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LAWRENCE LIVERMORE LABORATORY
University of California/Livermore, California

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S. M. Grimes

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S. M. Grimes
Lawrence Livermore Laboratory, Livermore California 94550

Abstract

The design of fusion reactors will require information about a large number of neutron cross sections in the MeV region. Because of the obvious experimental difficulties, it is probable that not all of the cross sections of interest will be measured. Current direct and pre-equilibrium models will be used to calculate non-statistical contributions to neutron cross sections from information available from charged particle reaction studies; these will be added to the calculated statistical contribution. Estimates of the reliability of such calculations will be derived from comparisons with the available data.

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Use of Nuclear Reaction Models in Cross Section Calculations

Because of the difficulty of cross section measurements involving neutrons, most studies of nuclear reaction mechanisms have utilized charged particles. It is normally argued that because of the similarity between the nuclear interactions of protons and neutrons with nuclei and because of the poorer quality of neutron data that it is more productive to concentrate on the charged particle studies. On the other hand, from a technological standpoint, the neutron cross sections are often the ones which are of greatest interest. I would like to summarize some procedures which are of value in estimating neutron induced cross sections based in large part on reaction systematics deduced from charged particle studies. Since neutron cross sections at 14 MeV are of particular interest to the CTR program, the emphasis will be on cross sections at that energy, although the same procedures would be useful both above and below that energy.

The most widely used model in estimating neutron cross sections is the statistical model (compound nucleus). This reaction mechanism yields (in general) spectra which are smooth in angular dependence and which are dominated by low energy neutrons (~1 MeV) and charged particles just above the Coulomb barrier. Extensive studies of the reaction mechanisms of nucleon induced reactions in the energy range below 20 MeV (and for $A \geq 20$) have indicated that a large fraction (>80%)of the reactions proceed through formation of a compound nucleus. Thus, this contribution must be included in calculating neutron cross sections. The parameters needed for such a calculation include transmission coefficients and level density parameters. Compilations listing average values for these quantities are available and many such calculations have shown that the averaged parameters produce

reasonable results.

The first transparency summarizes these requirements. Global optical parameters for alpha particles, protons and neutrons have been widely used in calculating transmission coefficients, but appropriate parameters are more difficult to find for deuterons, helium-3, or tritons. For nuclei in the range $A > 40$, these latter three channels typically represent less than 2% of the decay width and can be ignored without affecting the proton, alpha or neutron cross sections, but for $A \leq 25$ these channels could be important (depending on the Q values). Also, for light nuclei the use of averaged level density parameters may not be appropriate. Specific level schemes are required in situations where the level density is small. I will not discuss these calculations in detail because a previous speaker has discussed the Hauser-Feshbach formalism.

Although the remaining processes comprise a small fraction (<.2) of the reaction cross section they are of considerable importance. For example, if one looks at the neutron spectrum produced by 14-MeV neutron bombardment of Fe, it can be seen that only the low energy portion of the spectrum is fit by a compound nuclear calculation. From a neutron transport standpoint, a factor of five to ten error for inelastic neutrons above 8 MeV could be quite important.

Is there a procedure which can be used to predict the inelastic spectrum above 6 MeV on the basis of nuclear reaction systematics? To answer this question, we first examine (p,p') spectra on a number of targets at 14 MeV. The next transparency shows the (p,p') cross sections for a number of Ti and Mo isotopes. Each isotope chain includes one element for which the neutron number is magic. Although in these cases the first 2^+ state is populated

with a much smaller cross section than in the remaining isotopes, for each isotope the 2^+ and 3^- states are the two strongest inelastic states seen in the (p,p') reaction.

The systematics of the lowest 2^+ and 3^- states are reasonably well understood and a calculation of these cross sections depends only on information which is widely available (next transparency). Either a vibrational or a rotational model predicts a low-lying 2^+ state, with the difference between the two models appearing in the ordering of higher states.

To calculate the 2^+ cross section, optical model parameters and the deformation parameter β_2 are required. The precise location of the state does not affect the cross section significantly but an approximate location is needed to give the energy of the inelasticly scattered neutrons. Coulomb excitation measurements yield values for the parameter β_2 and the magnitudes of β_2 for over 150 nuclei have been tabulated by Stelson and Grodzins. More recently measured values are listed in the Nuclear Data Sheets. The 2^+ cross sections calculated for 14-MeV neutrons can be as small as 10 mb for magic nuclei but more typically are 20-50 mb and can be above 100 mb.

Many such calculations have been performed with distorted-wave-Born-approximation (DWBA) codes and good results are obtained with this approach. Somewhat more accurate results are obtained with a computer code which solves the coupled equations for the ground and 2^+ state. The differences in angular distributions between vibrational and rotational 2^+ states are not found in a DWBA calculation but are reproduced by a coupled channel calculation.

Similar calculations for the 3^- states require values for β_3. While the systematics of the dependence of β_3 on nucleon number are not as well known as those for β_2, these values have been measured for many nuclei. The Nuclear Data Sheets list the values for β_3 obtained from (p,p'), (α,α') or even (e,e') experiments.

Two additional comments regarding the uncertainty in such collective excitation calculations should be made. The calculated cross section depends not only on β but also the radius of the potential used in the calculation. Comparison of calculated values obtained with three well-known neutron potentials (Bjorklund-Fernbach, Rosen, Becchetti-Greenlees) indicates that the cross section for a given β varies less than 10% as a function of the optical parameters used.

A second potential problem lies in the proper choice of β when the values for β obtained using different reactions are inconsistent. It should be remembered that the β measured in electromagnetic measurements (e,e' or Coulomb excitation) could differ from that deduced from nuclear interactions ((p,p') or (α,α')) if the nuclear matter distribution is not the same as the charge distribution.

In general a Lane model analysis would predict that the β values for (p,p') and (n,n') might differ slightly because of an isovector component to β. These effects should be small--however, in cases where the electromagnetic and (p,p') β values differ the former (assuming no experimental errors) should be used in calculating an (n,n') cross section. The (p,p') and (n,n') β values would differ, while the electromagnetic β values will be closest to the latter values.

As has already been indicated, the ordering of higher excited states is in principle determined for a vibrational or rotational nucleus. The population of such states through two-step processes can be calculated with a coupled channel code.

Particularly for vibrational nuclei, such calculations are not always reliable because the "two-phonon" states contain significant admixtures of one-phonon states. Obviously, if the appropriate spectroscopic information is available, contributions from such states can be calculated but otherwise will be subject to considerably larger uncertainties than the 2^+ and 3^- state calculations.

In summary, reasonable estimates (accuracy ~ 20%) of cross sections for excitation of 2^+ and 3^- states may be made on the basis of parameters obtained from charged particle studies. The information available for other excited levels varies widely from nucleus to nucleus, making direct reaction calculations impossible in many cases.

An alternative approach to calculating non-equilibrium cross sections is to try to determine an average behavior and strength for them. Such a model has been developed and has been tested for a number of reactions.

The theoretical justification for such a procedure is that compound nuclear states are very complicated relative to the single particle levels serving as entrance channel states. I. as is generally believed, nuclear forces are primarily two-body, a compound nuclear state is reached only after a sequence of such interactions. The initial one-particle state is damped into a two-particle, one-hole state and this in turn into a three-particle, two-hole state. Only after a chain of five to ten such stages is a "compound nucleus" state reached. The additional assumption that each

of these intermediate states has a small decay width in addition to its damping width results in a "pre-equilibrium" contribution to emission spectra.

The first suggestion that the non-equilibrium portion of emission spectra be analyzed using such a model was made by Griffin and the model is often called the "Griffin" or exciton (where exciton denotes particle or hole) model. In its original form the formalism was able to predict that for small exciton numbers (n) the density of more complicated states (n + 2) was so large relative to the density of (n - 2) exciton states that the system would indeed proceed to equilibrium. In addition, the fraction of n exciton states with one particle unbound was easily shown to be a rapidly decreasing function of n. Thus, the decay either took place at an early stage in the equilibration process or occurred after the many transitions typical of an equilibrium process. (See transparency.)

A fundamental drawback to the first exciton models was that absolute cross sections were not predicted. By assuming a constant matrix element coupling all states related by a two-body interaction, the relative spectral shape could be obtained. A number of experiments established that predictions of the model were correct.

Within the last two years, two alternative approaches have extended the model to enable prediction of absolute cross sections. The "extended Griffin model" utilizes matrix elements whose dependence on excitation energy and mass number is deduced from fitting previous non-equilibrium spectra. An alternative procedure (called the hybrid model) is to determine the total damping width at each stage from the imaginary part of the optical potential. This model has the advantage of relying only on parameters determined from

other types of experiments (not from fitting non-equilibrium spectra) and also incorporates a dependence on geometry into the calculation. This model has provided a quantitative description of the non-equilibrium parts of nucleon-induced emission spectra.

The calculation of spectra requires only an assumption of the initial exciton configuration and an imaginary component to the optical potential. Since the values of both of these parameters are fairly well established, the calculation is effectively a no-free-parameter calculation.

The next transparency illustrates the quality of fit which can be obtained for a (p,n) spectrum. This reaction does not have strong collective states as an (n,n') or (p,p') spectrum; the analog state is the only prominent peak in these spectra and is only 1/3 to 1/4 as large as the typical 2^+ or 3^- state. Two general features of the hybrid calculation are worth noting. The predicted pre-equilibrium fraction (as a fraction of the total reaction cross section) is about 10% at 14 MeV and varies only slightly with A. It also increases with increasing bombarding energy, ranging from less than 5% at 8 MeV to about 15% at 25 MeV. Also, throughout this energy range, more than 80% of the pre-equilibrium cross section is produced by decays from the initial pre-equilibrium state. Thus, the shape of the pre-equilibrium spectrum is determined primarily by the assumed initial configuration, while the magnitude is sensitive to the value of the imaginary potential used.

Returning to the (n,n') reaction, we see in the next two transparencies the predictions of a combined pre-equilibrium and compound nuclear calculation. The comparisons for Fe and Ni show three sets of data, but only one of these extends higher than 8 MeV. Experimental points are denoted

by the circles and triangles and the solid lines denote a statistical calculation. The solid line with a diagonal mark ⫽ denotes the sum of the calculated statistical and the pre-equilibrium cross sections. For Fe, the discrepancy between the statistical prediction and the data is about 180 mb for neutrons above 5 MeV. The combined 2^+ and 3^- cross sections are about 70 mb and the pre-equilibrium prediction is 75 mb. Thus, for Fe, the high energy discrepancy is largely accounted for (≈80%) by the 2^+ and 3^- states and a pre-equilibrium contribution. The sum of these contributions for Fe is denoted ⋆. For the Ni target the calculations for the pre-equilibrium process and the direct contributions for the 2^+ and 3^- states have been supplemented by DWBA calculations for population of 8 additional excited states for which spectroscopic information is available from (p,p') studies. The addition of this cross section to the other non-statistical contribution produces very good agreement with the observed neutron spectrum--this is, however, more information than is usually available for a nucleus and the discrepancies seen in the Fe case will be more typical of estimated cross sections for nuclei for which detailed spectroscopic measurements are not available.

The previous discussion has pointed out that optical model parameters are required for evaluation of transmission coefficients as well as calculation of direct reaction cross sections. Widely used sets of optical model parameters for neutrons are due to Bjorklund and Fernbach, Rosen and Becchetti and Greenlees. The next transparency shows a comparison between the elastic scattering data of Coon et al. for Fe and the predictions of the above three compilations. The deviations seen are due to the fact

that the parameters were constrained to have a global dependence and are larger than would be obtained for a fit to a particular nucleus. They are presumably typical of those encountered in using global potentials, however.

Because neutron elastic scattering data are not as precise nor as extensive as proton elastic scattering cross section measurements, there is interest in determining the extent to which the latter data might be used to predict the former.

The next transparency lists the terms typically included in proton optical potentials. The V_0 and V_1 are the isoscalar and isovector components of the real potential and the $.4Z/A^{1/3}$ term is a Coulomb correction (correcting the optical model energy dependence for the effect of the Coulomb repulsion). The W_0 and W_1 are the isoscalar and isovector parts of the imaginary potential.

The neutron potentials deduced from these proton parameters assuming isospin conservation are shown on the bottom two lines. A comparison between the Coon data and the predictions of the Rosen and Becchetti-Greenlees "proton" parameters is presented in the last transparency. In each case the V_0, V_1, W_0, and W_1 are obtained from the proton optical analysis. For both potentials the fit is reasonably good and for the BG potential agreement with the data is better than for the corresponding neutron potential. The somewhat poorer fit for the Rosen potential may be due to the lack of a W_1 term in this potential. Particularly for the BG potential, the fit obtained for the "proton" potential is comparable in quality to those of the "neutron" global potentials.

In summary, application of our knowledge of reaction systematics enables reasonable estimates of compound nuclear, direct, and pre-equilibrium reaction contributions to neutron cross sections to be made. Until the specific needs of the CTR program are better defined, such calculated values will be of great value in preliminary design studies.

STATISTICAL:

HAUSER FESHBACH

$$\sigma = \pi \lambda^2 \frac{T_{in}\, T_{out}}{\Sigma\, T_{out}}$$

CALCULATION REQUIRES:

1. TRANSMISSION COEFFICIENTS (OPTICAL POTENTIAL)
2. BINDING ENERGIES
3. LEVEL DENSITY PARAMETERS

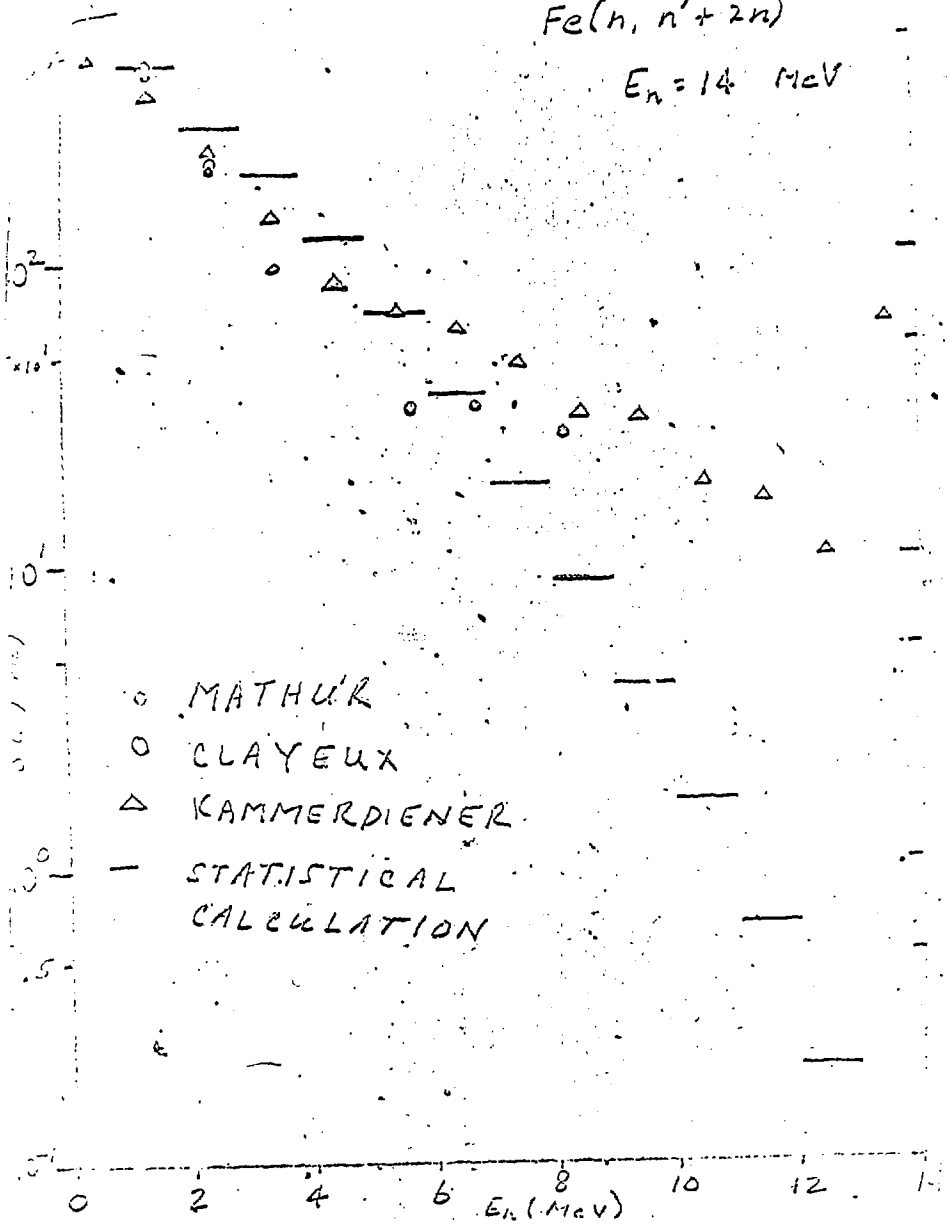
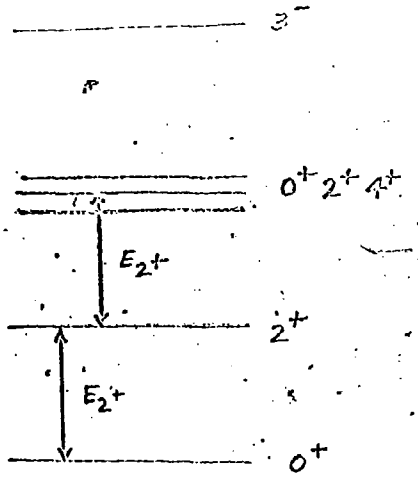

Fe(n, n'+2n)
E_n = 14 MeV
MATHUR
CLAYEUX
KAMMERDIENER
STATISTICAL CALCULATION
0
2
4
6
8
10
12
E_n (MeV)

TABLE II. Levels excited in the present experiment with their spins, parities, and integrated cross sections.

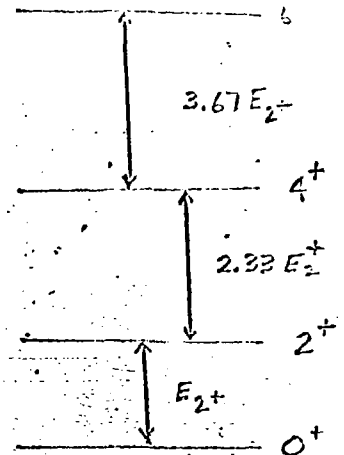
^{46}Ti			^{48}Ti			^{50}Ti		
Ex (keV)	J^π	σ (mb)	Ex (keV)	J^π	σ (mb)	Ex (keV)	J^π	σ (mb)
886	2^+	42.4	985	2^+	33.3	1550	2^+	16.8
2005	4^+	8.8	2301	4^+	2.7	2686	4^+	4.8
2603	0^+	2.4	2425	2^+	2.6	3208	6^+	1.1
2959	2^+	2.7	3004	0^+	1.9	3770		0.8
3056	3^-	6.5	3230, 3249	4^+	5.4	3880	0^+	1.5
3161	1^+	2.2				4138, 4184	4^+, 2^+	8.4
3435	(5)	1.4	3365, 3376	3^-, $2^{(+)}$	8.8	4322	2^+	3.3
3565	3^-	7.0	3520		0.7	4420	2^+	5.5
3715		1.4	3625	2^+	1.8	4738		0.8
3843	4^+	6.8	3707	1^-	1.2	4808	(2^+)	4.9
3929		3.1	3780	1^-	0.7	4898	(2^+)	2.9
4014		4.0	3850	3^-	2.1	4989		1.6
4177	3^-	8.6	4048, 4087	1^+	4.0	5206	(4^+)	2.4
4402		2.9	4203		1.0	5348		1.1
4681		5.2	4315		1.1	5417		1.8
4799		3.4	4385	(4^+)	2.8			
			4590	3^-	4.8			
			4806	2^+	2.6			
			4930	2^+	2.9			
			5160		1.8			
			5310		1.7			
			5400		1.2			
			5540	3^-	3.0			
			5630		3.1			
			5800	3^-	1.9			
			5900		1.6			
			6090		1.7			
			6240		1.4			
			6360		1.5			
			6470	(2^+)	2.3			

Table III. Energies, spins, parities and integrated cross sections of levels seen in this work.

^{92}Mo			^{94}Mo			^{96}Mo			^{98}Mo			^{100}Mo		
E_x (keV)	I^π	σ_t (mb)	E_x (keV)	I^π	σ_t (mb)	E_x (keV)	I^π	σ_t (mb)	E_x (keV)	I^π	σ_t (mb)	E_x (keV)	I^π	σ_t (mb)
g.s.	0^+		g.s.	0^+		g.s.	0^+		g.s.	0^+		g.s.	0^+	
1510	2^+	7.2	871	2^+	17.9	777	2^+	23.6	736	0^+	1.2	534	2^+	43.0
2283	4^+	3.1	1573	4^+	4.9	1147	(0^+)	0.7	788	2^+	20.8	694	(0^+)	1.8
2527	5^-	3.1	1864	2^+	1.8	1495	2^+	2.3	1433	2^+	2.3	800	(2^+)	0.8
2613	6^+	1.2	2066	(0^+)	1.9	1624	4^+	3.1	1510	4^+	1.9	1063	2^+	4.7
2850	3^-	11.1	2421	(2^+)	1.8	1865	4^+	3.8	1760	2^+	0.8	1140	(4^+)	2.3
3110	(2^+)	3.1	2533	3^-	9.9	2230	3^-	11.9	2024	3^-	13.3	1463	(2^+)	0.5
			2580	(5^-)	1.8	2616	(4^+)	1.1	2208	(4^+)	2.1	1500	?	0.5
			2830	(4^+)	1.8	2732	(6^+)	1.3	2343	?	3.2	1768	?	0.5
			2930	(2^+)	1.6	2810	?	1.5	2450	(4^+)	1.1	1910	3^-	16.0
			3090	(2^+)	1.9	2980	(4^+)	2.0	2500	(3^-)	2.0			



VIBRATIONAL



ROTATIONAL

CALCULATION REQUIRES:

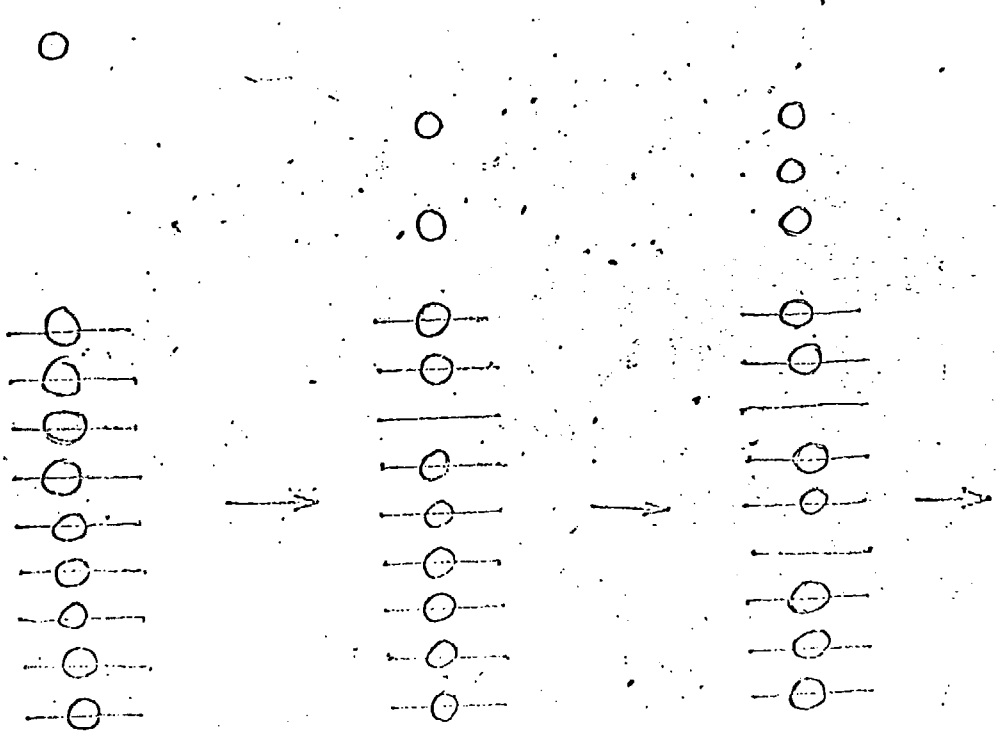
1. LEVEL POSITION
2. OPTICAL POTENTIAL
3. β VALUES

EXCITATION PROCESSES

1 PARTICLE
0 STATE

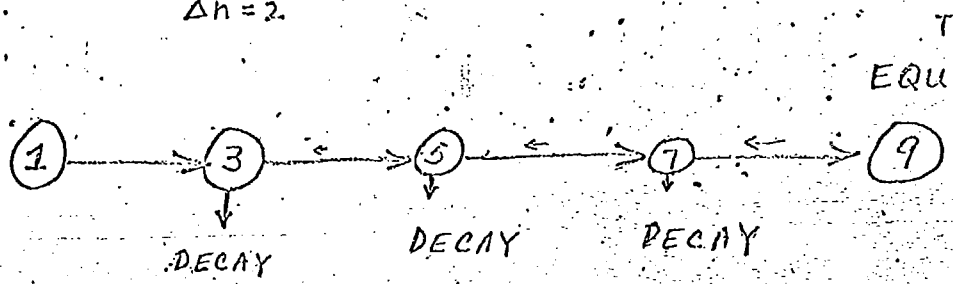
2 PARTICLE
1 HOLE
STATE

3 PARTICLE
2 HOLE
STATE

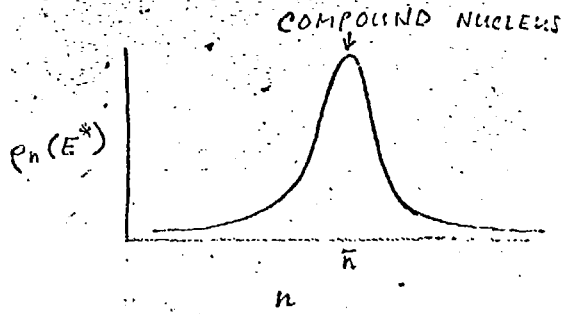


HYBRID MODEL

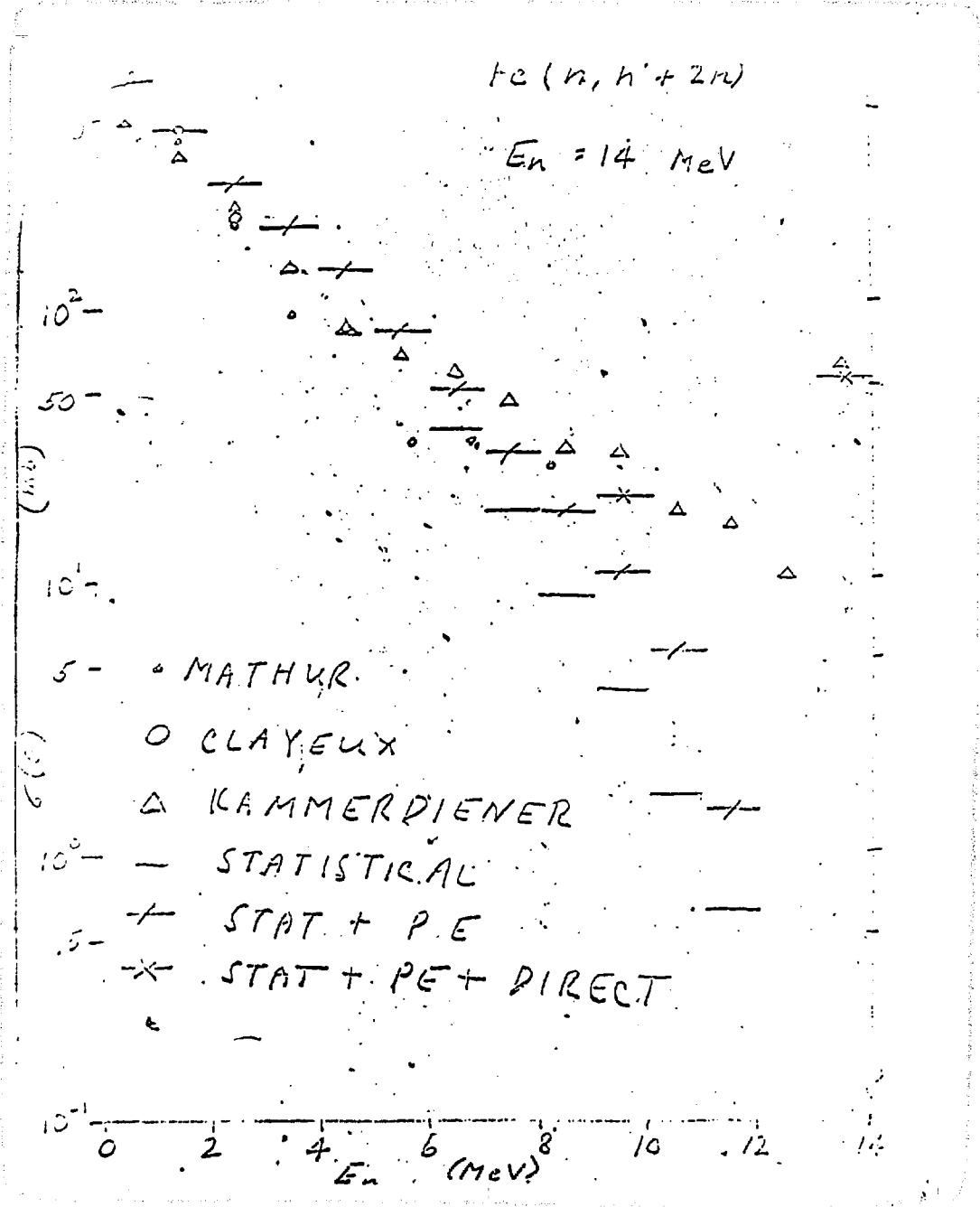
$$P_x(\epsilon) = \sum_{\substack{n=n_0 \\ \Delta n = 2}}^{\bar{n}} D_n \; {}_nP_x \; \frac{\rho_n(u,\epsilon)}{\rho_n(E^*)} \; g \, d\epsilon \left\{ \frac{\lambda_c(\epsilon)}{\lambda_c(\epsilon) + \lambda_+(\epsilon)} \right\}$$

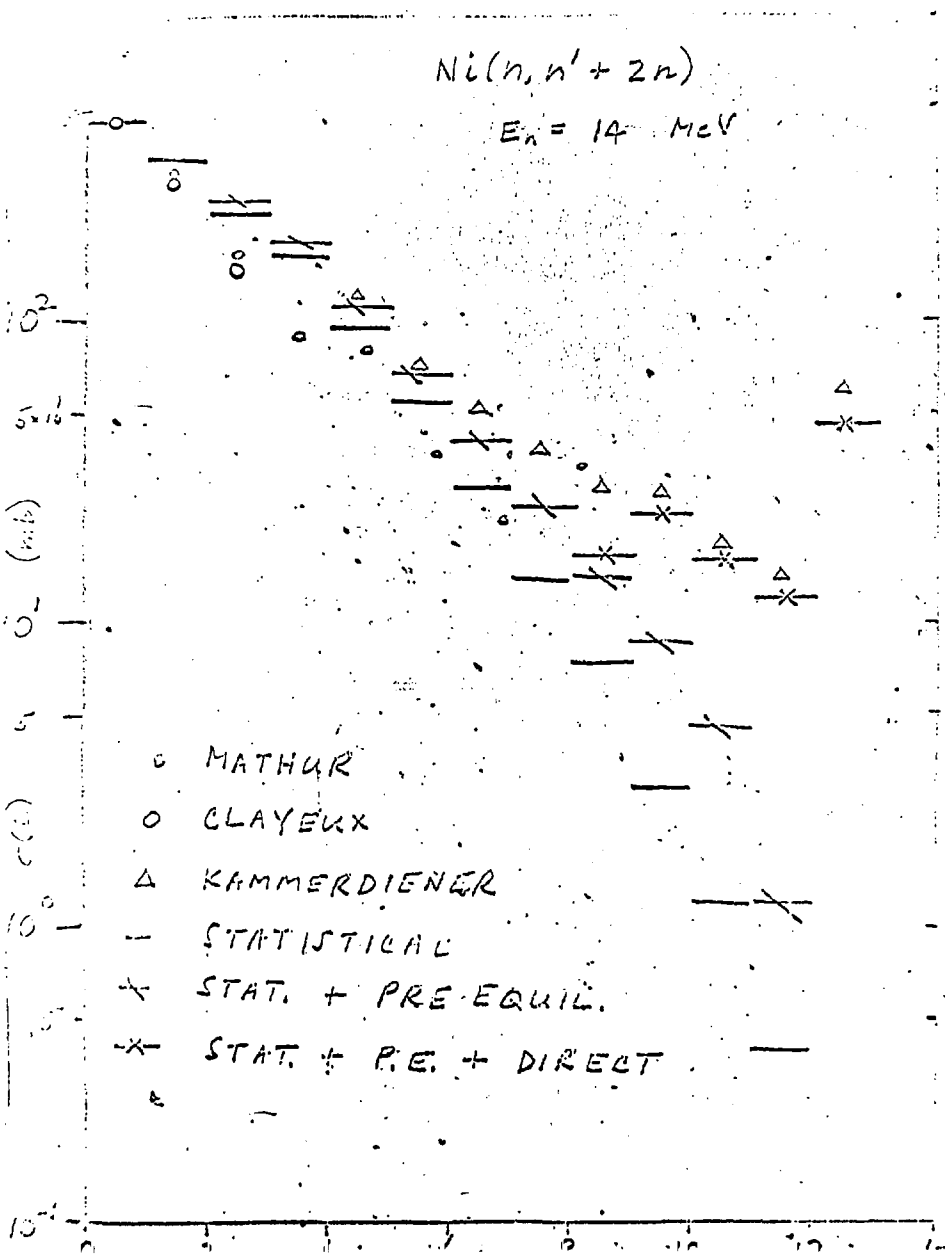


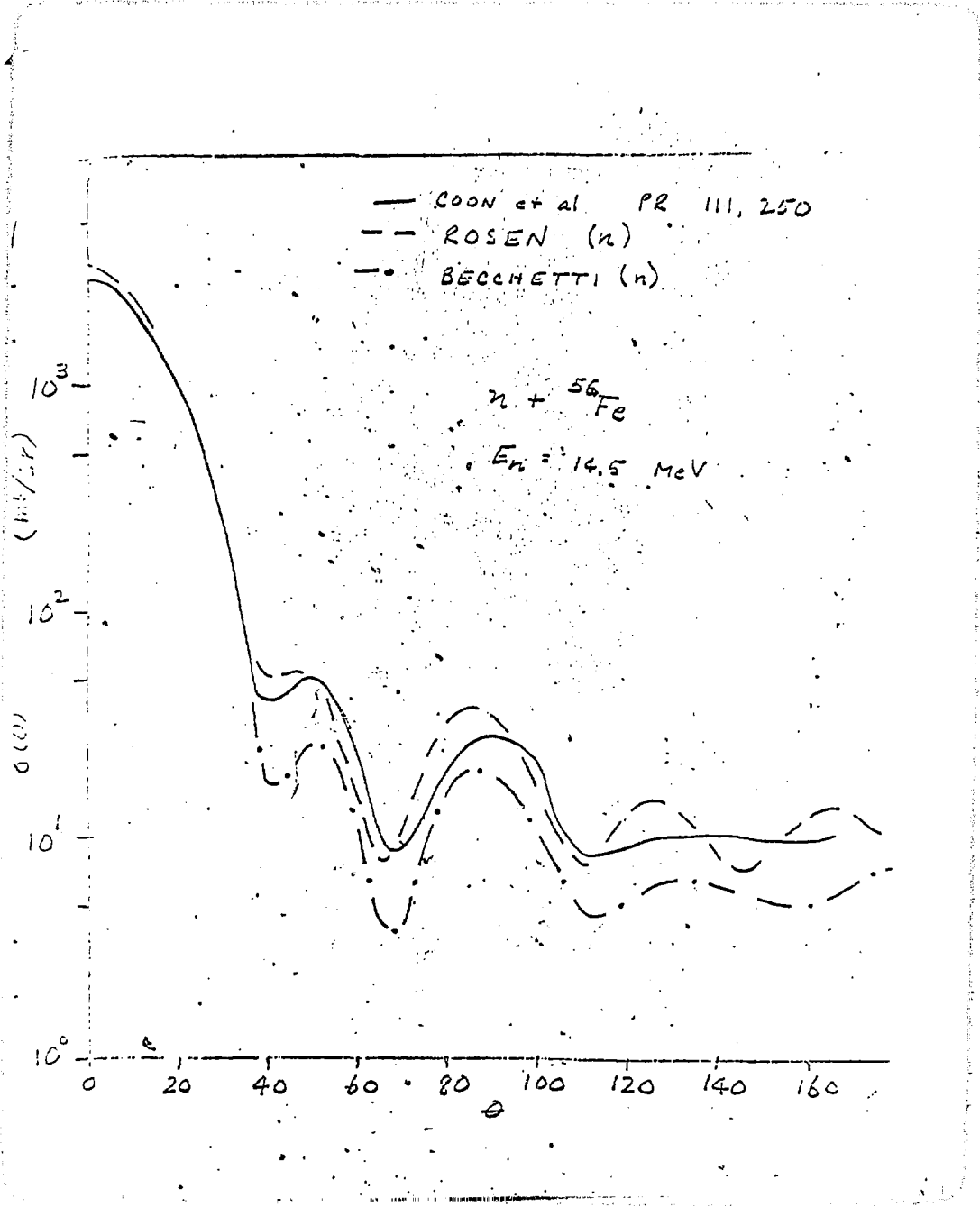
$$\rho_n(E^*) \propto \frac{g(gE^*)^{n-1}}{\bar{n}!\,(n-1)!}$$

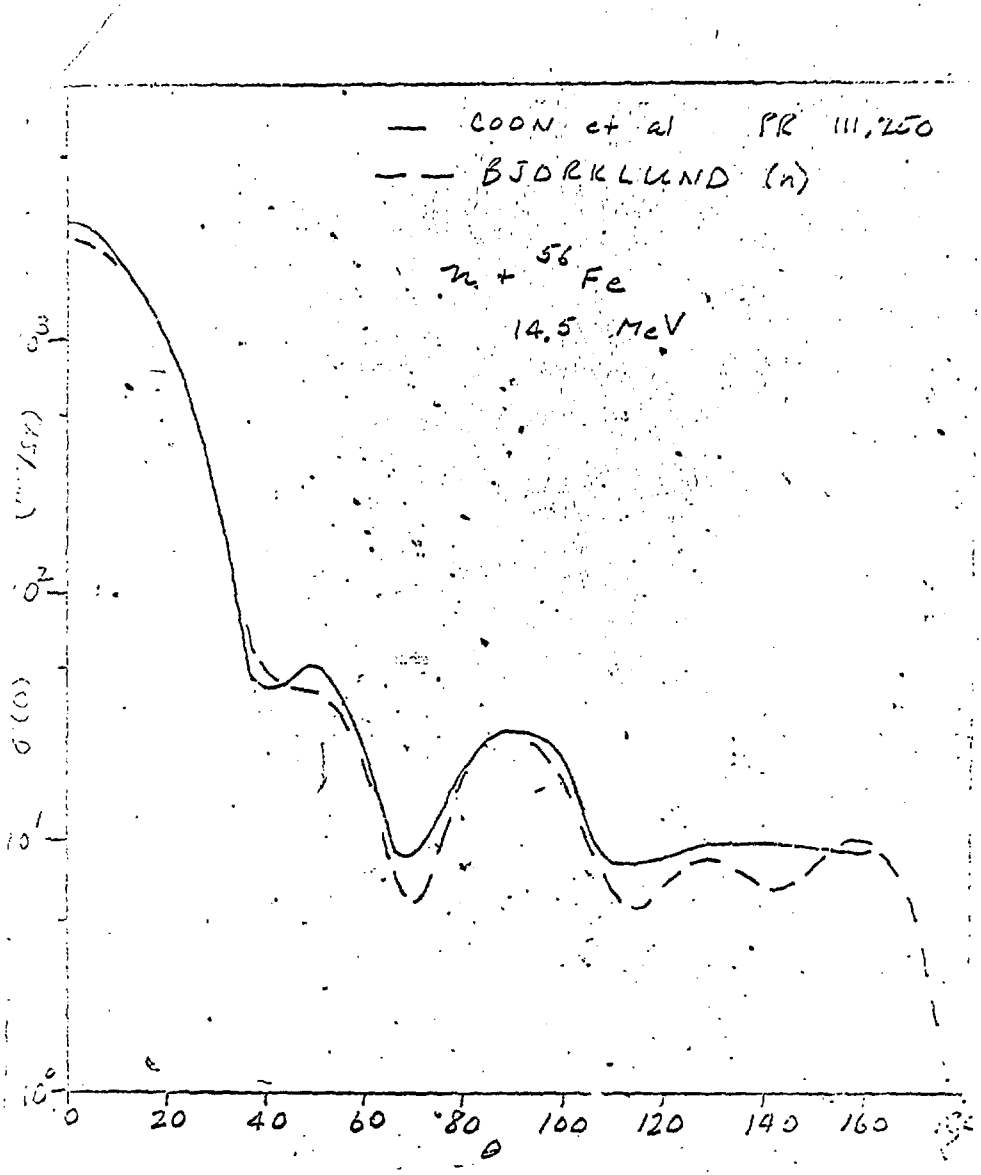



25 MeV
calculation
10
1
.1
10
15
20
22
24
(MeV)


Fe (n, n' + 2n)
En = 14 MeV
10²
50
10¹
5
10⁰
.5
10⁻¹
MATHUR
CLAYEUX
KAMMERDIENER
STATISTICAL
STAT + P.E
STAT + PE + DIRECT
0
2
4
6
8
10
12
14
En (MeV)


Ni(n, n' + 2n)
E_n = 14 MeV
MATHUR
CLAYEUX
KAMMERDIENER
STATISTICAL
STAT. + PRE-EQUIL.
STAT. + P.E. + DIRECT


COON et al PR 111, 250
ROSEN (n)
BECCHETTI (n)
n + 56Fe
En = 14.5 MeV
10^3
10^2
10^1
10^0
0
20
40
60
80
100
120
140
160
θ


— COON et al PR 111, 250
— — BJORKLUND (n)
n + 56 Fe
14.5 MeV
σ(θ) (mb/sr)
10^0
10^-1
10^-2
0
20
40
60
80
100
120
140
160
θ

PROTON POTENTIALS

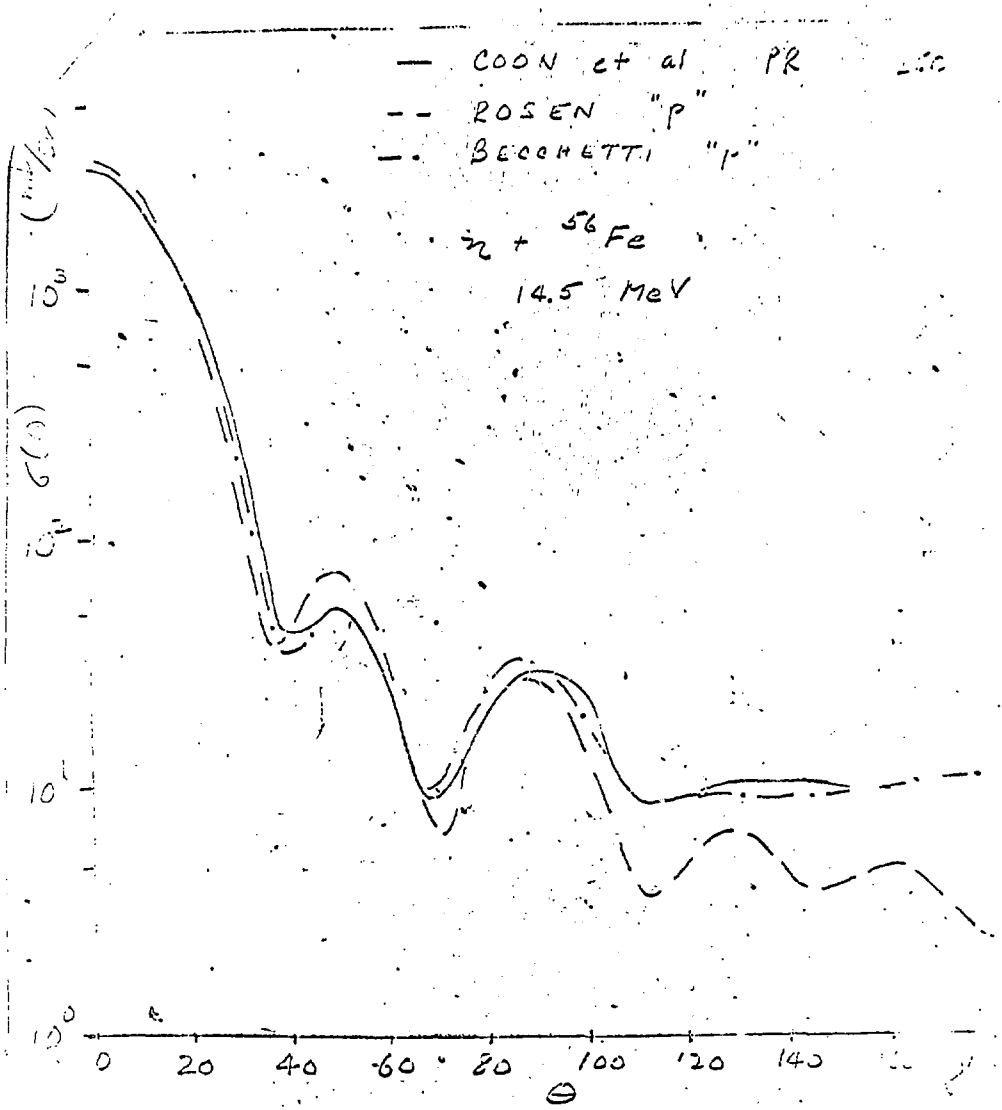
$$V_p(E) = V_0(E) + \frac{(N-Z)}{A} V_1(E) - \frac{.4Z}{A} V_3$$

$$W_p(E) = W_0(E) + \frac{(N-Z)}{A} W_1(E)$$

NEUTRON POTENTIALS

$$V_n(E) = V_0(E) - \frac{(N-Z)}{A} V_1(E)$$

$$W_n(E) = W_0(E) - \frac{(N-Z)}{A} W_1(E)$$


— COON et al PR
-- ROSEN "P"
-.- BECCHETTI "P"
n + 56Fe
14.5 MeV
10^0
10^-1
10^-2
10^-3
0
20
40
60
80
100
120
140
θ