

INELASTIC SCATTERING OF NEUTRONS

II.* COMPARISON OF QCN THEORY WITH EXPERIMENT

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Summary

The cross section for inelastic scattering of neutrons by medium and heavy target nuclei is derived using the quasi-compound nucleus theory. Calculations are carried out for ^{56}Fe and ^{60}Ni . The results of these calculations are compared with experiment. Agreement between theory and experiment is quite good for scattering to the continuum of high levels and to discrete levels with small spins. On the other hand the theory underestimates the scattering to levels with large spin values.

I. INTRODUCTION

In Part I (present issue, pp. 135–43) a formalism, the so-called quasi-compound nucleus (QCN) theory, was developed to describe inelastic scattering of neutrons. It was found that, with the expression obtained for the scattering amplitude, cross sections were rather difficult to evaluate.

In the present work certain assumptions concerning the nature of the nucleus make it possible to write the scattering cross sections in a form more amenable to numerical evaluation. These cross sections are calculated for ^{56}Fe and ^{60}Ni targets and are compared with the experimentally observed values.

II. SCATTERING CROSS SECTION

In the centre-of-mass frame the QCN contribution to the inelastic scattering amplitude is (see Part I)

$$M_{fi} = (4\pi)^{3/2} \sum_{\substack{J_1, J_2 \\ l_1, l_2}}^v X(J_A, J_1, l_1, J_B, l_2, J_2, J'_A | M_A, \mu_n, M'_A, \mu'_n) i^{l_2-l_1} \\ \times \left(\frac{M_B}{M_A} E_{ni} + (\mathcal{E}_v^B - \mathcal{E}_i^A) \right) \left(\int G_{v1}^{l_1 J_1*}(r) j_{l_1}(k_1 r) r^2 dr \right) \\ \times \left(\int G_{v1}^{l_2 J_2}(r) j_{l_2}(k_1 r) r^2 dr \right) Y_{l_2 m}(Q), \quad (1)$$

where

$$X(J_A, J_1, l_1, J_B, l_2, J_2, J'_A | M_A, \mu_n, M'_A, \mu'_n) \\ = (2l_1+1)^{1/2} \langle J_A, M_A, \frac{1}{2}, \mu_n | J_1, M_A + \mu_n \rangle \langle J_1, M_A + \mu_n, l_1, 0 | J_B, M_A + \mu_n \rangle \\ \times \langle J_2, M'_A + \mu'_n, l_2, m | J_B, M_A + \mu_n \rangle \langle J'_A, M'_A, \frac{1}{2}, \mu'_n | J_2, M'_A + \mu'_n \rangle, \quad (2)$$

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\mathbf{k}_i and \mathbf{k}_f are the momenta, in the centre-of-mass frame, of the incident and outgoing neutrons,

$$\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i, \quad \text{and} \quad E_i = k_i^2/2M_n.$$

The functions G_{vn}^{lJ} , which are solutions of a set of coupled differential equations, can be replaced by single-particle wavefunctions

$$G_{ni}^{lJ} \rightarrow \theta_{vn}^{lJ} R_{vn}^{lJ}(r). \quad (3)$$

The radical wavefunctions R_{vn}^{lJ} are real and are normalized to unity, and the quantities θ_{vn}^{lJ} are complex factors known as reduced width amplitudes.

The scattering cross section, integrated over all angles, is then (see e.g. Tobocman 1961)

$$\sigma_{fi} = \frac{1}{2(2J_A+1)} \frac{M_{An}^2}{(2\pi\hbar^2)^2 k_i} \sum_{M_A, \mu_n, M'_A, \mu'_n} \left(\int |M_{fi}|^2 d\Omega_Q \right), \quad (4)$$

where, owing to orthogonality of the spherical harmonics and to the presence of the factor $i^{l_2-l_1}$ in the amplitude,

$$\begin{aligned} \int |M_{fi}|^2 d\Omega_Q &= (4\pi)^3 \sum X(J_A, J_1, l_1, J_B, l_2, J_2, J'_A | M_A, \mu_n, M'_A, \mu'_n) \\ &\quad \times X(J_A, J'_1, l_1, J'_B, l_2, J'_2, J'_A | M_A, \mu_n, M'_A, \mu'_n) \\ &\quad \times \left(\frac{M_B}{M_A} E_i + (\mathcal{E}_v^B - \mathcal{E}_i^A) \right) \left(\frac{M_B}{M_A} E_i + (\mathcal{E}_v^B - \mathcal{E}_i^A) \right) \\ &\quad \times \theta_{v_1}^{l_1 J_1}{}^* \theta_{w_1}^{l_1 J'_1} \theta_{v_1}^{l_2 J_2} \theta_{w_1}^{l_2 J'_2}{}^* F_{v_1}^{l_1 J_1}(E_i) F_{w_1}^{l_1 J'_1}(E_i) F_{v_1}^{l_2 J_2}(E_f) F_{w_1}^{l_2 J'_2}(E_f). \end{aligned} \quad (5)$$

The summation is to be taken over the set of indices $(l_1, l_2, v, J_1, J_2, w, J'_1, J'_2)$, and

$$F_{vn}^{lJ}(E) = \int R_{vn}^{lJ}(r) j_l(r(2M_n E)^{\frac{1}{2}}) r^2 dr. \quad (6)$$

We shall assume that, owing to randomness of the phases of θ_{vn}^{lJ} in the summations over v, w, J_1, J_2, J'_1 , and J'_2 , the total contribution due to the terms with $(v, J_1, J_2) \neq (w, J'_1, J'_2)$ can be neglected. The cross section (4) can be written as

$$\begin{aligned} \sigma_{fi} &= \frac{M_{An}^2}{2(2J_A+1)(2\pi\hbar^2)^2 k_i} (4\pi)^3 \\ &\quad \times \sum_{M_A, \mu_n, M'_A, \mu'_n} \sum_{v, J_1, J_2, l_1, l_2} |X(J_A, J_1, l_1, l_2, J_2, J'_A | M_A, \mu_n, M'_A, \mu'_n)|^2 \\ &\quad \times \mathcal{F}(J_1, J_2, l_1, l_2, J_B; E_i, E_f, \mathcal{E}_v^B), \end{aligned} \quad (7)$$

where

$$\begin{aligned} \mathcal{F}(J_1, J_2, l_1, l_2, J_B; E_i, E_f, \mathcal{E}_v^B) &= |\theta_{v_1}^{l_1 J_1}|^2 |\theta_{w_1}^{l_2 J_2}|^2 \\ &\quad \times \left(\left(\frac{M_B}{M_A} E_i + (\mathcal{E}_v^B - \mathcal{E}_i^A) \right) F_{v_1}^{l_1 J_1}(E_i) F_{w_1}^{l_2 J_2}(E_f) \right)^2. \end{aligned} \quad (8)$$

When the number of levels per unit excitation energy is very large in the intermediate nucleus B , as is usually the case in medium and heavy nuclei, the sum over v in (7) may be replaced by an integral after inserting a suitable level density ρ on the right of (7). Thus,

$$\begin{aligned} \sigma_{fi} = & \frac{M_{An}^2}{2(2J_A+1)(2\pi\hbar^2)^2} \frac{k_f}{k_i} (4\pi)^3 \\ & \times \sum_{M_A, \mu_n, M'_A, \mu'_n} \sum_{J_1, J_2, l_1, l_2, J_B} |X(J_A, J_1, l_1, J_B, l_2, J_2, J'_A | M_A, \mu_n, M'_A, \mu'_n)|^2 \\ & \times \int_{\mathcal{E}_1}^{\mathcal{E}_0^B} \mathcal{F}(J_1, J_2, l_1, l_2, J_B; E_i, E_f, \mathcal{E}_v^B) \rho(J_B, \mathcal{E}_v^B) d\mathcal{E}_v^B. \end{aligned} \quad (9)$$

\mathcal{E}_0^B is the ground state binding energy of B . The lower limit of the integration is determined from the condition that all single-particle wavefunctions $R_{v_n}^{IJ}$ that occur in (9) must represent bound states. This also ensures that the singularities of the amplitude are confined to the negative part of the real E_i axis, i.e. the unphysical region.

For regions of excitation energy of the nucleus A , where the level density is large, we can write the cross section for scattering of neutrons with incident energy E_i to outgoing energies lying between E_f and $E_f + dE_f$ as

$$\sigma(E_i, E_f) dE_f = \sum_{J'_A} \sigma_{fi} \rho(J'_A, \mathcal{E}_f^A) dE_f. \quad (10)$$

The level density formula used here is one given by Gilbert and Cameron (1965). In their notation

$$\rho(E, J) = \frac{\pi^{\frac{1}{2}} \exp\{2(aU)^{\frac{1}{2}}\}}{12} \frac{(2J+1) \exp\{-(J+\frac{1}{2})^2/2\sigma^2\}}{a^{1/4} U^{5/4} 2(2\pi)^{\frac{1}{2}} \sigma^3}. \quad (11)$$

In our work it is advantageous to express ρ as a function of binding energy \mathcal{E} through the relation

$$E = \mathcal{E}_0 - \mathcal{E},$$

where \mathcal{E}_0 is the ground state binding energy.

III. REDUCED WIDTHS

The eigenfunctions $\Psi_v(X)$ of the total Hamiltonian of the system $(A+n)$, which correspond to bound states B , can be expanded in terms of the eigenfunctions ϕ_s of the Hamiltonian H_A for the internal motion of A :

$$\begin{aligned} \Psi_v(X) = & \sum_{sJlm} \langle J_A, M_A, \frac{1}{2}, \mu_n | J, M_A + \mu_n \rangle \langle J, M_A + \mu_n, l, m | J_B, M_A + \mu_n + m \rangle \\ & \times \psi_{vs}^{mJ}(\mathbf{r}) \phi_s(x) \end{aligned} \quad (12)$$

and

$$H_A \phi_s(x) = \mathcal{E}_s^A \phi_s(x). \quad (13)$$

The quantum number s is understood to include the spin quantum numbers J_A , M_A , and μ_n .

The reduced width amplitudes θ_{vs}^{lJ} were introduced by replacing ψ_{vs}^{lmJ} by the normalized single-particle wavefunctions

$$\psi_{vs}^{lmJ}(r) = \theta_{vs}^{lJ} R_{vs}^{lJ}(r) Y_{lm}(r). \quad (14)$$

The magnitude of θ_{vs}^{lJ} indicates the extent to which the wavefunction Ψ_v is represented by the single-particle wavefunction $R_{vs}^{lJ} Y_{lm}$.

When dealing with nuclei containing large numbers of nucleons, we assume that all single-particle states are equally represented in the compound nucleus B . We may then replace the quantities θ_{vs}^{lJ} in (9) by an average reduced width θ_v for each level v of the nucleus B .

From the condition

$$\Psi_v^*(X) \Psi_v(X) dX = 1, \quad (15)$$

we find

$$\sum_{s'lJ} (2J_B+1) |\theta_{vs}^{lJ}|^2 = 1. \quad (16)$$

The summation over s' is just the sum over s without the summations over the magnetic quantum numbers M_A and μ_n . The average reduced width $|\theta_v|^2$ is defined as

$$|\theta_v|^2 = \{(2J_B+1)N_v\}^{-1}, \quad (17)$$

where N_v is the total number of single-particle states with quantum numbers J_A , J , and l in the expansion of Ψ_v . The number of states of the core nucleus A of given spin J_A which can exist in B when B is in the state Ψ_v of energy \mathcal{E}_v^B is

$$N(v, J_A) = 2 \int_0^{\mathcal{E}_v^A} \rho(J_A, \mathcal{E}^A) d\mathcal{E}^A. \quad (18)$$

Using an approximate level density formula (Gilbert and Cameron 1965)

$$\rho(J, \mathcal{E}) = K(2J+1)U^{-2} \exp\{2(aU)^\dagger\}, \quad (19)$$

we find

$$N(v, J_A) = C'(2J_A+1), \quad (20)$$

where C' is some constant factor that is independent of v and J_A . The quantity N_v can now be expressed as

$$N_v = C' \sum_{J_A} (2J_A+1) \{N_1(J_A) + N_2(J_A)\}, \quad (21)$$

where $N_1(J_A)$ and $N_2(J_A)$ are the numbers of states of given J_A with $J = J_A + \frac{1}{2}$ and $J = J_A - \frac{1}{2}$ respectively, i.e.

$$N_1(J_A) = \begin{cases} 2(J_A+1), & \text{if } J_B > J_A + \frac{1}{2}, \\ 2J_B+1, & \text{if } J_B \leq J_A + \frac{1}{2}, \end{cases} \quad (22a)$$

$$N_2(J_A) = \begin{cases} 2J_A, & \text{if } J_B > J_A - \frac{1}{2}, \\ 2J_B+1, & \text{if } J_B \leq J_A - \frac{1}{2}. \end{cases} \quad (22b)$$

Using these, (21) becomes

$$N_v = 2C'\{P(J_B) + (2J_B + 1)Q(J_B)\}, \quad (23)$$

with

$$P(J_B) = \frac{1}{3}(2J_B + 3)(2J_B^2 + 6J_B + 4)$$

and

$$Q(J_B) = (J_M + J_B + 2)(J_M - J_B + 1),$$

where J_M is the upper limit of the summation over J_A in (21). If we denote N_v by $N(J_B)$, we find

$$\frac{N(J_B + 1)}{N(J_B)} = \frac{P(J_B) + (2J_B + 3)Q(J_B) + 2(2J_B + 1)(J_B + 1)}{P(J_B) + (2J_B + 1)Q(J_B)}. \quad (24)$$

If J_M is large compared with J_B this can be written approximately as

$$\frac{N(J_B + 1)}{N(J_B)} = \frac{2J_B + 3}{2J_B + 1}. \quad (25)$$

The average reduced width is thus of the form

$$|\theta_v|^2 = C(2J_B + 1)^{-2},$$

where C is some constant factor.

IV. RADIAL INTEGRALS

The radial wavefunctions $R_{vs}^{IJ}(r)$ which are required for the evaluation of the integrals (6) can be obtained by solving the equation

$$-d^2v_{nl}/dr^2 + [2M_{nA}\mathcal{E} - \nu(r) - \{l(l+1)\}/r^2]v_{nl} = 0, \quad (26)$$

where n is the principal quantum number of the wavefunction v . We assume that spin-orbit coupling effects are negligible so that $\nu(r)$ is a central potential, which we shall take to be of the Wood-Saxon form

$$\nu(r) = -V_0[1 + \exp\{(r - r_0)/a\}]^{-1}, \quad (27)$$

where r_0 and a are the radius and diffuseness parameters. The depth of the potential is variable so that wavefunctions for any given binding energy

$$\mathcal{E} = \mathcal{E}_v^B - \mathcal{E}_s^A$$

can be obtained.

For different values of the principal quantum number n , the radial integrals were found to differ from each other by factors that were almost independent of \mathcal{E} , E , and l . It is therefore possible to evaluate (6) using

$$R_{vs}^{IJ} = v_{nl}$$

for a fixed value of n .

Cross sections thus calculated will differ from the correct values by a constant factor, but their dependence on incident and outgoing energy is not affected.

One further assumption must be made concerning the parameters of the Wood-Saxon potential. We shall assume them to be independent of the state of the

TABLE 1
ENERGY LEVELS OF ^{56}Fe

Energy (MeV)	J^π	Energy (MeV)	J^π	Energy (MeV)	J^π	Energy (MeV)	J^π
0.0	0+	2.939	0+	3.368	2+	3.600	0+
0.846	2+	2.957	2+	3.388	6+	3.605	2+
2.084	4+	3.119	5-	3.445	3+	3.829	2+
2.654	2+	3.122	3+	3.450	1+	3.856	3+

TABLE 2
THEORETICAL σ_{th} AND EXPERIMENTAL $\sigma_{\text{exp}} = 4\pi\sigma$ (50°) CROSS SECTIONS FOR ^{56}Fe
In the calculations the parameters of the potential were $r_0 = 6\text{ f}$ and $a = 0.5\text{ f}$

Incident Energy (MeV)	Level (MeV)	σ_{exp} (bn)	σ_{th} (bn)	Incident Energy (MeV)	Level (MeV)	σ_{exp} (bn)	σ_{th} (bn)
3.00	0.845	0.96 \pm 0.08	1.030	4.50	2.939	0.166 \pm 0.008	0.343
	2.084	0.161 \pm 0.013	0.002		2.957		
	2.654	0.09 \pm 0.045	0.042		3.119		
3.50					3.122	0.148 \pm 0.010	0.018
	0.845	0.54 \pm 0.08	0.689	3.368	0.244 \pm 0.012	0.289	
	2.084	0.190 \pm 0.013	0.001	3.388			
	2.654	0.225 \pm 0.010	0.106	3.445			
	2.939	0.205 \pm 0.008	0.364	3.450	0.178 \pm 0.011	0.188	
	2.957			3.600			
	3.119	0.08 \pm 0.04	0.001	3.605	0.153 \pm 0.016	0.025	
	3.122			3.829			
			3.856				
4.00	0.845	0.47 \pm 0.08	0.502	5.00	0.845	0.43 \pm 0.08	0.197
	2.084	0.150 \pm 0.013	0.006		2.084	0.116 \pm 0.013	0.007
	2.654	0.167 \pm 0.010	0.138		2.654	0.116 \pm 0.010	0.104
	2.939	0.173 \pm 0.008	0.393		2.939	0.102 \pm 0.008	0.205
	2.957				2.957		
	3.119	0.197 \pm 0.010	0.013		3.119	0.126 \pm 0.010	0.016
	3.122				3.122		
	3.368	0.247 \pm 0.012	0.235		3.368	0.180 \pm 0.012	0.221
	3.388				3.388		
	3.445				3.445		
	3.450				3.450		
	3.600	0.068 \pm 0.035	0.117		3.600	0.166 \pm 0.011	0.144
	3.605				3.605		
					3.829		
	4.50	0.845	0.50 \pm 0.08		0.356	3.856	0.130 \pm 0.016
2.084		0.165 \pm 0.013	0.008				
2.654		0.132 \pm 0.010	0.143				

core nucleus, the integrals F_{vs}^{IJ} being calculated using fixed values of the parameters of the potential. From simple physical considerations one might expect the radius of the nucleus to increase with increasing excitation energy; however, such variations are probably small compared with the nuclear radius.

V. SCATTERING TO DISCRETE LEVELS

The cross sections for the excitation of the discrete levels of a nucleus are given by equation (9). Calculations were carried out for the low lying levels (up to 4 MeV excitation energy) of ^{56}Fe , with incident neutron energies between 3 and 5 MeV. The spin and parity assignments of the levels were taken to be the same as those used by Towle and Owens (1967) and are given in Table 1.

The results of these calculations and the experimentally observed cross sections (Hopkins and Silbert 1964) are listed in Table 2. The calculated cross sections were normalized to the correct total cross sections from Hopkins and Silbert:

Incident energy (MeV)	3.00	3.50	4.00	4.50	5.00
Total cross section (bn)	1.21 ± 0.09	1.27 ± 0.09	1.50 ± 0.09	1.74 ± 0.09	1.49 ± 0.09

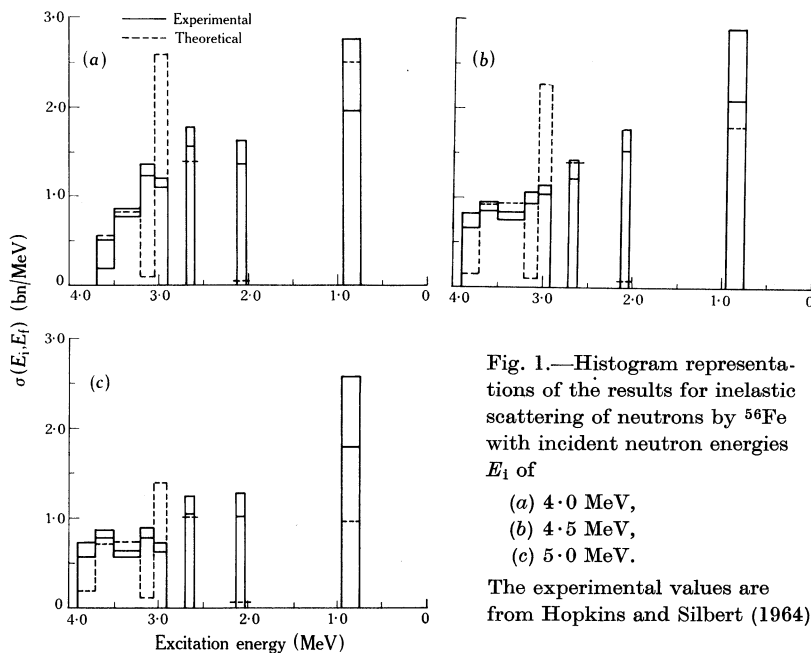


Fig. 1.—Histogram representations of the results for inelastic scattering of neutrons by ^{56}Fe with incident neutron energies E_i of

- (a) 4.0 MeV,
- (b) 4.5 MeV,
- (c) 5.0 MeV.

The experimental values are from Hopkins and Silbert (1964).

The outstanding features of the results in Table 2 (see also Fig. 1) are the large differences between the calculated and observed cross sections for scattering to the 2.084 MeV (4^+) and the 3.119 (5^-) plus 3.122 (3^+) MeV levels. On the other hand, the cross sections for scattering to the 2.939 (0^+) plus 2.957 (2^+) levels are overestimated. It is perhaps of some interest to observe that the amount by which the cross sections for the 2.939 plus 2.957 levels are overestimated is almost exactly equal to the amount by which the scattering to the 3.119 plus 3.122 levels is underestimated. The total cross sections for scattering to the 2.939 \rightarrow 3.122 MeV levels are very close to the observed ones.

The discrepancy between the calculated and observed cross sections for the first excited state when the energy of the incident neutrons increases has also been

noted by other authors when analysing scattering data with the Hauser-Feshbach method (see e.g. Towle and Owens 1967). This has been attributed to the rapid onset of a direct reaction mechanism when the energy of the incident neutrons is between 4 and 7 MeV.

VI. SCATTERING TO THE CONTINUUM

When we are considering scattering to final states where individual levels can no longer be resolved it is necessary to use a statistical model of the final nucleus to describe the scattering. The scattering cross section is then given by equation (10).

Cross sections were calculated for ^{56}Fe and ^{60}Ni with 7 MeV incident neutrons and were compared with the experimentally observed values of Towle and Owens (1967). The statistical model was used for scattering to levels above 3.7 MeV excitation energy for ^{56}Fe and 3.2 MeV excitation energy for ^{60}Ni . The parameters of the level density formula (11) were taken from the tabulations of Gilbert and Cameron (1965) and Cook, Ferguson, and Musgrove (1967).

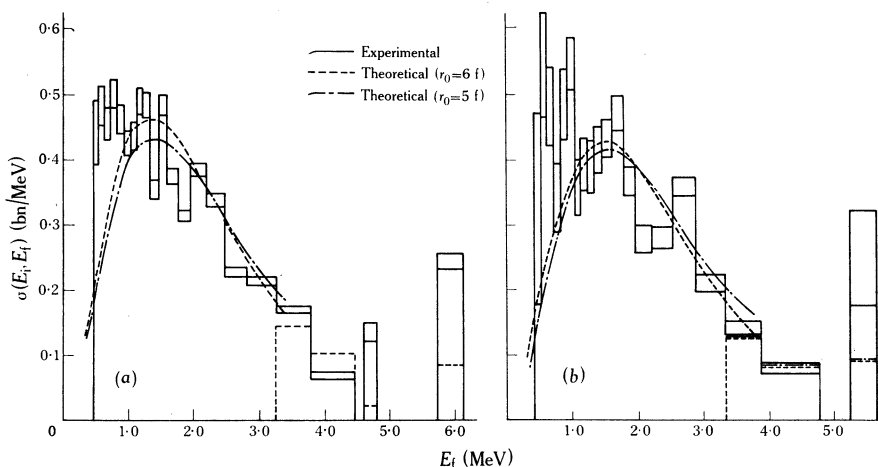


Fig. 2.—Results of calculations of $\sigma(E_i, E_f)$ for (a) ^{56}Fe and (b) ^{60}Ni compared with the experimentally observed values of $4\pi\sigma(E_i, E_f)$ at 90° by Towle and Owens (1967).

The calculated cross sections were found to be in good agreement with experiment (Fig. 2) except at very low outgoing neutron energies. The calculated cross section decreases when the excitation energy exceeds 5.5 MeV for ^{56}Fe and 5.3 MeV for ^{60}Ni . It is interesting to observe that the experimental values have peaks at almost precisely these energies, and decrease until the excitation energy reaches a value of about 5.8 MeV. The present calculations give an almost exact fit to the cross sections in those regions. It is also worth noting that the position of the peak in the theoretical cross section is almost independent of the parameters of the potential used for calculating the radial integrals (6).

The large values of the observed cross sections for scattering to levels beyond 5.8 MeV excitation energy is probably entirely due to the levels with large spin since, as we have observed in the previous section, it is for these levels that the QCN theory is inadequate, producing cross sections that are far too small.

VII. DISCUSSION

It was observed in Section V that the QCN theory underestimates the scattering to high spin levels. The radial integrals F_{vs}^{lJ} decrease rapidly with increasing l ; therefore, since levels with large spin values require incident or outgoing neutrons with high orbital angular momenta to excite them, the cross sections for the excitation of these levels will also be very small. It may be possible, by introducing a spin-orbit interaction in the potential (27), to eliminate some of the discrepancy between theory and experiment. The effect of an attractive spin-orbit potential would be to increase F_{vs}^{lJ} for higher orbital angular momenta, but it is doubtful that the inclusion of $l.s$ coupling will be sufficient to account for the difference between the calculated and the observed cross sections for, say, the 2.084 MeV (4^+) level of ^{56}Fe .

Another point worth commenting on is the good agreement between theory and experiment for scattering to levels in the continuum region between 5.3 and 5.8 MeV excitation energies. The results are quite remarkable in view of the already mentioned shortcomings of the theory. Although this agreement may be purely coincidental it appears from our results for ^{56}Fe and ^{60}Ni that at a certain excitation energy the distribution of levels in the nucleus undergoes a sudden change. It would be of great interest to see whether other nuclei in the medium to heavy region display similar behaviour.

VIII. ACKNOWLEDGMENT

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