STACK SPACE:  65 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
C
C   CALCULATION OF FUNCTIONS SIGMA L AND SIGMA LARGE
      SUBROUTINE SIGMA (YY,CDF,NU)
      Y = 0.0
      N = 0
      IF(NU - 2) 1,1,9
1     1 TERM = CDF/(NU + 1 + N) - ATAN(CDF/FLOAT(NU + 1 + N))
      Y = Y + TERM
      IF(ABS(TERM) - 1.0E-4) 3,3,2
2     2 N = N + 1
      GO TO 1
3     3 YY = Y + (-0.577215 * CDF)
      IF(NU - 1) 8,4,4
4     4 ZX = 0.0
      M = 0
5     5 TERM = (1/FLOAT(M + 1)) - (1/FLOAT(NU + M))
      ZX = ZX + TERM
      IF(ABS(TERM) - 1.0E-5) 7,7,6
6     6 M = M + 1
      GO TO 5
7     7 YY = YY + ZX
8     8 RETURN
      END
```

0 R84-00 SUBROUTINE SIGMA 14/02/87 15:43:50 TABLE SPACE: 2 KE
PER 20 LINES/1321 BYTES STACK SPACE: 154 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION

```
 C
        FUNCTION C(Y,QUE)
        REAL M
        C = COS(Y * QUE)
        RETURN
        END
```

```
D  R04-00     FUNCTION    C          14/02/87  15:43:51  TABLE SPACE:    1 KB
FER:    20 LINES/1321 BYTES    STACK SPACE:  59 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
      FUNCTION S(Y,QUE)
      REAL M
      S = SIN(Y * QUE)
      RETURN
      END
```

'D R84-00 FUNCTION S 14/02/87 15:43:51 TABLE SPACE: 1 KB
'FER: 20 LINES/1321 BYTES STACK SPACE: 59 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION

```
C
C
      FUNCTION Q(UK,E,H,VELL)
      REAL M
      Q = (UK + (E * 1.0E-6))/(H * VELL)
      RETURN
      END
```

```
D R04-00     FUNCTION    Q          14/02/97  15:43:51  TABLE SPACE:    1 KB
PER:    20 LINES/1321 BYTES    STACK SPACE: 117 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2002-2096-0  ***, SEE DOCUMENT.
  C
  C
        FUNCTION VCE,M,C)
        REAL M
        V =  SQRT((2.0 * E)/M) * C
        RETURN
        END

ID  A04-00     FUNCTION    V          14/02/87  15:47:52  TABLE SPACE:   1 KB
FER:   20 LINES/1321 BYTES    STACK SPACE: 121 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0002-3096-0  ***, SEE DOCUMENTA
  C
        FUNCTION  EEE(E,Z2,VEL,CO)
        EEE = ( - 1.0 * Z2 * CO )/(137.0 * VEL)
        RETURN
        END

D  R04-00     FUNCTION    EEE       14/02/87  15:43:52  TABLE SPACE    1 KB
FER:    20 LINES/1321 BYTES    STACK SPACE:  06 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
  LICENSED RESTRICTED RIGHTS AS     'CU IN 'ICENSE L-0202-3096-0  ***, SEE DOCUMENT-
   C
   C
   C
         FUNCTION D(Y,A0,ZC)
         D = EXP(( - 22/A0) * Y)/Y
         RETURN
         END

'D  R04-00     FUNCTION    D          14/02/87  15:43:52  TABLE SPACE:    1 KB
'FER:    20 LINES/1321 BYTES    STACK SPACE: 121 WORDS
;ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
V04-00                                                          14

: LICENSED RESTRICTED RIGHTS AS STATED IN .ICENSE L-2202-2096-0  ***, SEE DOCUMENT
      C
            FUNCTION AA(Y,A0,Z2)
            AA = Y * Y * EXP((- Z2/A0) * Y)
            RETURN
            END

7D  V04-00     FUNCTION    AA         14-02-87  15:43:53  TABLE SPACE:   1 KB
FFER:    20 LINES/1321 BYTES    STACK SPACE: 125 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2822-2896-2  ***, SEE DOCUMENT
  C
  C
        FUNCTION E(Y,A2,Z2)
        E = EXP(( - Z2/A2) * Y)
        RETURN
        END

'D  E84-B6     FUNCTION    E          14/02/87  15:43:53  TABLE SPACE:    1 KE
'FER:    28 LINES/1321 BYTES    STACK SPACE: 121 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
R04-0C                                                              14.

 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0222-3096-0  ***, SEE DOCUMENT
  C
        FUNCTION CWH(Y,A0,Z2)
        CWH = 1 * EXP(( - Z2/A0) * Y)
        RETURN
        END

0  R04-0C     FUNCTION    CWH       14/22/87  15:43:54  TABLE SPACE:   1 KB
FER:    20 LINES/1321 BYTES    STACK SPACE: 125 WORDS
ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0002-2096-2  ***. SEE DOCUMENT
   C
   C
         FUNCTION WN(X,SMALLM)
         WN = SQRT(SMALLM * X * 2.0E-06/(3.69360E+24))
         RETURN
         END

7D  R04-00     FUNCTION    WN        14/02/87  15:43:54  TABLE SPACE:    1 KB
FFER:    20 LINES/1321 BYTES    STACK SPACE: 113 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
R04-02                                                              14,

  LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2222-2096-2  ***, SEE DOCUMENT
   C
         FUNCTION EE(Y,Z2)
         EE = ( -  1.0 * Z2 * (3.68957489//(SQRT(Y)))
         RETURN
         END

'D  R04-00     FUNCTION    EE         14/02/87  15:43:54  TABLE SPACE:    1 KB
'FER:    20 LINES/1321 BYTES    STACK SPACE: 121 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
; LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2822-2896-8  ***, SEE DOCUMENT
      C
      C
      C
      C
            FUNCTION VV(X,CC)
            VV = 1.97835E-3 * CC * (SQRT(X))
            RETURN
            END

7D  R84-86     FUNCTION    VV        14/82/8,  15:43:55  TABLE SPACE:   1 KB
FFER:   20 LINES/1321 BYTES    STACK SPACE:  98 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0000-0096-0  ***, SEE DOCUMENT
  C
  C
        FUNCTION P(CC,ZZ,AB,VELL,VVEL,W)
        DE = (ZZ/(AB * 1.0E-10)) * * 1.5
        P  = (-2.0 * CC * DE )/(137.0 * VELL * (SQRT(VVEL)) * W)
        RETURN
        END

'D  R04-00     FUNCTION    P          14/02/87  13:43:55  TABLE SPACE:   1 KB
'FER:   20 LINES/1321 BYTES    STACK SPACE: 121 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
      C
      C
      C
            FUNCTION PG(EXX)
            COMPLEX XX,EXX,PG
            XX = (5,1)
            PG = XX * EXX * (SQRT(3.0))
            RETURN
            END
```

```
7D R84-00     FUNCTION    PG        14/02/87  15:43:56  TABLE SPACE:   1 KB
FFER:   28 LINES/1321 BYTES    STACK SPACE: 113 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
 LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2002-2096-2  ***, SEE DOCUMENT
  C
  C
  C
        FUNCTION GE(E,M,EXX,SMALLM)
        COMPLEX XX,EXX,GE
        REAL M
        XX = (Z,1)
        OG =  M * 197.32857
        GE = (XX * EXX * E * 2.0 * 137.0 * (SQRT(2.0)) * SMALLM)/(OG)
        RETURN
        END
```

```
'D  R04-00     FUNCTION    GE        14/02/87  15:43:56  TABLE SPACE:   2 KB
'FER:   20 LINES/1321 BYTES    STACK SPACE: 140 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2222-2896-2  ***. SEE DOCUMENT
   C
   C
   C
         FUNCTION HK(N,E)
         REAL M
         HK = (197.32857)/(2.0 * SQRT(2.0 * E * M))
         RETURN
         END

70  F84-00     FUNCTION    HK         14-02-87  15:43:57  TABLE SPACE:    1 KB
FFER:    20 LINES/1321 BYTES    STACK SPACE: 129 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
; LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0022-0096-0  ***) SEE DOCUMENT
      C
      C
      C    ETA IS CHOSEN TO BE NEGATIVE
             FUNCTION DD(Z2,E)
             DD = (1.0 * Z2 * 1.44)/(4.0 * E)
             RETURN
             END

'D  V04-00     FUNCTION    DD        14/02/87  15:43:57  TABLE SPACE:   1 KB
'FFER:   20 LINES/1321 BYTES    STACK SPACE:  99 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0202-2096-0  ***. SEE DOCUMENT
   C
   C
         FUNCTION ST(THETA)
         ST = 1.0/(SIN(THETA/2.0) * SIN(THETA/2.0))
         RETURN
         END

7D  R04-00     FUNCTION    ST        14/02/87  15:43:57  TABLE SPACE:    1 KB
FFER:    20 LINES/1321 BYTES    STACK SPACE: 124 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-0000-0096-0  ***, SEE DOCUMENT
  C
  C
        FUNCTION OWE(AS,ANGLE)
        COMPLEX XX,E,OWE
        XX   = (0,1)
        FF   = AS * LOG(ANGLE)
        B    = XX * FF
        OWE = EXP(B)
        RETURN
        END
```

```
7D  R04-00     FUNCTION    OWE       14/22/87  15:43:56  TABLE SPACE:   1 KB
FFER:   20 LINES/1321 BYTES    STALK SPACE:  25 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
! LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2882-2896-2  ***/ SEE DOCUMENT
      C
      C
      C
      C *** THIS SUBROUTINE CALCULATES THE COULOMB WAVE FUNCTION F(ETA,RHO)
            SUBROUTINE RCWFF(RHO,ETA,MINL,MAXL,FC,GC,FCP,GCP,ACCUR,STEP,NUMBER)
            REAL*4   K,K1,K2,K3,K4,M1,M2,M3,M4
            DIMENSION FC(2),FCP(2),GC(1),GCP(1)
      C *** COULOMB WAVEFUNCTIONS CALCULATED AT R = RHO BY THE
      C *** CONTINUED-FRACTION METHOD OF STEED   MINL,MAXL ARE ACTUAL
                              LMAX = MAXL
                              LMIN1= MINL + 1
                              XLL1 = FLOAT(MINL*LMIN1)
      C *** IF NUMER = 2 FC AND GC ARRAYS ARE RETURNED
      C *** IF NUMER = 3 FC,GC,FCP,GCP ARRAYS ARE RETURNED
            NUM = 1
            IF(NUMBER.GE.1 AND NUMBER.LE.3) NUM = NUMBR
            PACE = STEP
            ACC  = ACCUR
            IF(PACE.LT.100.0) PACE = 100.0
            IF(ACC.LT.1.0E-15.OR.ACC.GT.1.0E-3) ACC = 1.0E-6
            R    = RHO
            KTR  = 1
            LMAX = MAXL
            LMIN1= MINL + 1
            XLL1 = FLOAT(MINL*LMIN1)
            ETA2 = ETA*ETA
            TURN = ETA + SQRT(ETA2 + XLL1)
            IF(R.LT.TURN.AND.ABS(ETA).GE.1.0E-6) KTR = -1
            KTRP = KTR
            GO TO 2
      1     R    = TURN
            TF   = F
            TFP  = FP
            LMAX = MINL
            KTRP = 1
      2     ETAR = ETA*R
            RHO2 =   R*R
            FL   = FLOAT(LMAX + 1)
            FNU  = FL + 0.5
      C *** CONTINUED FRACTION FOR FP(MAXL)/F(MAXL)   FL IS F  XLFRINE IS FP **
            FF   = ETAR/FL + FL/R
            DK   = ETAR*2.0
            DEL  = 0.0
            D    = 0.0
            F    = 1.0
            K    = (FL*FL - FL + ETAR)*(2.0*FL - 1.0)
            IF(FL*FL+PL*ETAR.NE.0.0) GO TO 3
            R    = R + 1.0E-6
            GO TO 2
      3     H    = (FL*FL + ETA2)*(1.0 - FL*FL)*RHO2
            K    = K + DK + FL*FL*2.0
            D    =  1.0/(D*H + K)
            DEL =  DEL*(D*K - 1.0)
            IF(FL.LT.FNU) DEL = -R*(FL*FL + ETA2)*(FL + 1.0)*D/FL
            FL   = FL + 1.0
            FF   = FF + DEL
            IF(D.LT.0.0) F = -F
```

```
C LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2222-2096-0  ***. SEE DOCUMENT
      IF(PL .LT. 20000.) GO TO 11
      IF(ABS(DEL) .GE. ABS(FF*ACC)) GO TO 3
      FF  = F*FP
      IF( LMAX .EQ. MINL) GO TO 5
      FC (LMAX+1) = F
      FFL         = FF
      IF(NUM.EQ.2) FCF(LMAX+1) = FP
C *** STANDARD RECURSION TO MINL FOR F AND FP, ARRAYS GC,GCP ARE STORAGE
      L   = LMAX
      RI  = 1.0/R
      DO 4 LP  = LMIN1,LMAX
      FL = FLOAT(L)
      SL = ETA/FL + FL*RI
      RL = SQRT(1.0 + ETA2/(FL*FL))
      FC(L) = (SL*FC(L+1) + FPL)/RL
      FFL1 = SL*FC(L) - RL*FC(L+1)
      FPL  = FFL1
      IF(NUM.EQ.1) GO TO 4
      GC (L+1) = FL
      IF(NUM.LE.2) GO TO 4
      GCF(L+1) = SL
      FCF(L)   = FFL1
4     L  = L - 1
      F  = FC (LMIN1)
      FP = FFL1
5     IF(KTRF.EQ.1) GO TO 1
C *** REPEAT FOR R = TURN IF RHO LT TURN
C *** NOW OBTAIN P + I.Q FOR MINL FROM CONTINUED FRACTION (32)
C *** REAL ARITHMETIC TO FACILITATE CONVERSION TO IBM USING REAL*8
      P  = 0.0
      Q  = R - ETA
      PL = 0.0
      AR = -(ETA2 + XLL1)
      AI =   ETA
      BR = 2.0*Q
      BI = 2.0
      WI = 2.0*ETA
      DR =   BR/(BR*BR + BI*BI)
      DI =   BI/(BR*BR + BI*BI)
      DP = -(AR*DI + AI*DR)
      DQ =  (AR*DR - AI*DI)
6     P  =  P + DP
      Q  =  Q + DQ
      PL = PL + 2.0
      AR = AR + PL
      AI = AI + WI
      BI = BI + 2.0
      D  = AR*DR - AI*DI + BR
      DI = AI*DR + AR*DI + BI
      T  = 1.0/(D*D + DI*DI)
      DR =  T*D
      DI = -T*DI
      H  = BR*DR - BI*DI - 1.0
      K  = BI*DR + BR*DI
      T  = DP*H  - DQ*K
      DQ = DP*K  + DQ*H
      DP = T
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-8888-8888-8  ***) SEE DOCUMENT
      IF(PL.GT.46088.) GO TO 11
      IF(ABS(DF)+ABS(DG).GE.(ABS(F)+ABS(G))*ACC) GO TO 6
      F  = F/R
      G  = G/R
C *** SOLVE FOR FF,G,GF AND NORMALISE F  AT L=MINL
      G  = (FF - F*F)/G
      GF = F*G - G*F
      W  = 1.0/SQRT(FF*G - F*GF)
      G  = W*G
      GF = W*GF
      IF(KTR.EQ.1) GO TO 8
      F  = TF
      FF = TFF
      LMAX = MAXL
C *** RUNGE-KUTTA INTEGRATION OF G(MINL) AND GF(MINL) INWARDS FROM TURN
C ***                  SEE FOX AND MARTERS 1968 PG 202
      IF(RHO.LT.0.2*TURN) PACE = 999.0
      R1 = 1.0/3.0D0
      H  = (RHO - TURN)/(PACE + 1.0)
      H2 = 0.5D0*H
      I2 = IFIX(PACE + 0.001)
      ETAH = ET4*H
      H2LL = H2*YLL1
      S  = (ETAH + H2LL/R  )/R   - H2
7     RH2= R + H2
      T  = (ETAH + H2LL/RH2)/RH2 - H2
      K1 = H2*GF
      M1 = S*G
      K2 = H2*(GF + M1)
      M2 =  T*(G  + K1)
      K3 =  H*(GF + M2)
      M3 =  T*(G  + K2)
      M3 =     M3 + M2
      K4 = H2*(GF + M3)
      RH = R + H
      S  = (ETAH + H2LL/RH )/RH  - H2
      M4 =  S*(G + K3)
      G  = G  + (R1 + R2 + R2 + R3 + R4)*R1
      GF = GF + (M1 + M2 + M2 + M3 + M4)*R1
      R  = RH
      I2 = I2 - 1
C
C  1.0E300 TOO LARGE FOR PE 3220
C
C     IF(ABS(GF) GT 1.0E300) GO TO 11
      IF(ABS(GF).GT.1.0E75) GO TO 11
      IF(I2.GE.0) GO TO 7
      W  = 1.0/(FF*G - F*GF)
C *** UPWARD RECURSION FROM GC(MINL) AND GCF(MINL),STORED VALUES ARE R,S
C *** RENORMALISE FC,FCF FOR EACH L-VALUE
8     IF(NUM.GE.2) GC (LMIN1) = G
      IF(NUM.EQ.3) GCF(LMIN1) = GF
      IF(NUM.EQ.2) FCF(LMIN1) = FF*W
      FC(LMIN1) = F*W
      IF(LMAX.EQ.MINL) RETURN
      GFL = GF
      DO  9  L = LMIN1,LMAX
```

```
: LICENSED RESTRICTED RIGHTS AS STATED IN LICENSE L-2000-2096-0  ***, SEE DOCUMENT
        IF(NUM.EQ.1) GO TO 9
        IF(NUM.EQ.2) SL = ETA/FLOAT(L) + FLOAT(L)*RI
        IF(NUM.EQ.3) SL = GCP(L+1)
        RL = GC(L+1)
        GC(L+1) = (SL*GC(L) - GPL)/RL
        GPL1    =  RL*GC(L) - SL*GC(L+1)
        GPL     =  GPL1
        IF(NUM.LT.3) GO TO 9
        GCP(L+1) = GPL1
        FCP(L+1) = FCP(L+1)*W
   9    FC(L+1)  = FC(L+1)*W
        RETURN
  11    W  = 0.0
        G  = 0.0
        GP = 0.0
        GO TO 6
        END

?D  R84-00     SUBROUTINE  RCWFF     14/02/87  15:44:25  TABLE SPACE:   5 KB
FFER:    20 LINES/1321 BYTES    STACK SPACE: 167 WORDS
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
SION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
        IF(NUM.EQ.1) GO TO 9
        IF(NUM.EQ.2) SL = ETA/FLOAT(L) + FLOAT(L)*RI
        IF(NUM.EQ.3) SL = GCP(L+1)
        RL = GC(L+1)
        GC(L+1) = (SL*GC(L) - GPL)/RL
        GPL1    =  RL*GC(L) - SL*GC(L+1)
        GPL     =  GPL1
        IF(NUM.LT.3) GO TO 9
        GCP(L+1) = GPL1
        FCP(L+1) = FCP(L+1)*W
    9   FC(L+1)  = FC(L+1)*W
        RETURN
   11   W  = 0.0
        G  = 0.0
        GP = 0.0
        GO TO 6
        END
```

?D R84-00 SUBROUTINE RCWFF 14/02/87 15:41:25 TABLE SPACE: 5 KB
?PER: 28 LINES/1321 BYTES STACK SPACE: 167 WORDS
?ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION
?ION FLOATING PT SUPPORT REQUIRED FOR EXECUTION

```
V4-02                                                                    14

LICENSED RESTRICTED RIGHTS AS STATED IN  LICENSE L-2220-2896-8  ***. SEE DOCUMENT
        IF(NUM EQ 1) GO TO 6
        IF(NUM EQ 2) SL = ETA(FLOAT(L) * FLOAT(L))*RI
        IF(NUM EQ 3) SL = GCF(L+1)
        RL = GCF(L+1)
        GCF(L+1) = (SL*GCF(L) + GFL)/RL
        GFL1     =  RL*GCF(L) - SL*GCF(L+1)
        GFL      =  GFL1
        IF(NUM.LT.3) GO TO 5
        GCF(L+1) = GFL1
        FCF(L+1) = FCF(L+1)*W
6       FC(L+1)  = FC(L+1)*W
        RETURN
11      S  = 0.0
        G  = 0.0
        GP = 0.0
        GO TO 1
        END

  FOR-BJ     SUBROUTINE  PCOFF     14-FEB-87  15:44:25  TABLE SPACE:   5 KB
BP     28 LINES/1321 BYTES     STACK SPACE: 167 WORDS
%% FLOATING PT SUPPORT REQUIRED FOR EXECUTION
%% FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C       THIS SUBROUTINE DOES THE INTEGRATION OVER THE WHOLE INTEGRAND
        SUBROUTINE QTFE(H,Y,Z,NDIM)
C
C
        DIMENSION Y(1),Z(1)
C
        SUM2=0.
        IF(NDIM-1)4,3,1
      1 HH=.5*H
C
C       INTEGRATION LOOP
        DO 2 I=2,NDIM
        SUM1=SUM2
        SUM2=SUM2+HH*(Y(I)+Y(I-1))
      2 Z(I-1)=SUM1
      3 Z(NDIM)=SUM2
      4 RETURN
        END
```

```
0 FOR-22     SUBROUTINE  QTFE       14/02/87  15:44:26  TABLE SPACE:   1 KB
FOR     23 LINES/1321 BYTES     STACK SPACE: 173 WORDS
NO FLOATING PT SUPPORT REQUIRED FOR EXECUTION
```

```
C
C
C
      SUBROUTINE QTFE(H,Y,Z,NDIM,N)                                    70
C                                                                      71
C                                                                      71
      DIMENSION Y(1),Z(1)                                              71
C                                                                      71
      SUM2=0.                                                          71
      IF(NDIM-1)4,3,1                                                  71
    1 HH=.5*H                                                           7
C                                                                      71
C     INTEGRATION LOOP                                                 71
      DO 2 I=N,NDIM,1
      SUM1=SUM2                                                        71
      SUM2=SUM2+HH*(Y(I)+Y(I-1))                                       72
    2 Z(I-1)=SUM1                                                      72
    3 Z(NDIM)=SUM2                                                     72
    4 RETURN                                                           72
      END                                                              72
```

F04-00 SUBROUTINE QTFE 14/02/87 15:44:28 TABLE SPACE 1 KB
... 22 LINES/1321 BYTES STACK SPACE 175 WORDS
... FLOATING PT SUPPORT REQUIRED FOR EXECUTION