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THEORETICAL CALCULATIONS OF INELASTIC SCATTERING
MATRICES FOR MULTIGROUP REACTOR ANALYSIS.

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Reactor Development

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TOTAL 42

TABLE OF CONTENTS

PAGE NO.

LIST OF TABLES - - - - -	ii
LIST OF FIGURES - - - - -	iii
ABSTRACT - - - - -	iv
I. INTRODUCTION - - - - -	1
II. BASIS OF PHYSICAL MODEL - - - - -	2
III. TREATMENT OF KNOWN NUCLEAR LEVELS - - - - -	4
IV. INELASTIC SCATTERING PROBABILITY IN STATISTICAL REGIONS - - - - -	8
V. A CALCULATIONAL PROCEDURE - - - - -	12
VI. CALCULATION OF INELASTIC SCATTERING MATRIX FOR Fe^{56} - - - - -	17
A. Experimental Data and Theoretical Formulas - - - - -	17
B. Numerical Results for Known Nuclear Levels (Fe^{56}) - - - - -	20
C. Normalization - - - - -	22
D. Calculations of Inelastic Scattering Probability (Fe^{56}) $E_{\text{incident}} < 2.86 \text{ Mev}$ - - - - -	26
E. Calculation of Inelastic Scattering Matrix (Fe^{56}) - - - - -	33
APPENDIX A - Inelastic Scattering Probabilities in the Statistical Region - - - - -	A-1
APPENDIX B - Summary of Nuclear Level Density - - - - -	B-1
I. Models for Nuclear Level Density - - - - -	B-3
A. Fermi Degenerate Gas Model - - - - -	B-3
B. Newton's Model - - - - -	B-5
C. Cameron's Method - - - - -	B-9
II. Discussion and Conclusions - - - - -	B-11
REFERENCES - - - - -	37

LIST OF TABLES

<u>Table No.</u>	<u>Title</u>	<u>Page No.</u>
I	The Denominator Factors vs. Energy (Eqs. 21-27) for Fe ⁵⁶	24
II	Calculated Inelastic Scattering Cross Section for Various Levels of Fe ⁵⁶	25
III	Inelastic Scattering Probability Matrix for Fe ⁵⁶	34
IV	Inelastic Scattering Probability Matrix for Fe ⁵⁶ in the Statistical Region	36
A-I	Values of t_1 for MUFT Energy Groups	A-2
A-II	Normalized Inelastic Scattering Probabilities	A-8
A-III	Normalized Inelastic Scattering Probabilities	A-9
B-I	Effective Proton Spin Parameters	B-7
B-II	Effective Neutron Spin Parameters	B-8

LIST OF FIGURES

<u>Fig. No.</u>	<u>Title</u>	<u>Page No.</u>
1	The Level Scheme of Fe ⁵⁶	
2	Transmission Coefficients for Fe ⁵⁶ from Emmerich's Calculation	21
3	Comparison of Experimental Data and Calculated Inelastic Scattering Cross Section for Fe ⁵⁶	23
4	Normalized σ_1 , Normalized σ_2 , σ_3 , σ_4 and σ_5 versus incident neutron lethargy	27
5	Normalized σ_1 , Normalized σ_2 , σ_3 , σ_4 and σ_5 versus Exit Neutron Lethargy	28
6(a)	Calculated and Normalized σ_1 and σ_2 versus Permissible Values of Exit Neutron Lethargy for Incident Neutrons in MUFT Group 6	31
6(b)	Calculated and Normalized σ_2 and σ_3 versus Permissible Values of Exit Neutron Lethargy for Incident Neutrons in MUFT Group 6	32
A-1	Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature	A-3
A-2	Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature	A-4
A-3	Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature	A-5
A-4	Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature	A-6
A-5	Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature	A-7
B-1	Level Spacing per Spin State versus Number of Neutrons in Compound Nucleus (Harvey 1961)	B-2
B-2	The Parameter, a, versus Mass Number (after Ericson)	B-10

ABSTRACT

A calculational procedure for obtaining the inelastic scattering probabilities, which are required for MUFT-4 - A Multigroup Fast Neutron Spectrum Code, is described. The relevant theoretical considerations are summarized. The formulation of Hauser and Feshbach is used when known nuclear levels can be excited. In all other cases, the statistical model is recommended. To elucidate the procedure an illustration is given for Fe^{56} . In addition, general inelastic scattering probabilities are presented as a function of nuclear temperatures, and a critical discussion of the theoretical developments in the statistical model is given.

I. INTRODUCTION

The treatment of neutron slowing-down is of significant importance in the design of thermal power reactors. There are two main mechanisms by which fission neutrons lose energy: (1) the elastic scattering and (2) the inelastic scattering processes. In this report, only the inelastic scattering of neutrons is discussed. By inelastic neutron scattering, it is implied that a neutron loses part of its energy by exciting the nucleus (in the ground state) to one of its excited levels. The probability of this process depends upon the specific nuclear levels of a nucleus. It turns out that all the nuclear levels, which can in principle be excited, are not known. Sometimes the relevant information like spins, parities and excitation energies may be known experimentally only for a few nuclear levels. Consequently, a nuclear model has to be used in such calculations.

It is the purpose of this report to document a calculational procedure by which the inelastic-scattering-probability matrices, which appear in a multigroup code,¹ could be calculated. It may be remarked at this stage that most of the formalism used appears already in the literature. For the sake of clarity and convenience, this report is divided into six sections. First, a treatment of the known nuclear levels is given in Section 3, followed by a discussion of the statistical region in Section 4. Section 5 contains an illustration, and the numerical results are given for Fe⁵⁶. A summary of the statistical model and the general numerical results are given in the Appendices A and B respectively.

II. BASIS OF PHYSICAL MODEL

In 1936, N. Bohr presented a very simple idea for the mechanism of nuclear reactions - namely, the concept of compound nucleus formation. Since then, this idea has been investigated thoroughly and surprisingly enough this concept, with some minor changes, is still considered valid. The formation of a compound nucleus implies that when a neutron (or any other particle, e.g. proton, α particle) is incident on a target nucleus, a compound system (consisting of the incident particle and the target nucleus) is formed. The decay time of such a compound system is generally large compared to the nuclear time scale. Because of this reason, an incident neutron loses its identity in the compound system. Thus, in the compound system formation, it is explicitly assumed that the properties of this compound system are independent of how it was formed. For example, whether a compound system with certain quantum numbers (total angular momentum, parity and energy) is formed by an incident neutron or a proton, the decay of this system is independent of the incident particle. As is to be expected, this compound system prefers to decay giving off neutrons compared to protons, because of the strong coulomb effects in the case of a charged particle.

In many cases, a large number of compound states can be excited because of the following two reasons:

- 1) the nuclear level spacing may be less than the width of these levels and,
- 2) the spread in the incident energy of neutrons is larger than the level spacing.

If, in addition, numerous nuclear levels of a residual nucleus can be excited, we can treat the decay of the compound system in a statistical fashion. A strict test of the formation of a compound system is the prediction of isotropic angular distributions of emergent particles around $\theta = \pi/2$.

(This means terms with only $2L$ appear in the Legendere polynomial). This isotropy has been observed in more than 90% of the cases.

At this stage, we point out that the inelastic scattering calculations become more difficult when the statistical assumption of compound-system decay is not valid. For example, when only a few nuclear levels can be excited (because of the incident neutron energy) one has to use a different (physical) nuclear model. The ground work of such analyses was first proposed² by Hauser and Feshbach in 1952. In this nuclear model, an average nuclear potential is assumed and then the wave-equation is solved so that "transmission coefficients" can be calculated.^{3,4} It became obvious that this average nuclear potential should have at least two parts, namely a real part and an imaginary part. In most calculations, it has been assumed that this imaginary part of the nuclear potential is related to the real part. Further refinements - like a diffusive boundary of the nuclear potential were incorporated later on. A detailed account of these new developments appear in the review articles⁵ by Bodansky⁶ (1962), Feshbach⁷ (1960) and the original reports of Emmerich⁴ (1962).

Another new process has been discovered recently. It is called the "direct interaction" or "nuclear stripping." In this process, an incident particle does not spend so much time in the compound system and consequently retains most of its identity. This results in a strong peak in the angular distributions of emergent particles. However, it turns out that there are relatively few cases (less than 10%). So far this process has been ignored in reactor calculations. In our opinion, this cannot lead to any significant effects in a typical reactor calculations. A summary^{8,9} of the physical model for nuclear stripping is given by Bannerjee (1960) and Levinson (1960).

III. TREATMENT OF KNOWN NUCLEAR LEVELS

In this report, by known nuclear levels, we will imply that the spin excitation energy and parity of the levels have been deduced from experimental data. In this section, we consider the case when the incident neutron energy is such that only known levels can be excited. We will define $\sigma(i \rightarrow i', E \rightarrow E')$ as the cross section for the inelastic scattering of incident neutrons with energy E from a target nucleus with ground state spin i and parity $P_{(i)}$ with the target nucleus being left in an excited state with spin i' , parity $P_{(i')}$ and excitation energy $E-E'$. The energies of the incident and the inelastically scattered neutron, namely E and E' , are in Mev and in the center of mass system. Following Hauser and Feshbach, one gets:

$$\sigma(i \rightarrow i', E \rightarrow E') = \frac{\pi}{2(2i+1)} \kappa^2 \sum_{\ell=0}^{\infty} T_{\ell}(E) \sum_{J=1-(\ell+\frac{1}{2})}^{1+\ell+\frac{1}{2}} \epsilon_{i,\ell}^J (2J+1) N^J \quad (1)$$

where:

$$N^J = \frac{\sum_{\ell'=0}^{\infty} \epsilon_{i',\ell'}^J T_{\ell'}(E') \left| (-1)^{P_{(i)}+\ell} + (-1)^{P_{(i')}+\ell'} \right|}{\sum_q \sum_{\ell''=0}^{\infty} \epsilon_{i(q),\ell''}^J T_{\ell''}(E-E_q) \left| (-1)^{P_{(i)}+\ell} + (-1)^{P_{(q)}+\ell''} \right|} \quad (2)$$

with the following definitions:

κ = de Broglie wavelength of the incident neutron divided by 2π

i = spin of the ground state of the target nucleus

$P_{(i)}$ = parity of the ground state of the target nucleus

i' = spin of the excited level of the nucleus

$P(i')$ = parity of the excited level of the nucleus

q = this index implies appropriate quantum numbers of all the levels up to $E_q \leq E$.

E = energy (in Mev) of the incident neutron in C-system.

E' = energy (in Mev) of the inelastically scattered neutron in D-system.

$E_1 = E - E'$ = energy (in Mev) of the excited level

l = orbital angular momentum of the incident neutron

l' = orbital angular momentum of the inelastically scattered neutron

J = total angular momentum of the compound system.

$T_l(E)$ = transmission coefficient corresponding to a particular orbital angular momentum l and energy (in Mev) of a neutron. E is in C-system.

$\sigma(i \rightarrow i', E \rightarrow E')$ = cross section in cm^2 for neutrons with energy E in Mev inelastically scattering from a target nucleus with spin i and parity $P(i)$ leaving the target nucleus in an excited state with spin i' , parity $P(i')$ and excitation energy $E_1 = E - E'$.

$$\epsilon_{i,l}^J = \begin{cases} 2, & \text{if conditions I and II are satisfied} \\ 1, & \text{if either condition I or condition II is satisfied} \\ 0, & \text{if neither condition I or II is satisfied} \end{cases} \quad (3)$$

$$\text{Condition I } J-l \leq i + \frac{1}{2} \leq J + l$$

$$\text{Condition II } J-l \leq i - \frac{1}{2} \leq J + l$$

It may be noted that the permissible values of J are obtained by vector addition of $\vec{i}$ and $(\vec{l} + \vec{s})$, where $\vec{l}$ and $\vec{s}$ are the orbital angular momentum and spin of the incident neutron.

The calculation of the transmission coefficients, $T_\ell(E)$, involves an assumption of an average nuclear potential with real and imaginary parts. Emmerich⁴ has tabulated the transmission coefficients for a wide range of parameters. Emmerich uses the following potential:

$$V(r) = -V_c \text{ for } r < R_c$$

$$V(r) = -V_c \left(1 - i \lambda \frac{d}{dx}\right) \left[e^{-x}\right]^{-1} \text{ for } r > R_c$$

where

$$x = \frac{r - R_c}{\tau}$$

The diffusive edge is determined by the value of τ . Note that the imaginary part of the nuclear potential was taken to zero in the core and λ times the derivative of the real part with respect to x in the surface region. The mean radius, $\bar{R}$, was defined as follows:

$$\bar{R} = \int_0^\infty \frac{V(r)}{V_c} dr$$

The above equation leads to $\bar{R} = R_c + 1.359 \tau$

Then, we have four parameters to describe the potential, namely $\bar{R}$, τ , V_c and λ . By a comparison with experimental data, it was found for an isotope of mass number A (See for example, Emmerich reference 4)

$$\bar{R} = (1.25 A^{\frac{1}{3}} + 0.5) \cdot 10^{-13} \text{ cm} \quad (4)$$

Emmerich has tabulated the transmission coefficient up to $\ell=8$ for the following cases for $\bar{R}$ from 4.0 to 8.2 in intervals of 0.3 (units of 10^{-13} cm).

V_c	λ	$E(\text{in Mev})$
44	0.34	0.1, 0.4, 0.7, 1.0
43	0.37	1.5, 2.0, 2.5, 3.0
42	0.40	4.0, 5.0, 6.0
41	0.43	7.0, 8.0, 9.0, 10.0
40	0.46	12.0, 14.0

It should be noted that it has been assumed that the transmission coefficients do not depend on the total angular momentum of the compound system.

At this stage, we give detailed expressions of Eq. (1) for one case of interest. The summations in Eq. (1) and Eq. (2) are rather intricate, and some care must be used in obtaining appropriate results for the case of interest.

If we have the 1st excited state (2+) and the ground state (0+) and the neutron energy is such that only 1st excited state can be excited, we have

$$\begin{aligned} \sigma(0^+ \rightarrow 2^+) = & \frac{\pi \chi^2}{2} \left[T_0(E) \frac{2T_2(E')}{2T_2(E') + T_0(E)} \right. \\ & + T_1(E) \left\{ \frac{2[T_1(E') + T_3(E')]}{T_1(E') + T_3(E') + T_1(E)} + \frac{4[2T_1(E') + 2T_3(E')]}{2T_1(E') + 2T_3(E') + T_1(E)} \right\} \\ & + T_2(E) \left\{ \frac{4[T_0(E') + 2T_2(E')]}{T_0(E') + 2T_2(E') + T_2(E)} + \frac{6[T_0(E') + 2T_2(E')]}{T_0(E') + 2T_2(E') + T_2(E)} \right\} \\ & \left. + T_3(E) \left\{ \frac{6[2T_1(E') + 2T_3(E')]}{2T_1(E') + 2T_3(E') + T_3(E)} + \frac{8[T_1(E') + 2T_3(E')]}{T_1(E') + 2T_3(E') + T_3(E)} \right\} \right] \end{aligned} \quad (5)$$

Here $E' = E - E_1$, where E and E_1 are the incident neutrons energy and the excitation energy of 2^+ level respectively. All these energies are in the center of mass system. In heavy materials, where recoil energy of the residual nucleus is very small, the energies in C-system are essentially the same as in the laboratory frame. It should be noted that energy-groups in MUFT correspond to the laboratory frame of reference.

$$E_c = \left(\frac{A}{A+1} \right) E_L$$

In Eq. (5)

$$\chi^2 = \frac{.20728}{E \text{ (in Mev)}} \cdot 10^{-24} \text{ cm}^2$$

where E is the neutron incident energy in C-system.

IV. INELASTIC SCATTERING PROBABILITY IN STATISTICAL REGIONS

By a statistical region, we imply the energy region of excited nuclear levels whenever these nuclear levels are so numerous (and close to each other) that a statistical treatment of a compound system can be made. At the very outset, it may be noted that very little experimental information as regards spins and parities of the nuclear levels is available beyond 3 mev or so. Consequently, some sort of nuclear model must be used for a description of the nuclear levels above 3 mev. Usually the particular choice of the dependence of level density of excitation energies is dictated by experimental measurements of either the γ -ray measurements or energy distribution of inelastically scattered neutrons. The measurements of γ -ray intensities give information about inelastic scattering because one can "identify" the γ -ray which results from the transition between the excited nuclear states to the ground state. The statistical approach of the decay of a compound system (consisting of the incident neutron and the target nucleus) is sometimes compared to the evaporation of a liquid drop, where evaporation is governed by purely statistical consideration. Thus, in analogy with thermodynamics, it has become customary to define a nuclear temperature. These considerations give us an expression for the relative intensity of a particle from a statistical decay of a compound system.⁶

$$I_v(E, E^*) dE = \frac{(2S_v + 1) E \sigma_v(E, U) \rho_v(u) M_v dE}{\pi^2 h^3 \rho_c(E^*)} \quad (6)$$

where:

$I_v(E, E^*) dE$ = relative yield of particle v with energy E when a compound system with total energy E^* decays.

$U = E^* - E$ = Excitation energy of a level

M_v = mass of the particle v

S_v = spin of the particle v

$\rho_v(U)$ = nuclear level density at excitation energy of U .

$\hbar$ = Planck's constant divided by 2π

$\sigma_v(E, U)$ = cross section for formation of a compound system when a particle, v , is incident upon the excited (residual) nucleus.

v = symbol, designating a particle e.g. a neutron, a proton, α particle etc. etc.

In a reactor calculation, we are concerned mainly with neutron fluxes. Thus, we get for neutrons

$$I(E) = C E \sigma_c(E, U) \rho(U) dE \quad (7)$$

Here, we have absorbed the various constant factors in the constant C . Let us make another assumption i.e. $\sigma_c(E, U)$ has very weak energy dependence, and therefore can also be absorbed in the constant C . We wish to point out this assumption appears to be valid. However, this validity is based upon certain other assumptions. This is because it is extremely difficult (if not impossible) to measure a capture cross section for a certain incident neutron energy on an "excited" nuclear level. This has led to the assumption that perhaps this cross section can be given by the corresponding cross section for the ground state. For the ground state, the reaction cross section, σ_r , is given by the following:

$$\sigma_r(E) = \pi \lambda^2 \sum_{l=0}^{\infty} (2l+1) T_l(E) \quad (8)$$

where $T_l(E)$ is the transmission coefficient for neutron energy E and orbital angular momentum l , and λ is neutron wave length divided by 2π . By explicit calculations, it can be seen that $\sigma_r(E)$ does not vary significantly with energy above 4 mev or so. In this statistical region (neutrons above 3 mev incident energies), Eq. (7) leads to the following:

$$I(E, E_0) dE = C E \rho(E_0 - E) dE \quad (9)$$

In Eq. (9), we have shown the functional dependence of relative neutron flux with energy E for incident neutrons of energy E_0 .

In one of the simplest forms, which has been used widely, we have

$$\rho(E_0 - E) = C_1 e^{(E_0 - E)/T} \quad (10)$$

where C_1 is a normalizing constant. The nuclear temperature, T , is considered as a function of the incident neutron energy E_0 . This particular form of the nuclear level density implies that the energy-dependence is contained in the exponential term. Though there are no theoretical arguments to support this form, yet most of the experimental results have been used in arriving at the values of nuclear temperature. Using Eqs. (9) and (10), we get the probability of a neutron (with lethargy u) to be inelastically scattered with final lethargy value u' .

$$P(u \rightarrow u') = \frac{1}{T^2} \left[E'^2 e^{-E'/T} \right] du' \quad (11)$$

The nuclear temperature, T , can be expressed as a function of the incident neutron energy.

$$T = aE^{\frac{1}{2}} \quad (12)$$

where the parameter a is determined from experimental data. It should be noted that this parameter, a , is different for each isotope. In MUFT¹, the energy-groups are defined from a certain energy E_i to E_{i-1} . For the calculation of inelastic scattering probabilities from a group i to other groups, we need an "average" nuclear temperature for the groups, designated by i . This should be done by the following equation.

$$T_i = \frac{2a}{\Delta u_i} \left[E_i^{\frac{1}{2}} - E_{i-1}^{\frac{1}{2}} \right] \quad (13)$$

where E_i is the larger energy value in group i and Δu_i is the lethargy interval of group i . The nuclear temperature is a positive definite number.

Thus, we get the probability of inelastic neutron scattering from group i to energy group j , where $j > i$.

$$P_{ij} = \left(\frac{E_{j-1}}{T_i} + 1\right) e^{-E_{j-1}/T_i} - \left(\frac{E_j}{T_i} + 1\right) e^{-E_j/T_i} \quad (14)$$

Again, it must be noted that $E_{j-1} < E_j$ and this leads to the obvious statement that $P_{ij} > 0$ for $j > i$.

At this stage, it is to be noted that several other forms of the nuclear level density have been proposed. For example,

$$\rho(U) \propto U^{-n} e^{2\sqrt{bU}} \quad (15)$$

where n has been given values of $5/4$, 2 and 0 . For the case $n=0$, (as in Eq. 10) it is tacitly assumed that only the exponential term governs the dependence of the nuclear level density on the excitation energy. In this formulation the temperature, T , is related to n and b by

$$\frac{1}{T} = \left(\frac{b}{U}\right)^{\frac{1}{2}} - \frac{n}{U} \quad (16)$$

It may be noted, here, that only when $n=0$ and b is constant we get the relation

$$T = \frac{1}{bU^2}$$

Another interesting point is that the value of the level density at a certain energy is not the same for odd-odd nuclei and even-odd nuclei. In fact, we have the relationship approximation:

$$0.5 C_1 (\text{odd-odd}) = C_1 (\text{odd-even, even-odd}) \quad (17)$$

C_1 is a parameter in Eq. (10)

A summary of the expressions for the nuclear level density is given in Appendix B.

V. A CALCULATIONAL PROCEDURE

In this section, a calculational procedure for obtaining an inelastic scattering matrix for a certain isotope is summarized. For more detailed information than given below, original papers and the recent review article should be consulted.

Step 1: Make a literature search on the experimental data for an isotope.

The following sources should be consulted first:

- (a) Nuclear Data Sheets
- (b) Reviews of Modern Physics, 30, No. 2 Part II (1958)
- (c) BNL - 325 (and supplements)

The above references should, at least, establish the nuclear level scheme. It may be of a great help if the same information is requested from: Sigma Center, Brookhaven National Laboratory. Perhaps, the Sigma Center can also supply the references to other later experimental data. In any case, some recent Physical Reviews and Nuclear Science Abstracts should also be searched. The following information must be compiled:

- (1) Nuclear level structure of an isotope,
- (2) Experimental $\sigma_{n,n'}$ cross section for the measured levels
- (3) The nuclear temperature, T , at a certain energy.

If some of these data are not available, it will be necessary to use similar information concerning a neighboring isotope.

Step 2: Obtain the appropriate transmission coefficients. This can be done by first calculating

$$\bar{R} = (1.25 A^{\frac{1}{3}} + 0.5) 10^{-13} \text{ cm}$$

and interpolating between the values from Emmerich's calculations (Westinghouse Research Report 62-118-540-P1, 1962). Alternatively, the values

of transmission coefficients can be obtained from Los Alamos Scientific Report LA-2099 (April 1957), MIT - LNS No. 73 (February 1960) or by running a code. It may be noted that these transmission coefficients depend very much on the nature of the average nuclear potentials used. It turns out that most of these calculations use slightly different models and also the results are presented differently.

It is suggested that the transmission coefficients, calculated by using any of the above methods, be plotted versus neutron energy for the isotope of interest.

Step 3: If the nuclear temperature is not known experimentally (as in Step 1) one can use a value either from an empirical fit of Newton^{13,14} (Canadian J. of Physics 34, 804 (1956)), or a value may be calculated by using the more recent curves of b in Eq. (16) (Ericson, Proceeding of the International Conference on Nuclear Structure, University of Toronto Press (1960)).

Step 4: Consider the contributions of all known nuclear levels. (This means that one knows the spin, the parity and energy of excitation of the relevant nuclear levels.) Using Eq. (1) and the curves (Transmission Coefficients vs Energy), calculate σ_{in} for the first excited level and denote it as $\sigma_{in}(1)$. It may be noted that the energy factor in Eq. (1) refers to the center of mass system. We suggest that all calculations be done in this c-system, and later on, if need be, neutron energies be converted to the laboratory system. It may be recalled that since $E_c = (\frac{A}{A+1}) E_L$ we can ignore the distinction between E_L and E_c when A is large ($A > 50$).

Plot $\sigma_{in}(1)$, the calculated inelastic cross section for the first excited level, versus neutron lethargy. Similarly plot $\sigma_{in}(j)$ vs-neutron lethargy for all known nuclear levels i.e. $j = 2, 3, 4 \dots$ lethargy,

$$u_j = \log \frac{10}{E(\text{in Mev})}$$

Step 5: Since MUFT does not allow inelastic scattering within a group, this contribution has to be properly considered in the values of σ_{in} . The appropriate method is to calculate

$$f_i = \frac{\sum' \sigma_{i,j}}{\sum \sigma_{i,j}}$$

where the prime over the summation denotes $j \neq i$. These fractions, f_i , should be calculated for all the relevant energy groups. The entries σ_{in}^j (for an energy-group designated by j) should be calculated as follows:

$$\sigma_{in}^j(\text{MUFT}) = f_j \sigma_{in}^j(\text{expt})$$

Note that $(1-f_j) \sigma_{in}^j(\text{expt.})$ should be put in MUFT as symmetric scattering.

Step 6: From Step 4, we have σ_{in} (for various known levels) versus neutron energy (generally up to 3 Mev or so.) Now it may turn out that these respective cross sections do not agree with experimental information. The experimental cross sections may be available only at a certain energy. In such a case, normalize the calculated σ_{in} to the experimental value.

Step 7: Calculate the inelastic scattering probabilities for the known nuclear levels as follows:

$$p_{1j} = \frac{\sigma_{1j}}{\sum' \sigma_{1,j}}$$

$\sigma_{1,j}$ is the lethargy averaged cross sections (calculated from the theoretical curves normalized to experimental data), so that a neutron incident in group 1 can be scattered (inelastically) into energy group j . It should be noted that this step is not difficult, because for a certain incident energy (in group 1) only discrete values of exit neutron energies are possible.

Therefore, sometimes group j may not be completely subscribed by the neutrons in group 1.

Since MUFT energy-groups are defined in a simple fashion in units of lethargy, these calculations can be done conveniently when σ_{in} (for all the nuclear levels) is plotted versus lethargy.

Step 8: When the incident neutron energy is greater than the last resolved level (spin & parity known), we cannot continue the above procedure because some levels, where spins and parities are not known, can now be excited. This results in the usual difficulty because the appropriate transmission coefficients (in the denominator of Eq. (2)) cannot be calculated. The procedure recommended is that above 3 (or 4) Mev energies, one should use the statistical model. We will remark on this interference between the resolved and the unresolved nuclear level regions in Part C of the report. However, we suggest that this interference contribution be ignored at least for the immediate future.

Step 9: When all the inelastic scattering probabilities of the known levels have been computed, use the appropriate nuclear temperature from Step 1 in the equation.

$$T = a E^{\frac{1}{2}}$$

to determine the parameter a . The nuclear temperature for each energy group should then be computed from the following:

$$T_1 = \frac{2a}{\Delta u_1} \left[\frac{1}{E_1^2} - \frac{1}{E_{i-1}^2} \right]$$

where E_i and E_{i-1} are the upper and the lower limits of energy specifying the group i . Δu_i is the width of group i .

Step 10: With the nuclear temperatures calculated for all groups (above 3 Mev or so), one calculates the inelastic scattering probabilities from the following equation:

$$P_{ij} = \left(\frac{E_{j-1}}{T_i} + 1 \right) e^{-E_{j-1}/T_i} - \left(\frac{E_j}{T_i} + 1 \right) e^{-E_j/T_i}$$

Step 11: Any finite contribution of inelastic probability to groups beyond energy-group 25 of MUFT can either be lumped in group 25 or can be distributed uniformly over all the energy groups.

Step 12: Summations of probabilities should be normalized to 1.000. This is a strict condition in MUFT library.

$$\sum_j p_{ij} = 1.0000$$

VI. CALCULATION OF INELASTIC SCATTERING MATRIX FOR Fe^{56}

In our calculations, we make the assumption that a statistical description is valid above 2.86 Mev. Furthermore, since $E_c = (\frac{56}{56+1}) E_L$ we ignore the distinction between E_c (energy in C-System) and E_L (energy in the laboratory frame of reference). As it can be easily seen in the calculations presented here, this approximation can be easily dispensed with.

A. Experimental Data and Theoretical Formulas

The level Scheme of Fe^{56} was taken³ as in Fig. 1.

Fig. 1'

3+		3.4
4+		3.1
2+		2.9
2+		2.6
4+		2.1
2+		0.84
0+		0

In this scheme, the ground state has spin zero and even parity. The first level (2+), the second level (4+), the third level (2+), the fourth level (2+), the fifth level (4+) and the sixth level (3+) are respectively at the following energies (with respect to the ground state): 0.84 Mev, 2.1 Mev, 2.6 Mev, 2.9 Mev, 3.1 Mev and 3.4 Mev. It may be noted that the spin of the nuclear level at 3.1 Mev is not completely established. In fact, it has been suggested¹⁵ that this spin may be 2 instead of 4. Thomas¹⁶ and Bodansky⁶ have summarized the recent experimental information. It has been found⁶ that the value of nuclear temperature $T = 0.95$ for incident energy of 7 Mev. It should be noted that this nuclear temperature for Fe^{56} may be in error. There are conflicting experimental data in the literature. In fact, at the present time, the nuclear temperature (for Fe^{56}) calculated from (n,n') reactions is not consistent with the corresponding temperature

for (p, p') and (p, α) reactions. The reasons for this discrepancy are not quite understood. See reference (17) for further discussion of this point.

In Fig. 1, we can have the following types of transitions:

$$0+ \rightarrow 2+, 0+ \rightarrow 4+, \text{ and } 0+ \rightarrow 3+.$$

We give below the inelastic cross sections for these combinations up to ℓ and ℓ' equal* to 3. ℓ and ℓ' are the orbital angular momentum of the incident and the (inelastically) scattered neutron respectively.

From Eq. (1), one obtains:

$$\begin{aligned} \sigma(0+ \rightarrow 2+) &= \frac{\pi \chi^2}{2} \left[T_0(E) \frac{4}{A} T_2(E') \right. \\ &+ T_1(E) \left\{ \frac{2}{B} [T_1(E') + T_3(E')] + \frac{8}{C} [2T_1(E') + 2T_3(E')] \right\} \\ &+ T_2(E) \left\{ \frac{4}{D} [T_0(E') + 2T_2(E')] + \frac{6}{F} [T_0(E') + 2T_2(E')] \right\} \\ &+ T_3(E) \left\{ \frac{12}{H} [T_1(E') + T_3(E')] + \frac{8}{K} [T_1(E') + 2T_3(E')] \right\} \Big] \end{aligned} \quad (18)$$

$$\begin{aligned} \sigma(0+ \rightarrow 3+) &= \frac{\pi \chi^2}{2} \left[T_0(E) \frac{2}{A} T_2(E') \right. \\ &+ T_1(E) \left\{ \frac{4}{B} T_3(E') + \frac{4}{C} [T_1(E') + 2T_3(E')] \right\} \\ &+ T_2(E) \left\{ \frac{8}{D} T_2(E') + \frac{6}{F} [T_0(E') + 2T_2(E')] \right\} \\ &+ T_3(E) \left\{ \frac{12}{H} [T_1(E') + T_3(E')] + \frac{16}{K} [T_1(E') + T_3(E')] \right\} \Big] \end{aligned} \quad (19)$$

* The values of the relevant transmission coefficients for $\ell > 3$ are negligibly small for $E \leq 2.86$ Mev. See for example Fig. (2).

$$\begin{aligned}
\sigma(0 \rightarrow 4+) &= \frac{\pi \lambda^2}{2} \left[T_1(E) \left[\frac{2}{B} T_3(E') + \frac{8}{C} T_3(E') \right] \right. \\
&+ T_2(E) \left[\frac{4}{D} T_2(E') + \frac{12}{F} T_2(E') \right] \\
&+ T_2(E) \left\{ \frac{6}{H} [T_1(E') + 2T_3(E')] + \frac{16}{K} [T_1(E') + T_3(E')] \right\} \left. \right] \quad (20)
\end{aligned}$$

where: *

$$A = T_0(E) + 2T_2(E_1) + 2T_2(E_3) + 2T_2(E_4) + T_2(E_6) \quad (21)$$

$$\begin{aligned}
B &= T_1(E) + T_1(E_1) + T_3(E_1) + T_3(E_2) + T_1(E_3) + T_3(E_3) + T_1(E_4) \\
&+ T_2(E_4) + T_3(E_5) + 2T_3(E_6) \quad (22)
\end{aligned}$$

$$\begin{aligned}
C &= T_1(E) + 2T_1(E_1) + 2T_3(E_1) + 2T_3(E_2) + 2T_1(E_3) + 2T_3(E_3) \\
&+ 2T_1(E_4) + 2T_3(E_4) + 2T_3(E_5) + T_1(E_6) + 2T_3(E_6) \quad (23)
\end{aligned}$$

$$\begin{aligned}
D &= T_2(E) + T_0(E_1) + 2T_2(E_1) + T_2(E_2) + T_0(E_3) + 2T_2(E_3) \\
&+ T_0(E_4) + 2T_2(E_4) + T_2(E_5) + 2T_2(E_6) \quad (24)
\end{aligned}$$

$$\begin{aligned}
F &= T_2(E) + T_0(E_1) + 2T_2(E_2) + T_0(E_3) + 2T_2(E_3) + T_0(E_4) \\
&+ 2T_2(E_4) + 2T_2(E_5) + T_0(E_6) + 2T_2(E_6) \quad (25)
\end{aligned}$$

$$\begin{aligned}
H &= T_3(E) + 2T_1(E_1) + 2T_3(E_1) + T_1(E_2) + 2T_3(E_2) + 2T_1(E_3) \\
&+ 2T_3(E_3) + 2T_1(E_4) + 2T_3(E_4) + T_1(E_5) + 2T_3(E_5) + 2T_1(E_6) + 2T_3(E_6) \quad (26)
\end{aligned}$$

$$\begin{aligned}
K &= T_3(E) + T_1(E_1) + 2T_3(E_1) + 2T_1(E_2) + 2T_3(E_2) + T_1(E_3) + 2T_3(E_3) \\
&+ T_1(E_4) + 2T_3(E_4) + 2T_1(E_5) + 2T_3(E_5) + 2T_1(E_6) + 2T_3(E_6) \quad (27)
\end{aligned}$$

* It should be noted that Eq. (21) through Eq. (27) need be calculated only once for a particular level scheme of an isotope.

and E is the incident neutron energy in the c-system (Mev).

$$E_1 = E - 0.84$$

$$E_2 = E - 2.1$$

$$E_3 = E - 2.6$$

$$E_4 = E - 2.9$$

$$E_5 = E - 3.1$$

$$E_6 = E - 3.4$$

B. Numerical Results for Known Nuclear Levels (Fe^{56})

With this ground work, we still need the appropriate transmission coefficients for further numerical results.

$$\bar{R} = (1.25 A^{\frac{1}{3}} + 0.5) 10^{-13} \text{ cm.}$$

$$\text{For } \text{Fe}^{56}, \bar{R} = 5.28 10^{-13} \text{ cm.}$$

From Emmerich's Calculations,⁴ we look up the transmission coefficients and plot these versus neutron energy. The calculated values of the transmission coefficients are plotted in Figure 2. It should be noted that these values are calculated for a certain average nuclear potential. Other calculations¹⁰ are available for different physical parameters.

Using Emmerich's calculations as presented in Figure 2, we give the values of A , B , C , D , F , H and K (as defined in Eq. 21 through Eq. 27) in Table I. The calculated inelastic scattering cross sections are given in Table II. In Table II, $\sigma_{(1)}$ denotes the inelastic cross section for level 1 at a particular energy, E_c . We have given these energies in Mev and they

$$\bar{R} = 5.28 \times 10^{-13} \text{ cm}$$

Fig. 2 Transmission Coefficients for Fe^{56} from Emmerich's Calculations.

are in the center-of-mass system. However, for Fe^{56} the distinction between E_c and E_L can be ignored.*

C. Normalization

At this stage, a comparison of the calculated inelastic scattering cross section (for the various nuclear levels) is made with the existing experimental data. The experimental information¹⁸ is summarized below.

$\text{Fe}^{56} (n,n')$	
$E(\text{Mev})$	$\sigma_{in}(\text{barns})$
1.0	0.5 ± 0.06
1.2	0.6 ± 0.06
1.75	0.75 ± 0.05
2.25	1.00 ± 0.05
2.45	1.10 ± 0.05
2.50	1.18 ± 0.05
2.51	1.00 ± 0.04
3.25	1.21 ± 0.06
3.48	1.23 ± 0.07

It may be noted that when the incident neutron energy is 1.75 Mev, only the first level (at 0.84 Mev) can be excited. However, for the incident neutron energy equal to 2.45 Mev both the first and the second levels can be excited. This suggests the normalization procedure for the calculated cross sections in Table II. We normalize $\sigma_{(1)}$ (at $E = 1.75$ Mev) to a value of 0.75 barns. $\sigma_{(2)}$ is normalized at $E = 2.45$ to a value given by the difference of 1.10 barns ($\sigma_{in}(\text{expt})$ at $E = 2.45$) and the normalized $\sigma_{(1)}$ at $E = 2.45$. The calculated inelastic scattering cross section vs incident energy is given in Figure 3 after this normalization. In Figure 3, the experimental inelastic scattering cross section versus energy is given; the flags denote the experimental errors.

* This is because $E_c = \left(\frac{A}{A+1}\right) E_L$

Fig. 3 Comparison of experimental data and calculated cross section for Fe^{56} (σ_1 and σ_2 were properly normalized).

TABLE I THE DENOMINATOR FACTORS VS. ENERGY (EQS. 21-27) FOR Fe^{56}

E	π^2	A	B	C	D	F	H	K
(Mev)	barns							
.90	.2303	.93	.2475	.2650	.980	.980	.0350	.0175
1.10	.1884	.983	.3310	.3920	1.3110	1.3110	.1220	.061
1.30	.1594	1.124	.4150	.5300	1.5640	1.5640	.230	.115
1.60	.1296	1.40	.5400	.7400	1.960	1.9600	.4250	.225
1.80	.1152	1.60	.6100	.8500	2.220	2.220	.515	.275
2.00	.1036	1.76	.6700	.9500	2.450	2.450	.609	.329
2.20	.09422	1.94	.7335	1.0570	2.660	2.660	.7285	.436
2.30	.09012	2.02	.7525	1.0900	2.7710	2.7820	.793	.517
2.50	.08291	2.14	.8065	1.1830	2.9610	3.0220	.958	.713
2.70	.07677	2.20	.8655	1.2910	3.8350	3.980	1.136	.9085
2.80	.07403	2.262	.9190	1.3880	4.0870	4.2820	1.278	1.039
3.00	.06909	2.442	1.0425	1.6250	5.1420	5.4320	1.575	1.2925
3.30	.06281	2.902	1.2720	2.0640	6.0020	6.4320	2.133	1.777
3.35	.06187	2.98	1.3320	2.1850	6.120	6.5900	2.279	2.201
3.42	.06061	3.115	1.3840	2.2880	6.2960	6.8120	2.423	2.373
3.50	.05922	3.36	1.5855	2.6810	6.6210	7.2020	2.861	2.77

TABLE II CALCULATED INELASTIC SCATTERING CROSS SECTION FOR VARIOUS LEVELS OF Fe^{56}

E_c (Mev)	σ_1 barns	σ_2 barns	σ_3 barns	σ_4 barns	σ_5 barns
.9	.7725				
1.1	.9129				
1.3	1.010				
1.6	1.1536				
1.8	1.1714				
2.0	1.1679				
2.2	1.1428	.007463			
2.3	1.1239	.02421			
2.5	1.0704	.07052			
2.7	.8878	.10913	.1714		
2.8	.8578	.1339	.2091		
3.0	.7044	.1450	.2257	.1199	
3.3	.5901	.1713	.2622	.1796	.01348
3.35				.1813	.01617
3.42				.1864	.02272
3.50				.1910	.07891

It should be noted, however, that the calculated inelastic cross sections of the various levels were based on the transmission coefficients as tabulated by Emmerich⁴. If we had used the transmission coefficients tabulated by Beyster et. al.¹⁹ the calculated results would have been different. This fact is not surprising because Emmerich and Beyster et. al have used different nuclear potentials.

D. Calculations of Inelastic Scattering Probability (Fe^{56}) $E_{\text{incident}} < 2.86 \text{ Mev}$

It is convenient to perform these calculations in the lethargy units. In the following, we will denote by u and u' the incident and the exit neutron lethargies respectively. In Figure 4, we give the normalized $\sigma_{(1)}$ and $\sigma_{(2)}$ versus lethargy u . Also, $\sigma_{(3)}$, $\sigma_{(4)}$, and $\sigma_{(5)}$ are plotted. It may be noted that level 6 cannot make any contributions for incident neutron energy ≤ 2.8 Mev. We are using the same notation as in the preceeding sections, i.e. $\sigma_{(i)}$ denotes the inelastic scattering cross section for a nuclear level, designated by i . Similarly in Figure 5 we plot $\sigma_{(i)}$ vs lethargy corresponding to exit neutron energies. Here, some care must be used. The important point to remember is that

$$E_{\text{exit}} = E_{\text{incident}} - E_i$$

where E_i is the excitation energy of a nuclear level designated by subscript i . Thus for the various levels, E_{exit} (and therefore u') is not the same for a fixed incident neutron lethargy, u .

The inelastic scattering probability from group i to group j , $P_{i,j}$, is given by Eq. (11)

$$P_{i,j} = \frac{\sum_k \bar{\sigma}_k(i,j) \Delta u_{j,i}}{\sum_k \sum_j \bar{\sigma}_k(i,j) \Delta u_{j,i}} \quad (28)$$

Fig. 4 Normalized σ_1 , Normalized σ_2 , σ_3 , σ_4 and σ_5 vs. incident neutron lethargy.

barns

Fig. 5 Normalized σ_1 , normalized σ_2 , σ_3 , σ_4 and σ_5 v.s. exit neutron lethargy.

where

k = summation index for the nuclear levels

$\bar{\sigma}_k(i,j)$ = average inelastic scattering cross section (for neutron incident in group i) from nuclear level designated by the subscript k so that the exit neutrons are in group j . The bar denotes an average over exit neutron lethargy interval, permissible by energy conservation. (i.e. $\Delta u_{j,i}$).

$\Delta u_{j,i}$ = permissible lethargy interval of exit neutrons in group j for neutrons incident in group i .

It should be noted that strict normalization condition

$$\sum_j P_{i,j} = 1.00000$$

must be satisfied.

For the sake of clarity and completeness, we present the details of the calculations for neutrons incident in MUFT energy-group 6. It may be recalled that energy group 6 has 2.23 Mev and 2.86 Mev as the lower and the upper energy limits. The following steps were followed:

- (i) We can see from the level scheme in Fig. 1 that only level 1, level 2, and level 3 can be excited when the incident neutron energy lies in group 6. It can be immediately seen that for nuclear level 4 to be excited, incident neutron energy must be greater than 2.9 Mev.
- (ii) We calculated the permissible ranges of exit neutron energies for these levels. For example, the energy range is 1.39 (=2.23 - 0.84) Mev to 2.02 (=2.86 - 0.84) Mev for nuclear level 1. Similarly, the permissible exit neutron energy ranges are from 0.12 Mev to 0.76 Mev, and 0.76 Mev to 0.0 Mev for nuclear levels 2 and 3 respectively. Since it is most convenient to perform the calculations in lethargy units, these energy limits were converted to

lethargy limits by using the familiar formula

$$u = \ln \frac{10}{E}, \text{ E is in Mev.}$$

(iii) In Fig. 6(a) and Fig. 6(b) the inelastic scattering cross sections (normalized, wherever necessary) are plotted as a function of exit neutron lethargy. These curves are relevant only for incident neutrons in group 6. The thick lines represent the permissible ranges of lethargies for the various levels. The dotted (vertical) lines represent the boundaries of the MUFT energy groups. It can be seen from Fig. 6(a) that the inelastic scattering cross section (and hence, the inelastic scattering probabilities) are identically zeros for the energy group 9 ($u = 2.0$ to $u = 2.25$) and the energy group 10 ($u = 2.25$ to $u = 2.50$). This result is not surprising because one can arrive at this conclusion by purely energy-conservation arguments. It may be noted that the calculated values of σ_j , where j specifies a nuclear level, are sometimes extrapolated for large values of u' (and up to a maximum value of $u' = 7.5$).

(iv) It will be convenient to define

$$D = \sum_{j=7}^8 \bar{\sigma}_1(6,j) \Delta u'_{j,6} + \sum_{j=11}^{18} \bar{\sigma}_2(6,j) \Delta u''_{j,6} + \sum_{j=15}^{23} \bar{\sigma}_3(6,j) \Delta u'''_{j,6}$$

We have used primes over the permissible ranges of lethargy because these may be different for each level. It should be noted that $\Delta u_{j,6}$ depends on the lethargy limits of group j .

For groups $j \leq 6$, $P_{ij} = 0$

For group j given by $7 \leq j \leq 8$, we have by using Eq. (28) and the above definition of D .

$$P_{6,j} = \frac{\bar{\sigma}_1(6,j) \Delta u'_{j,6}}{D}$$

Similarly,

$$P_{6,j} = \frac{\bar{\sigma}_2(6,j) \Delta u_{j,6}''}{D} \quad \text{for } 11 \leq j \leq 14,$$

$$P_{6,j} = \frac{\bar{\sigma}_2(6,j) \Delta u_{j,6}'' + \bar{\sigma}_3(6,j) \Delta u_{j,6}''}{D} \quad \text{for } 15 \leq j \leq 18,$$

and,

$$P_{6,j} = \frac{\bar{\sigma}_3(6,j) \Delta u_{j,6}''}{D} \quad \text{for } 19 \leq j \leq 23.$$

The results of our calculations are presented in Table III.

E. Calculation of Inelastic Scattering Matrix (Fe^{56}). $E_{\text{incident}} > 2.86 \text{ Mev.}$

Above 2.86 Mev incident neutron energy, it is appropriate to use the statistical model.¹ The nuclear temperature, T , is equal to 0.95 Mev corresponding to neutron incident energy of 7 Mev. It may be recalled that

$$T = a E^{\frac{1}{2}} \quad (29)$$

The average nuclear temperature for each MUFT energy group is given by

$$T_i = a t_i \quad (30)$$

where

$$t_i = \frac{2}{\Delta u_i} \left[E_i^{\frac{1}{2}} - E_{i-1}^{\frac{1}{2}} \right]$$

and E_i and E_{i-1} are the upper limit and the lower limit of energy group i .

For Fe^{56} , we get the following values of the nuclear temperature:

$$T_1 = 1.066$$

$$T_2 = 0.9402$$

TABLE III INELASTIC SCATTERING PROBABILITY MATRIX FOR Fe⁵⁶

E < 2.86 Mev

MUFT Group J	P _{6,j}	P _{7,j}	P _{8,j}	P _{9,j}
1				
2				
3				
4				
5				
6				
7	.09337			
8	.1577	.05599		
9	.0000	.5327	.0000	
10	.0000	.3389	.1665	.0000
11	.09907	.0000	.4435	.0000
12	.1220	.0000	.3900	.02920
13	.09337	.0000	.0000	.2965
14	.06847	.0000	.0000	.2847
15	.06648	.0000	.0000	.2717
16	.03486	.0000	.0000	.1179
17	.02490	.0000	.0000	.0000
18	.05059	.02270	.0000	.0000
19	.04108	.02841	.0000	.0000
20	.03859	.01420	.0000	.0000
21	.06224	.00710	.0000	.0000
22	.03735	.0000	.0000	.0000
23	.00993	.0000	.0000	.0000
24	.0000	.0000	.0000	.0000
25	.0000	.0000	.0000	.0000
$\sum_j P_{i,j}$	1.00000	1.00000	1.00000	1.00000

All entries not given above group 9 are zeros.

$$T_3 = 0.8364$$

$$T_4 = 0.7303$$

$$T_5 = 0.6526$$

The inelastic scattering probabilities for Fe^{56} in the statistical region are given in Table IV. These were calculated from the following:

$$P_{ij} = \left(\frac{E_j - 1}{T_i} + 1 \right) e^{-E_j - 1/T_i} - \left(\frac{E_j}{T_i} + 1 \right) e^{-E_j/T_i}$$

The entries in Table V are normalized so that

$$\sum_j P_{ij} = 1.00000.$$

Thus, for Fe^{56} , the complete inelastic scattering probability matrix is given by Table III and Table IV.

TABLE IV. INELASTIC SCATTERING PROBABILITY MATRIX FOR Fe^{56} IN THE STATISTICAL REGION*

MUFT Group j	$P_{1,j}$ T=1.066	$P_{2,j}$ T=.9402	$P_{3,j}$ T=.8364	$P_{4,j}$ T=.7303	$P_{5,j}$ T=.6526
1					
2	.0712				
3	.04225	.02819			
4	.07694	.05926	.0440		
5	.1104	.09515	.07946	.0606	
6	.13122	.12363	.1133	.09749	.08344
7	.13462	.13594	.1339	.1269	.1187
8	.1231	.13134	.1369	.1398	.1403
9	.1028	.1144	.1248	.1351	.1433
10	.08006	.09209	.1040	.1178	.1305
11	.05900	.06963	.0809	.0950	.1087
12	.04165	.05016	.05950	.07185	.08443
13	.02844	.03479	.04196	.05178	.06211
14	.01891	.02343	.02862	.03593	.04379
15	.01233	.01541	.01903	.02420	.02986
16	.00790	.00996	.01239	.01593	.01985
17	.00501	.00634	.00795	.01029	.01292
18	.00315	.00400	.00503	.00656	.00828
19	.00196	.00250	.00315	.00413	.00525
20	.00122	.00155	.00197	.00258	.00329
21	.00122	.00155	.00197	.00259	.00331
22	.00045	.00059	.00074	.00098	.00126
23	.00017	.00021	.00028	.00033	.00047
24	.00006	.00008	.00010	.00011	.00017
25	.00002	.00002	.00005	.00005	.00007

*The normalization condition, $\sum_j P_{1,j} = 1.00000$, is satisfied for all energy groups.

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APPENDIX A

Inelastic Scattering Probabilities in the Statistical Region

In the statistical region (when the incident neutron energy is > 3 Mev), general results can be obtained for a multigroup fast neutron spectrum code. The numerical results depend upon the nuclear temperature. It is necessary to define an average nuclear temperature for incident neutrons in an energy group in the MUFT IV scheme. E_i and E_{i-1} will denote the upper and the lower energy limits of a MUFT group designated by i . The average nuclear temperature, T_i , for energy group i is as follows:

$$T_i = t_i a \quad (A-1)$$

where

$$t_i = \frac{2}{\Delta u_i} \left(E_i^{\frac{1}{2}} - E_{i-1}^{\frac{1}{2}} \right)$$

In Eq. (A-1), Δu_i is the lethargy interval for energy group i . The probability of neutron inelastic scattering incident in an energy group i to an energy group j is denoted by $P_{i,j}$.

$$P_{i,j} = (E_{j-1}/T_i + 1)e^{-E_{j-1}/T_i} - (E_j/T_i + 1)e^{-E_j/T_i} \quad (A-2)$$

It should be noted that all references in Eq. (A-2) to the incident energy group i come through T_i . Thus, general results can be computed as a function of the values of the nuclear temperatures.

For the purposes of convenience, t_i in Eq. (1-1) is tabulated in Table A-I for MUFT energy groups. Once the value of the constant a is known, the appropriate average nuclear temperatures can be immediately calculated.

In Figures A-1 through A-5, the values of inelastic scattering probabilities are given as a function of the nuclear temperature. The calculated values are also given in Tables A-II and A-III.

TABLE A-I: VALUES OF t_1 FOR MUFT ENERGY GROUPS

Energy Group	Lower Limit of Energy Group	Upper Limit of Lethargy	$t_1 = \frac{2}{\Delta U_1} \left(E_1^{\frac{1}{2}} - E_{1-1}^{\frac{1}{2}} \right)$
1	7.79 Mev	0.25	2.9698
2	6.07	0.50	2.6186
3	4.72	0.75	2.3294
4	3.68	1.00	2.0338
5	2.86	1.25	1.8174
6	2.23	1.50	1.5827
7	1.74	1.75	1.3938
8	1.35	2.00	1.2576
9	1.05	2.25	1.0976
10	.821	2.50	.9488
11	.639	2.75	.8537
12	.498	3.00	.7495
13	.388	3.25	.6624
14	.302	3.50	.5868
15	.235	3.75	.5182
16	.183	4.00	.4559
17	.143	4.25	.3970
18	.111	4.50	.3599
19	.0865	4.75	.3125
20	.0674	5.00	.2759
21	.0409	5.50	.2295
22	.0248	6.00	.1790
23	.015	6.50	.1400
24	.00912	7.00	.1079
25*	.00553	7.50	-

* Since energy group 25 is the last group for which inelastic scattering probability is entered and no inelastic scattering within a group is allowed, we do not need t_{25} .

Fig.A1 Calculated Inelastic Scattering Probabilities for Various MUFT Groups versus Nuclear Temperature

TABLE A-II: NORMALIZED INELASTIC SCATTERING PROBABILITIES

MUFT GROUP	T=.2	T=.25	T=.27	T=.30	T=.35	T=.4
1	.00	.00	.00	.00	.00	.00
2	.00	.00	.00	.00	.00	.00
3	.00	.00	.00	.00	.00	.00
4	.00	.00	.00	.00	.0003	.0009
5	.00	.0001	.0003	.0007	.0022	.0053
6	.0002	.0012	.0021	.0042	.0100	.0185
7	.0015	.0063	.0095	.0158	.0291	.0445
8	.0073	.0210	.0281	.0398	.0602	.0794
9	.0233	.0484	.0589	.0739	.0956	.1120
10	.0520	.0836	.0943	.1077	.1232	.1314
11	.0874	.1151	.1223	.1294	.1345	.1334
12	.1178	.1326	.1343	.1341	.1292	.1211
13	.1335	.1327	.1296	.1234	.1122	.1005
14	.1318	.1190	.1128	.1038	.0899	.0779
15	.1168	.0978	.0908	.0812	.0678	.0572
16	.0953	.0752	.0686	.0601	.0488	.0402
17	.0729	.0549	.0494	.0425	.0338	.0274
18	.0530	.0385	.0343	.0291	.0227	.0182
19	.0370	.0261	.0231	.0194	.0149	.0118
20	.0250	.0173	.0152	.0126	.0096	.0076
21	.0272	.0184	.0161	.0138	.0100	.0078
22	.0112	.0074	.0064	.0052	.0039	.0030
23	.0044	.0029	.0025	.0020	.0013	.0012
24	.0017	.0011	.0009	.0008	.0006	.0005
25	.0007	.0004	.0005	.0005	.0002	.0002

TABLE A-III: NORMALIZED INELASTIC SCATTERING PROBABILITIES

MUFT Group	T=.5	T=.6	T=.7	T=.8	T=.9
1	.00	.00	.00	.00	.0015
2	.00	.00	.00	.00	.0075
3	.0008	.0029	.0074	.0145	.0237
4	.0045	.0121	.0236	.0377	.0525
5	.0165	.0332	.0524	.0715	.0880
6	.0411	.0658	.0880	.1059	.1182
7	.0755	.1007	.1183	.1291	.1336
8	.1089	.1261	.1337	.1350	.1316
9	.1302	.1348	.1319	.1254	.1166
10	.1341	.1272	.1169	.1060	.0950
11	.1229	.1088	.0953	.0833	.0725
12	.1029	.0864	.0727	.0619	.0527
13	.0802	.0646	.0529	.0439	.0367
14	.0592	.0462	.0369	.0301	.0248
15	.0419	.0318	.0249	.0201	.0164
16	.0286	.0213	.0164	.0132	.0106
17	.0190	.0140	.0107	.0084	.0068
18	.0124	.0090	.0068	.0053	.0043
19	.0080	.0057	.0043	.0033	.0027
20	.0050	.0036	.0027	.0021	.0017
21	.0051	.0036	.0027	.0021	.0017
22	.0020	.0014	.0010	.0008	.0006
23	.0007	.0005	.0004	.0003	.0002
24	.0003	.0002	.0001	.0001	.0001
25	.0002	.0001	.00	.00	.00

APPENDIX B

Summary of Nuclear Level Density

It would be helpful for the purpose of a discussion to list some experimental points concerning the nuclear level density:

- (i) For a given nucleus, the nuclear level spacing decreases rapidly with the increase in the excitation energy.
- (ii) For a fixed excitation energy the level spacing decreases rapidly with an increase in the mass number A .
- (iii) It has been found that the nuclear level density depends, at least, on the following three effects:
 - (a) Magic Nuclei: It has been observed that the level spacing increases by several orders of magnitude, when the number of neutrons and, or, protons are magic. In nuclear physics, a magic number is denoted by the following: 8, 28, 50, 82 and 128. This effect can be seen in Fig. B-1. In this figure, the level spacing per spin state is plotted versus the number of neutrons in compound nucleus.
 - (b) Odd-Even Effect: The nuclear level spacing (or the nuclear level density) is also influenced by the number of neutrons being odd and the number of protons being even, or other combinations. For example, one would expect that the level spacing of an even-even nucleus is different from those of an odd-even nucleus.
 - (c) Pairing Effect: In a highly successful model of a nucleus - the nuclear shell model - the neutrons (and the protons) prefer to occupy states in pairs consistent with the Pauli's exclusion principle. It has been proposed that an additional energy is required to break a pair, so that one of the nucleons can be excited to a higher level. In other words, the excitation energy effectively becomes $E_n - \delta$ rather than E_n , where δ is the pairing energy.

Fig. B-I. Level Spacing per Spin State Versus Number of Neutrons in Compound Nucleus. (Harvey 1961).

I. MODELS FOR NUCLEAR LEVEL DENSITY

The calculation of the inelastic scattering probability depends upon the number of nuclear levels (and on the assignment of their spins and parities), which lie below an excitation energy - the energy of the incident neutron. All this information being not always available, there arises a need for a theoretical description of nuclear levels by a nuclear model. A comparison of theoretical calculations and experimental data is generally made for a justification of a particular nuclear model. Only in recent years²⁰, enough experimental data on the nuclear level spacing has been accumulated for such a comparison. However, experimental information is far from being complete.

A. Fermi Degenerate Gas Model

In an extremely simplified picture, a nucleus can be described as a Fermi degenerate gas²¹. Thus, we can ignore the Coulomb effects i.e., we can consider the protons and neutrons as just nucleons. With such a description, the problem of nuclear level density simply reduces to the following: in how many ways a given excitation energy can be distributed amongst all the nucleons in a nucleus. It should be noted that we are not concerned with a single nucleon excitation, because the nuclear level spacing, computed from such a consideration, would be constant (with respect to the excitation energy) - contrary to the experimental facts. Therefore, we are dealing with a statistical description of the nuclear level density in terms of many-particle excitations.

For the range of neutron energy of interest (to the reactor problems), the decay time of the compound nucleus is much larger than the nuclear relaxation time. As a consequence of this fact, there is no phase relation between the formation of the compound nucleus and its decay. Therefore, the decay of this system is governed by the statistical considerations. In this regard, the process may be compared to the classical process of evaporation of heated liquid drops.

Bethe²¹ gives for the level density $\rho(E)$

$$\rho(E) = C e^{2(aE)^{1/2}} \quad (B-1)$$

where C is a numerical constant and E is the excitation energy. The simplified theory predicts that the level density parameter a is proportional to the mass number A .

Weinberg and Blatt²² proposed Eq. (B-2)

$$\rho(E) = C e^{2(aE')^{1/2}} \quad (B-2)$$

where

$$E' = E - \delta / [1 - \exp[-a(E - \delta)]] \quad (B-2a)$$

with δ equal to the pairing energy of a nucleus. It should be pointed out that the level density is essentially governed by $2\sqrt{aE}$ at high excitation energies. However, some difficulties arise when $E \rightarrow 0$. Lang and Le Couteur²³ have modified the analytical expression so as to get a finite result for the case $E \rightarrow 0$.

It must be noted that the single Fermion states are also characterized by the projection of the angular momentum, m , on the z axis. The projection of the total angular momentum, M , on the z axis of the system is the sum of projections of the n excited particles. The application of random coupling to the problem gives essentially a Gaussian distribution $\exp[-M^2/2\sigma^2]$, where the mean square deviation

$$\sigma^2 = n \langle m^2 \rangle$$

The density of states of a certain M is therefore given by

$$\rho(E, M) = \rho(E) \frac{e^{-M^2/2\sigma^2}}{\sqrt{2\pi} \sigma}$$

which gives

$$\rho(E, j) = \frac{(2j+1) \rho(E)}{2\sqrt{2\pi} \sigma^3} e^{-\frac{j(j+1)}{2\sigma^2}} \quad (B-3)$$

The approximation used in Eq. (B-3) is excellent for a very large range of j . The value of σ lies between 2 and 5. Ericson²⁴ gives $\sigma \sim 4$ for nuclides around atomic weight 55. σ^2 is also related to the nuclear moment of inertia, I , and the nuclear temperature, t

$$\sigma^2 = It/\hbar^2.$$

Since $I \sim A^{5/3}$ and $t \sim A^{-1/2}$, $\sigma \sim A^{1/2}$. However, not enough experimental information is available to verify this theoretical prediction. It should be noted that the nuclear temperature is defined as follows

$$\frac{1}{t} = \frac{d}{dE} \ln \rho(E).$$

B. Newton's Model

It was observed that the important region of a single particle level spacing is near the Fermi surface. Newton²⁵ assumes that $\bar{g}_0(t)$, the average single particle (nuclear) level density at a temperature t , is a slowly varying function of the temperature. Whereas no effect of magic nuclei was considered in the treatment described in the preceding section, Newton considers these effects by calculating $g(E)$ from Eq. (B-4).

$$g(E) = 2 \alpha A^{2/3} (j_N + j_Z + 1) \quad (B-4)$$

j_Z and j_N are the spins of the proton and neutron shell model states, which correspond to the atomic number $A (=N+Z)$. α is adjusted by an empirical fit to the experimental data, and j_N and j_Z are calculated from Klinkenberg's scheme²⁶. The level density $\rho(E, j)$ is related to $D(E, j)$, the level spacing by the following

$$\rho(E, j) = 1/D(E, j)$$

Newton gives

$$D = C(2j+1)^{-1} A [G_1 G_2]^{1/2} (2u+3t)^2 \exp \left\{ -2(\pi^2 G u/6)^{1/2} \right\} \quad (B-5)$$

where: $G_1 = \alpha(2\bar{j}_N+1)A^{2/3}$

$$G_2 = \alpha(2\bar{j}_Z+1)A^{2/3} \quad (B-6)$$

$$G = 2\alpha(\bar{j}_N+\bar{j}_Z+1)A^{2/3}$$

The temperature t is given by Eq. (6):

$$t = (6u/\pi^2 G)^{1/2} \quad (B-7)$$

The effective $\bar{j}_Z$ and $\bar{j}_N$ are given in Tables B-I and B-II. u is the effective excitation energy.

$$u = E - \delta$$

where E may correspond to the energy of the incident neutron in the process of inelastic scattering and δ is the pairing energy.

For $A > 40$, $\delta \approx 0.82 (4-A/100)$ Mev. δ may be taken to be (approximately) as 3.5 Mev for $A < 40$, or $\delta \approx A^{-1/2}$ Mev, as recommended by Green and Edwards²⁷.

Newton was able to fit the experimental data on level spacing (including the magic nuclei) within an uncertainty of a factor of three.

Ericson²⁴ followed Newton's method and found a fit given by Eq. (B-8):

$$\rho(u, j) = C \frac{j(j+1)}{u^2} \exp \left[-\frac{j(j+1)}{2\sigma^2} \right] \exp 2[a u]^{1/2} \quad (B-8)$$

where u is the effective excitation energy. The value of the parameter a was found to be

$$a = 0.056 (\bar{j}_Z+\bar{j}_N+1) A^{2/3} \quad (B-9)$$

TABLE B-I
Effective Proton Spin Parameters

z	Effective ($2\bar{j}_z+1$)	z	Effective ($2\bar{j}_z+1$)
1	2.0	49	9.6
2	2.67	50	9.2
3	3.33	51	8.8
4-5	4.0	52	8.4
6	3.33	53-56	8.0
7	2.67	57	8.2
8	3.33	58	8.4
9	4.67	59	8.6
10-13	6.0	60	8.8
14	4.67	61-64	9.0
15	3.33	65-74	9.0
16	2.67	75	8.0
17	3.33	76	7.0
18-19	4.0	77	6.0
20	5.33	78	5.0
21	6.67	79	3.6
22-27	8.0	80	3.2
28	6.67	81	4.4
29	5.33	82	5.6
30-31	4.0	83	6.8
32	4.67	84	8.4
33	5.33	85-90	10.0
34-37	6.0	91	9.867
38	4.67	92	9.733
39	3.33	93	9.6
40	4.67	94	9.467
41	7.33	95-98	9.33
42-48	10.0		

TABLE B-II

Effective Neutron Spin Parameters

N	Effective ($2j_N+1$)	N	Effective ($2j_N+1$)	N	Effective ($2j_N+1$)
1	2.0	42-48	10.0	93-100	10.0
2	2.67	49	9.2	101-106	10.0
3	3.33	50	8.4	107-118	10.0
4-5	4.0	51	7.6	119	8.8
6	3.33	52	6.8	120	7.6
7	2.67	53-54	6.0	121	6.4
8	3.33	55	6.8	122	5.2
9	4.67	56	7.6	123	3.6
10-13	6.0	57	8.4	124	3.2
14	4.67	58	9.2	125	4.4
15	3.33	59-64	10.0	126	5.6
16	2.67	65-74	10.0	127	6.8
17	3.33	75	8.8	128	8.4
18-19	4.0	76	7.6	129-134	10.0
20	5.33	77	6.4	135	10.4
21	6.67	78	5.2	136	10.8
22-27	8.0	79	3.6	137	11.2
28	6.67	80	3.2	138	11.6
29	5.33	81	4.0	139-148	12.0
30-31	4.0	82	4.8		
32	4.67	83	5.6		
33	5.33	84	6.8		
34-37	6.0	85-88	8.0		
38	4.67	89	8.4		
39	3.33	90	8.8		
40	4.67	91	9.2		
41	7.33	92	9.6		

As before, $\bar{j}_z$ and $\bar{j}_N$ are given in Tables B-I and B-II. a is plotted versus the mass number in Fig. B-2. The solid curve corresponds to Eq. (B-9).

C. Cameron's Method

Whereas Newton tried to find a theoretical fit to the experimental data on the nuclear level density and explained the general variation with the shell structure by using Klinkenberg's model, Cameron²⁸ considers these effects by a semiempirical atomic mass formula. The expression for the level density, as given by Cameron, is very complicated for calculation purposes.

$$D(u, j) = \frac{3.26 \cdot 10^5}{(2j+1)} \left[G_z G_N G^3 A^2 \left(\frac{\pi^2}{3} Gt - \frac{3}{2} \right) t^7 \right]^{1/2} \exp - \frac{\pi^2 Gt}{3} \quad (B-10)$$

where

$$t = \frac{3}{\pi^2 G} \left[\frac{3}{2} + \left(\frac{9}{4} + \frac{2 \pi^2 G u}{3} \right)^{1/2} \right] \quad (B-11)$$

and

$$G_k(t) = \frac{a_0(k) + a_1(k)t + a_2(k)t^2 + a_3(k)t^3 + a_4(k)t^4}{1 + t + t^2 + t^3 + t^4} \quad (B-12)$$

$$G = G_N + G_z. \quad (B-13)$$

In Eq. (B-12), k stands for N or z . Cameron fitted the fine coefficients namely $a_0(k)$ ----, $a_4(k)$ by a least square fit to 15 values of $G_k(t)$. These coefficients are tabulated for $10 \leq z \leq 109$ and $10 \leq N \leq 189$. However, it must be noted that for G and t to be determined simultaneously some iterative procedure is to be followed. Cameron recommends Eq. (B-14)

$$G(t)_{\text{initial}} = a_4(z) + a_4(N). \quad (B-14)$$

Near the closed shells it is often better to choose an initial value of about one half of the amount given by Eq. (B-14).

Fig. B-II The Parameter a Versus Mass Number (See Eqs. B-8 and B-9 of the text, (after Ericson).)

The root mean square error for Cameron's model is 1.74 in contrast to a corresponding value of 3 obtained from Newton's model. It may be noted that the Newton's method corresponds to a ratio of the moment of inertia to the rigid body value of 0.13 in contrast to the corresponding ratio by Cameron's model of 0.03. Part of the reason for such a reduction is that the cut-off term in angular momentum is not justified.

II. DISCUSSION AND CONCLUSIONS

In the first place, most of the existing experimental data on the nuclear level density can be explained by the various theoretical models. For example, it should be noted that the Newton's method (as well as Cameron's model) can effectively explain the large variation of the nuclear level spacings with the mass number A . However, a great caution is to be exercised in particular cases especially when accurate computations of the inelastic scattering matrix are desirable. Though the nuclear level density has generally been taken to be proportional to $\exp[2 a E]^{1/2}$, yet this is valid only for high excitation energies (neutron energy above 9 Mev or so).

The most convenient and quite accurate treatment is due to Ericson, who followed the basic model of Newton. The relevant expression is given in Eq. (B-8). However, Eq. (B-1) can be profitably used whenever an accurate determination of the parameter a is available from a detailed analysis of the experimental data in particular cases.