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# INTERNATIONAL NUCLEAR DATA COMMITTEE

Proceedings of the IAEA Research Coordination Meeting

on

## METHODS FOR THE CALCULATIONS OF

NEUTRON NUCLEAR DATA FOR STRUCTURAL MATERIALS

in co-operation with the Centro di Calcolo del ENEA Bologna, Italy, 7-10 October 1986

> Edited by V. Goulo Nuclear Data Section International Atomic Energy Agency

> > January 1988

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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# CONTENTS

I. Organization of the meeting	5
II. List of participants	7
III. Working Group I Report	9
IV. Working Group II Report	11
SESSION: DEVELOPMENT OF MULTISTEP COMPOUND REACTION MODELS	
Recent development of the multistep compound reaction model A. Marcinkowski (INS, Warsaw, Poland)	19
A unified compound and pre-equilibrium model for reactor structural	
materialsZhang Jingshang (IAE, Beijing, China)	51
The first steps toward a more precise multistep compound model of nucleon induced reactions B.V. Carlson (CTA/IEAV, Brazil)	30
SESSION: EXITON, HYBRID, UNIFIED PRE-EQUILIBRIUM MODELS	
Count of p-h configurations by combinatorial method in the frame of BCS theory G. Reffo (ENEA, Bologna, Italy)	47
Single-particle effects in precompound decay reactions	53
Effects of angular-momentum conservation in unified pre-equilibrium and equilibrium reaction model H. Gruppelaar (ECN, Netherlands)	61
Neutron capture in the frame of exiton model G. Reffo (ENEA, Bologna, Italy)	73
SESSION: DESCRIPTION OF DIRECT PROCESSES	
Role of direct and pre-equilibrium processes in the description of threshold reaction exitation functions A.V. Ignatyuk (FEI, Obninsk, USSR)	81
Analysis of neutron induced reactions in Cr isotopes and the calculations of direct contribution to neutron inelastic spectra S. Gmuca (INP, Bratislava, Czechoslovakia)	84
Angular distributions of photons following the capture of fast neutronsG. Longo (ENEA, Bologna, Italy)	93

<u>SESSION</u> :	PARAMETRIZATION OF OPTICAL MODEL, LEVEL DENSITY FUNCTION GAMMA-RAY STRENGTH FUNCTIONS	S,
Gamma-ray	spectra as calculated with code ALICE	107
Consisten effects in	t description of shell, superconductive and collective n the level density of structural materials	113
Geometry conservat: materials	dependent hybrid model including angular momentum ion and statistical model parameters for structural fast neutron data calculationsav	127
SESSION:	METHODS OF CROSS-SECTION EVALUATIONS	
Neutron so	cattering on nuclei near A=60 and A=90 R.D. Lawson (ANL, Argonne, USA)	137
Neutron i 1-20 MeV:	nduced reaction cross-sections of iron in the energy range A work programme (Abstract only) S.B. Garg (BARC, India)	148
Transform different	ation formulae for Legendre coefficients of double ial cross-sections Shi Xiangjun (IAE, Beijing, China)	148
Neutron p A1-27	oroduction and gamma-ray production from 14-MeV neutrons on G. Reffo (ENEA, Bologna, Italy)	156
Optical-s sections	tatistical calculations of the chromium neutron cross V.A. Konshin, V.P. Korennoj, A.V. Ulanovsky, Yu.G. Fokov, O.V. Khatkevich	161

## I. ORGANIZATION OF THE MEETING

I. First Reasearch Coordination Meeting on METHODS FOR THE CALCULATION OF FAST NEUTRON NUCLEAR DATA FOR STRUCTURAL MATERIALS in co-operation with the Centro di Calcolo del E.N.E.A.

## Bologna, Italy, 7-10 October 1986

The first meeting of the IAEA CRP was convened by the IAEA Nuclear Data Section in co-operation with the Centro di Calcolo del ENEA in Bologna, Italy. It was run by the Scientific Secretary V. Goulo with the assistance of Dr. D.E. Cullen (NDS) and the local organizing committee consisting of Dr. G. Reffo (Chairman), Dr. E. Menapace, Ms. P. Cenni.

The main objectives of the meeting were the following:

- 1. Bringing together all participants to review the status of the activities of the CRP.
- 2. Discussion and intercomparison of the various calculation methods used.
- 3. Summary of the results of these intercomparison assessments of the reliability of the calculational methods to recommend them for use in calculations of neutron cross sections of the structural materials of fission and fusion reactors.

The programme of the meeting based on the Adopted Agenda (enclosed in Appendix 1) consisted of 9 sessions including opening, presentation of reports and working groups. Presentation of reports was divided among 5 sessions devoted to different aspects of nuclear theory for evaluation of fast neutron data:

Session II.	Development of Multistep Compound Reaction Models
Session III.	Exiton, Hybrid, Unified Pre-equilibrium Models
Session IV.	Description of Direct Processes
Session V.	Parametrization of Optical Model, Level Density Functions, Gamma-Ray Strength Functions

Session VI. Methods of Cross Section Evaluation

Two working groups dealt with methods for the calculations, their parametrization, and working programme for next year and international co-operation.

Reports of the Working Groups were done by their Chairmen: Dr. M. Blann (Lawrence Livermore Laboratory, USA) and Dr. H. Gruppelaar (ECN, Petten, the Netherlands).

The meeting was attended by 18 participants. (The List of Participants is attached). Three participants of the CRP were absent.

The next RCM in the frame of the CRP is planned to be convened 8-11 February 1988 in Vienna.

The Working Group 1 was devoted to the discussion of the status of semi-classical and quantum mechanical theories of multistep compound and multistep direct processes, the use of neutron and proton induced reaction data for model calculation testing, problems of level density functions.

During Working Group 2 number of unified model aspects, description of photon production spectra, parametrization of models were discussed.

Working programme for the next year has included the following items:

- 1. Improvement and parametrization of pre-compound models for the main structural material elements, Al, Fe, Cr, Ni, Nb, Pb.
- 2. There was an interest expressed by different scientific groups in calculations of double differential neutron and particle emission spectra and photon production data.
- 3. It was decided to try to make some intercomparison of model calculations to demonstrate their reliability but not to overlap this work with NEA-DB intercomparison exercises.
- 4. Special interest was expressed in the planned programme of the forthcoming CRP on the measurement and analysis of 14 MeV neutron induced double differential neutron emission cross sections and (n,n'x) cross sections.

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## III. WORKING GROUP 1 REPORT

## Dr. M. Blann Lawrence Livermore Laboratory, USA

We have enjoyed and learned from the presentation of members of the CRP during the past three days. We have focused on areas which have promise for the future, on problem areas for immediate scrutiny. and perhaps, most importantly have, with help from Dr. Gruppelaar, mapped out a program for the next year which should both provide some of the evaluated data and encourage collaborations between members of this group. The latter exchange of ideas is very important, as there is usually a coherent addition of ideas with a constructive interference pattern.

We had an interesting discussion with help from Adrian Marcinkowski on the status of quantum mechanical theories such as due to Feshbach, Kerman and Koonin or to Tamura, Udagawa and Lenske. The conclusions were that these theories are not yet developed to the point of being trustworthy, predictive tools for data evaluation. Rather, if they work reasonably well for (p,n) reactions, they may give very poor results for (p,p') or (n,n') reactions. Prof. Ignatyuk emphasized the importance of a thorough testing and further development of the multistep direct and multistep compound models so that they may become useful applied tools for the future. The consensus was that we must rely on our present semi-classical models for our current data needs, while continuing development of the quantum mechanical treatment.

The models we use for continuum precompound phenomena provide good angle integrated cross sections, but have difficulty in reproducing the back angle yields of the angular distributions. The quantum theoretical formulations have shown that this is a reasonable result, as the extreme back angle yields result from nucleon-potential rather than nucleon-nucleon scattering processes. Nonetheless, we realize that the back angle yields which we do not get well in our semi-classical models are not important for purposes of evaluation, so that our models which are computationally fast and easy to perform and which permit large "throughput", are well suited to providing evaluated data. We recognize that we must link our calculated results very well with experimental results when the latter are available.

Prof. Ignatyuk stressed the importance of treating transitions to collective levels by appropriate means, e.g., DWBA. We heard several examples of this and saw a good illustration in Dr. Reffo's calculations for Al. In this example, few quasi-particle densities were used to identify the collective excitations by their absence in calculated intrinsic excitations. Inclusion of these provided a great improvement in the calculated result. Other members of this CRP have also emphasized the importance of treating transitions to collective levels.

An important general point was made by Dr. Jahn: there is a much broader range of data available, and of higher quality, for proton induced reactions than for neutron induced reactions. We should make use of these data for testing our model calculations, in addition to use of good quality neutron data when available. We had a good discussion on the topic of precompound decay models as to the way that the single particle level density "g" and single particle level density parameter "a" should be defined. We found a broad range of ideas on this topic. A good computer experiment to help resolve this question and form a consensus of opinion would involve computer generation of few quasiparticle densities using realistic single particle levels using the approach of Williams or of Reffo, and of fitting these results with an Ericson-Williams particle hole prescription. We can then see what "g" values for precompound states are necessary to reproduce the more realistically generated densities, and see how these values compare with corresponding "a" values for the equilibrated nuclei.

It was suggested that it would also be a worthwhile exercise to test the energy dependence of the exciton model "k" parameter by analysing data at higher energy than 14 MeV. Likely candidates are high quality data sets measured by Galonsky on a series of targets for incident proton energies of 25, 35 and 45 MeV (Nucl. Phys. A 257, 15 (1976).

A problem of compound nucleus decay for 50 years has been the question of level densities. A major contributor to good answers on this problem has been Prof. Ignatyuk, and several of the model codes represented by members of this CRP have incorporated his theories. We have, however, heard here of his additional new contributions in this area, and several groups hope to collaborate more closely with Prof.<Ignatyuk in order to incorporate his latest work into their modeling codes, and also to cooperate on further developments on theory of level densities.

Most importantly, we have met and gotten to know one another. We have tasks for the next year with some overlap. It is important that we exchange correspondence on progress with those with whom we have an overlap in assignments. From this and from meetings of this CRP, we will forge mutually beneficial collaborative efforts.

## IV. WORKING GROUP 2 REPORT

Dr. H. Gruppelaar ECN, Petten, the Netherlands

#### 1. UNIFIED - MODEL ASPECTS

At the meeting there was considerable interest in the unification of the Hauser-Feshbach and the exciton model (see papers of Zhang, Avrigeanu, Reffo, Gruppelaar et al.). Progress was reported on the simplification of Iwamoto's cluster method for practical use (Zhang), the use of spin-dependent GDHM models (Avrigeanu) the introduction of microscopic level densities into PENELOPE (Reffo) and computational procedures that speed-up the calculations, while satisfying consistency requirements (Gruppelaar et al.).

Also the physical basis of the model is better understood (Gruppelaar et al.): there is a close relation with the model of Agassi et al. and the MSC model of FKK (Feshbach, Kerman, Koonin).

In practice the "HF - models with pre-equilibrium correction" such as GNASH or STAPRE may give results similar to the more unified models (PENELOPE, etc.) for the energy spectra. However, the unified models are more attractive from a conceptual point of view and may be easier to extend to predict angular distributions.

It was stressed that in order to describe multi-particle emission near thresholds discrete levels are required (HF-type model).

For further development of the unified model simple parametrizations of the particle-hole level-density formula are required that are consistent with microscopic calculations and experimental data, cf. Sect. 3. In particular it is required that the sum over (p,h) states gives the experimental level density.

From calculations of Gruppelaar et al. it follows that  $\sigma^2(n,E)$  is a crucial parameter that determines the spin-dependence of calculated quantities.

## 2. PHOTON PRODUCTION SPECTRA

There were four reports on  $\gamma$ -ray emission.

The simple method described by Blann is useful for very fast calculations and yet there are quite good results. Zhang reported on the introduction of pre-equilibrium  $\gamma$ -ray emission based upon Betak's method. A slightly better method, that is consistent with the Brink-Axel approach in equilibrium calculation, is that of Akkermans et al.

Reffo has extended this method for use into the unified model by adding the J-dependence. This was also performed recently by Oblozinski for inclusion in MSC-type of calculations (FKK-model). The results are surprisingly good, in agreement with experimental data (the data base may be too small) and with direct/semi-direct model calculations reported by Longo. In fact the calculations with pre-equilibrium  $\gamma$ -ray emission also explain the left-hand part of the giant-dipole peak in the spectrum, where previous methods gave large underpredictions. It was concluded that the "Akkerman's method" (with J-dependence) is a simple and useful method to introduce  $\gamma$ -ray emission into the pre-equilibrium models.

## 3. PARAMETRIZATION

## 3.1. Optical model

Details on the optical-model parametrization were presented by Lawson (this meeting) and on previous meetings (CRP, Optical-model meeting in Paris). Some observations of this meeting are:

- 1) for the structural materials regional model parameters are needed.
- 2) Spherical optical-model parameters can be used to fit  $\sigma_t$ ,  $\sigma_{e1}(\theta)$ .
- 3) Due to collective effects the imaginary part may be enhanced, if a spherical model is used.

Work at Argonne was reported (Lawson) for the A=90 and A=60 regions with substantial differences in the real potential. For both regions different parametrizations are required. Within each region the imaginary part may change from nucleus to nucleus.

Although the energy range may be extended up to 20 MeV the extrapolation down to low energies is probably limited to about 1 MeV. Below this range an unresolved-resonance treatment could be followed.

#### 3.2. Level density

In various papers the topic of level density was discussed. Ignatyuk gave a description of collective enhancement factors; Reffo discussed his combinatorial calculations and Avrigeanu focused on phenomenological descriptions of the energy dependence of  $\rho$  for practical use. In many discussions the level density played a central role.

With respect to the energy dependence of  $\rho$  (usually described in the HF-model with the Gilbert-Cameron or BSFG formulae) it is clear that above about 10 MeV the BSFC model gives too low results. Better descriptions are available: see the paper of Avrigeanu and recent work of Ignatyuk. There is also work going on at Karlsruhe in this direction (Anzaldo).

The (p,h)-densities, presently described in EM by the Williams formula with various corrections (e.g. for finite-hole depth to include geometry dependence) were discussed by Reffo. The shape of the results of combinatorial calculations is very much like the Williams prediction, apart from the low-energy side where the gap ( $\Delta$ ) is difficult to parametrize. Also the absolute values turn out to be quite different, but in EM calculations often only ratios of level densities are the critical quantities. The spin cut-off parameter is easy to parametrize and was shown to be proportional to n. At high n-values, near equilibrium,  $\sigma^2(n,E)$  is expected to become close to the value used in HF calculations, see work of Fu and of Ignatyuk. The parity-distribution, important in  $\gamma$ -ray cascade calculations, is irregular and difficult to parametrize. The large amount of microscopic results needs to be summarized in a simple form, useful for applications. Also existing schemes such as the methods of Ignatyuk, Fu and the Williams recursive formula (part of the ALICE subroutine library) need to be considered.

## 3.3. $\gamma$ -ray strength functions

For modification of the approach of Gardner the reader is referred to the paper of Avrigeanu. There was no further discussion on this topic.

## 4. WORKING PROGRAMME FOR NEXT YEAR AND INTERNATIONAL CO-OPERATION

Table 1 lists the various topics on which the CRP laboratories are active. Most of the work is performed on improvement and parametrization of pre-compound models, in particular for Al, Fe, Cr, Ni, Nb and Pb, but also for some other materials. It was decided that the emphasis for the next period is still on further development of methods and models, although the final goal of application of these tools to obtain reliable nuclear-data evaluations is nearby.

In this respect some intercomparisons of produced data files may become possible at the next meeting. Most groups are working on data in the high-energy range above a few MeV, concentrating on doubledifferential neutron and particle emission spectra and on photonproduction data.

It was decided to try to make some comparisons between calculated data at the next meeting, in particular for Fe at 14.6 MeV and at 25.7 MeV, where measurements are available. Without specifying all parameters (in order to avoid duplication with the NEA-DB intercomparison activities already performed for Nb and Co) it was suggested that one calculation at least should be made with g=A/13 MeV. This would allow the experts to relate the differences in the results (if any) to differences in the models. Also photon-production data should be included in this intercomparison.

Table 1 may also serve as a guide for the participants to contact the various CRP-members for information and exchange of data. It is recommended to optimize the contacts.

In order to compare results of microscopic level-density calculations it was recommended to use at different institutes a common shell-model base. Blann, Reffo, Ignatyuk and Anzaldo (KFK) are interested in such an intercomparison.

For practical applications results of microscopic level-density calculations are needed. Available material for Fe, Cr, Ni will be distributed by Reffo, whereas Blann will make available a version of a code to perform calculations with Williams recursive formula. Finally, it was stressed that the situation with respect to experimental data is not always ideal. There may be large discrepancies in experimental (n,n'x) data and also there may be substantial differences between the angular distributions measured in the lab. and c.m. systems (relation with other CRPs). For theoretical studies the (p,nx) data base may have to be preferred.

Material	Optical Model	Coupled Channels	FKK type	Other micr. methods, MSDirect	Preeq.   models +   unified	Comment	Level density	Gamma-ray problems, photon-emission cross sections
A1			INS (Wars.)		Braz.   Bol.   LLL   JAE		Braz.	Bol.   LLL   Braz.
Fe		(Kiev)		Brat. 54, 56 Braz. 56	LASL JAE KfK LLL Beijing Buch. FEI BARC	alfa emission cluster model alfa emission + collective	Bol. -transfer syst. FEI-collective proc. KfK	LLL Brat. Beijing BARC
Cr	Minsk	(Kiev)			LLL   BARC   Brat.   JAE	alfa emission	Bol. -transfer syst. FEI-collective processes	LLL
Ni	(ANL)	 Pei			JAE   LASL   BARC   Petten   LLL   Buch.		Bol. -transfer syst. FEI-collective processes	LLL Brat. (Petten) BARC
Other Pb	ANL Bi, ANL	       PEI	   INS     (Wars.)	     Brat. 	   Dresden   Nb   Dresden	   collective     collective	Dresden-par. Nb Dresden-par.	

## Table 1 CRP Working Programmes

# SESSION

# DEVELOPMENT OF MULTISTEP COMPOUND REACTION MODELS

RECENT DEVELOPMENT OF THE MULTI-STEP COMPOUND REACTION MODEL

A. Marcinkovski Institute for Nuclear Studies, Warsaw, Poland

#### ABSTRACT

Two-body interaction matrix elements in the frame of multi-step-compound reaction theory of Feshbach-Kermann-Koonin taking into amount the Pauli blocking and the Fermi energy constraint have been obtained for practical computations of nuclear data of structural materials.

#### 1. Introduction

19

Since the quantum theory of precompound reactions has been formulated by Feshbach. Kerman and Koonin in 1980<sup>1)</sup> several model calculations of multi-step compound (MSC) emission in (p,n), (n,p),  $({}^{3}$ He,p) and (n,2n)reactions have been reported  $^{2-5)}$ . The experimental verification is in favour of the MSC mechanism, which describes the symmetric portions of the angular distributions of reaction products emitted from a sequence of states of increasing complexity, involving only bound particle orbitals. The application of the quantum-theory in practical computations of the MSC reaction yield contains numerous abbreviations, e.g. use of the two-body interaction matrix elements for spin-less particles or the well-known Ericson formula for unconditional particle-hole state densities. Quite recently these problems have been addressed in a few papers. The matrix elements of a 5-function interaction for one-half spin particles have been derived and subsequently the X-factors of all widths  $\langle \Gamma(U) \rho(U) \rangle = X_{a,T}^{sjn} Y(U)$  involved in the process containing the angular momentum structure embodied in the  $\delta$ -force and the assumed spin distribution of the single-particle levels were obtained in closed analytical form. Similarly formulae were obtained for the Y-functions, being the densities of particle-hole bound states accessible in different MSC emission modes. The latter factors have been derived recursively by Stankiewicz et al.<sup>6)</sup> who ignored the Pauli exclusion principle and effect of the finite potential well on hole scattering. These drawbacks have been removed in ref.<sup>7)</sup>, were Oblozinsky derived the densities of the particle-hole bound states by applying the equidistant-spacing approximation and the Darwin-Fowler statistical method. The Pauli blocking and the Fermi energy constraint are consistently observed within this theoretical approach. The final relations are compact and can be viewed as built of the usual Ericson state densities with additional correction term.

#### 2. The Energy Dependence of the Widths for the MSC Process

The Y-functions contain all the excitation energy U dependence of the width originating in the final-state level density. The energy dependence of the X-factors is weaker and due to the angular momentum barrier for the outgoing nucleon. In evaluating of the Y-function one considers it to be a product of three terms: the number of ways to choose the interacting exciton pair in a system of p-particles and h-holes, the density of states for the active excitons remaining in the system after emission and the probability that the noninteracting core-excitons have appropriate energy. The latter probabilities are expressed as simple ratios of state densities<sup>6,7)</sup>.

Let us consider for simplicity a particle emission mode involving a creation of a particle-hole pair in the system via scattering of a hole. In this case one obtains

$$Y_{m}^{n+1} = \frac{1}{2}h(h+1)g - \frac{\omega^{8}(p,h+1,U)}{\omega^{8}(p,h,E)}, \qquad (1)$$

when neglecting the finite depth F of the potential well<sup>6)</sup> or

$$Y_{n}^{n+1} = \frac{1}{2} \frac{q^{3} \delta}{\omega^{3F}(p,h,E)} \frac{\left(\omega^{8F}(p,h-1,U^{p+h})\right)}{(p+h)(p+h-1)} + \frac{\omega^{8F}(p,h-1,(E-F)^{p+h})}{(p+h)} - \frac{\omega^{8F}(p,h-1,(E-F)^{p+h-1})}{(p+h-1)}$$
(2)

20 when the F constraint on hole scattering is imposed. In eq.(2)  $\delta = 1$ for F + U = E > 0 and equals 0 otherwise. The particle-hole bound state densities  $\omega^{B}$  and  $\omega^{BF}$  are reported in ref.<sup>6)</sup> and ref.<sup>7)</sup> respectively. The symbol  $\omega^{BF*}$  denotes a modified density notation explained in ref.<sup>7)</sup>. In fig. 1 the effect of the finite well depth (solid lines) is compared with the results of eq.(1) (dashed lines). It is seen that if F < E the phase space for emission is reduced and the energies available after emission are limited.

Accounting for Pauli blocking brings into the state density expression a correction term  $-\alpha_{p,h}^{2} - \frac{1}{2}\left(\frac{p^{2}+p}{g} + \frac{h^{2}-h}{g}\right)$  in addition to the excitation energy shift introduced already by Williams<sup>8)</sup>.



Figure 1. Taken from ref.<sup>7)</sup>

#### 3. The Angular Momentum Structure of the MSC Widths



Figure 2. The angular diagram for particle-particle scattering reads<sup>9)</sup>

for  $1 + 1_3 + Q$  and  $1_1 + 1_2 + Q$  even and 0 otherwise. Here  $j = (2j + 1)^{1/2}$  and I is the overlap radial-integral of wavefunctions U for the four interacting orbitals,

$$I_{l_{4}} \mathcal{L}_{l_{3}} = \frac{V_{0}}{4\pi} \left(\frac{4}{3} T_{7} T_{0}^{3}\right) \int U_{l_{4}} U_{l_{4}} U_{l_{3}} \frac{d\tau}{\tau^{2}} .$$
 (4)

Assuming Bethe's spin distribution  $R_N$  of nuclear states, with a spin cut-off factor depending on the number of excitons N, one obtains, following the prescription of Feshbach, Kerman and Koonin, the X-functions for damping as well as for the possible exit modes in the MSC process<sup>5)</sup>. For the particle-particle scattering case, which does not alter the number of excitons, the X-function is

$$\begin{split} \chi_{m\gamma}^{sjen} &= 2\pi \frac{j_{L}\hat{s}}{R_{pq}(7)} I_{\ell_{1}LL_{2}L_{3}}^{2} \sum_{\substack{Q \neq 0 \neq 1 \\ R_{pq}(7)}} \hat{Q} F(Q)_{j_{3}} R_{1}(j_{3}) R_{pq}(j_{3}) (j_{2} \neq 0) (j_{2} \neq 0)^{2} (j_{2} \neq 0)^{2}$$

For the interaction creating a particle-hole pair, considered in the preceding section, one gets

$$\begin{array}{l} \times s_{jen+1} = 2\pi \int e^{\frac{1}{2}} \int I_{2,e_{2}f_{3}} \sum_{Q_{j_{3}}j_{4}} (\widehat{Q}R_{f}Q)_{j_{3}} F_{(j_{3}}) R_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} - \frac{1}{2}O \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) S_{M}(j_{4}) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big) S_{M}(j_{4}) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big) S_{M}(j_{4}) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big) S_{M}(j_{4}) \Big( \frac{1}{2} + \frac{1}{2}S \Big) \Big) \Big)$$

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FORMATION AND EMISSION OF LIGHT PARTICLES IN FAST NEUTRON INDUCED REACTION---A UNIFIED COMPOUND PRE-EQUILIBRIUM MODEL(2)

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#### Abstract

For fast neutron-induced reactions for structural materials by using the unified compound pre-equilibrium model, the light composite particles emissions have to be taken into account properly. The mechanism of cluster formation and emission have been investigated. Estimated results with considering secondary emission process have compared with experimental data. It shows that the unified compound pre-equilibrium model can be successfully used to evalute nuclear data.

## Key words: low energy nuclear reaction, exciton model cluster formation factor

#### 1. Introduction

In fast neutron-induced reactions for structural materials the charged particles emissions estimation has to be taken into account properly. Besides the proton emissions, the other light composite particles emission, for instance,  $\alpha$ , <sup>3</sup>He, d,t emissions will be taken place during the reaction process. Thus, how to form such composite particles inside the excited compound system needs to be described. Although pre-equilibrium emission of light composite particles in the framework of the exciton model has gotten some success for years, there still remains some ambiguties in the formulation. C.K. Cline first derived the formulation of composite particle formation probability in ref.(1). The main idea in ref(1) is that while the particle number above Fermi sea is equal to or greater than the composite particle number, the composite particle will be cons-: tituted and its formation probability will be given according to

21

22

some simple arrangement factors. The calculated composite particle spectra are much smaller in absolute values than the experimental data. In order to improve the results, several formulisms have been E. Betak et al.<sup>(2)</sup> proposed the intrinsic phase space considered. factor concept and derived the factor and the formation probability for each configuration. Although their results are quite good in fitting the experimental data, the assumption of constant formation probability is reasonless from the physical point of view. A.Iwamoto et al.[6] proposed a model based on the statistical phase space argument by means of the Fermi gas model to derive the analytical expression of the formation probability of the complex particle. Their main physical point is that some of particles which form the complex particle may come from the levels below Fermi sea. The consideration is quite similar to the pick-up process in direct reaction theory. This physical picture is more reasonable. The calculated results have been improved a lot and the experimental data can be reproduced well. It may be seen that their derivations of the formulation are very complicated and todious In the paper . we adopted their physical idea and simplified the derivations. Almost the same results have been obtained. The physical assumption of the formation probability, calculated results as well as their dependance on some physical parameters are given in sec.2. In order to emphasize the considering formation factor, we only calculated emitted particles cross section. In sec.3 the emitted charged particles spectrium, cross section formulations and calculated results are presented. As the matter of convenince, we have calculated cross section for structural material: <sup>54</sup>Fe induced reactions by neutron with energy in the range of En 20 MeV to avoid the third particle emission process. Finally a brief summary discussion is illustrated.

## 2. Formation Probability of Light Nuclear Cluster in Excited Compound System

As in cluster model, we define the center of mass coordinate of a cluster composed of N nucleons at R as the coordinate system of the cluster associated with a harmonic oscillator potential.

$$\vec{R} = \frac{1}{N} \sum_{i=1}^{N} \vec{r_i}$$
(2.1)

Suppose the intrinsic wave function of the cluster corresponds to the ground state of the potential. Thus the total wave function of the cluster reads

$$\Psi = \prod_{i=1}^{N} \phi(r_i) = \phi(R) \phi_{int} \qquad (2.2)$$

with

$$\phi(\gamma) = \left(\frac{\beta}{\pi}\right)^{3/4} \exp\left\{-\frac{\beta}{2}\gamma^2\right\}$$
(2.3)

$$\Phi(R) = \left(\frac{N\beta}{\pi}\right)^{3/4} \exp\left\{-\frac{\beta}{2}NR^{3}\right\}$$
(2.4)

Here  $\phi(R)$ ,  $\phi_{int}$ ,  $\phi(r_i)$  stand for the mass center normalized wave function, intrinsic wave function, single particle wave function, of the cluster, respectively. The relative coordinates for N=2,3,4 are defined as follows

$$N = 2; \quad \vec{r} = \vec{r}_{1} - \vec{r}_{2} .$$

$$N = 3; \quad \vec{r} = \vec{r}_{1} - \vec{r}_{2} , \quad \vec{r}' = \frac{1}{2}(\vec{r}_{1} + \vec{r}_{2}) - \vec{r}_{3} .$$

$$N = 4; \quad \vec{r} = \vec{r}_{1} - \vec{r}_{1} , \quad \vec{r}' = \vec{r}_{3} - \vec{r}_{4} , \quad \vec{r}'' = \frac{1}{2} \left[ (\vec{r}_{1} + \vec{r}_{2}) - (\vec{r}_{3} - \vec{r}_{4}) \right] . \quad (2.5)$$

The corresponding momentum for N=2,3,4 are given by

$$N=2: \vec{F}_{r} = \pm \vec{F}_{r} - \pm \vec{F}_{r} .$$

$$N=3: \vec{F}_{r} = \pm \vec{F}_{r} - \pm \vec{F}_{r} ,$$

$$\vec{F}_{r} = \pm \vec{F}_{r} ,$$

$$\vec{F}_{$$

Thus the intrinsic wave function can be expressed as

$$N=2; \qquad \phi_{int} = \left(\frac{B}{2\pi}\right)^{3/4} \exp\left\{-\frac{B}{4}r^{4}\right\}, \\ N=3: \qquad \phi_{int} = \left(\frac{B^{2}}{3\pi^{2}}\right)^{3/4} \exp\left\{-\frac{B}{4}r^{2} - \frac{B}{3}rr^{4}\right\}, \\ N=4: \qquad \phi_{int} = \left(\frac{B^{3}}{4\pi^{2}}\right)^{3/4} \exp\left\{-\frac{B}{4}rr^{4}r^{4}\right\}.$$
(2.7)

The r.m.s. radius of the cluster is  $exp(-\frac{1}{4\pi^3}) = exp(-\frac{1}{4}(r+r') - \frac{1}{2}r'')$ 

$$Y_{H}^{2} = \frac{1}{N} \int_{L^{2}}^{\infty} (\vec{r}_{c} - \vec{R})^{2} |\phi_{int}|^{2} d\vec{s}_{N}$$
(2.8)

Here  $d_{J_N}$  stands for 3(N-1) dimensions of intrinsic coordinate.

Substituting the intrinsic wave function into eq.(2.8), we have the relation between the r.m.s. radius and the parameters of the cluster harmonic oscillator potential.

$$Y_{N=2}^{2} = \frac{3}{\beta} = \frac{3\pi}{m\omega_{N=2}},$$

$$Y_{N=3}^{2} = \frac{1}{\beta} = \frac{\pi}{m\omega_{N=3}},$$

$$Y_{N=4}^{2} = \frac{9}{\beta\beta} = \frac{9\pi}{\beta}.$$
(2.9)

Thus, the parameter  $\omega_{_{
m N}}$  of the cluster harmonic oscillator can be determined by the r.m.s. radius of the cluster. Because of the condition of the energy conservation in the harmonic oscillator potential, each related degrees of freedom provides energy of  $\frac{3}{2 \pi \omega_{\rm N}}$ , i.e.,

Here

We take  $\xi_{\mu}$  as the emitted energy of the cluster composed of N nucleons. According to the energy conservation we have

$$\mathcal{E}_{N} = \frac{\mathcal{P}^{2}}{2Nm} + \frac{3}{4} \frac{1}{4} \frac{1}{4$$

Here, P is the momentum of mass center of the cluster.  $\vec{p} = \sum_{i=1}^{4} \vec{p}_i$   $\mathcal{E}_F$  is the single-particle Fermi energy(30-35MeV) and  $B_N$  is the binding energy of the cluster in the composite nucleus. It can be see clear from eq.(2.11) that after determining emitting energy  ${\cal E}_{\rm N}$ 

the momentum of the mass center of the cluster also can be determined. On the restriction one can count the number of states of the intrinsic freedom of the cluster to obtain the formation factor of

the cluster. In the present model, we take the mass center coordinate R is arbitrary. By means of this condition the derivation of the formation factor of the cluster can be simplified more obviously, and the formulation is very much similar to the one of ref(4-5). Thus it can be concluded that the derivation with the restriction of R is more tedious, but no more physical results could be obtained.

Some of particles which form the cluster come from the levels above as well as below the Fermi surface have been taken into account. We take [1,m] to express the particle number above and below the Fermi surface, respectively, and have 1+m=N. Thus the conditions are following.

$$|\overline{p}_i| > P_F$$
,  $i = 1, 2 \cdots d$ ,

$$[\bar{p}_{i}] < P_{\bar{p}}$$
,  $j = 1, 2, \dots, m$ .

The formation factor of the cluster can be obtaine by the integration of phase space, which take the form of

$$N=2: \quad \overline{F}_{lm}(E_{\perp}) = \frac{1}{(2\pi\pi)^2} \int_{\overline{L}} d\overline{p} r d\overline{r}$$

$$N=3; \quad \overline{F}_{2m}(\mathcal{E}_3) = \frac{1}{(2\pi\pi)^4} \int_{\vec{p}} d\vec{p}_i d\vec{p}_i, d\vec{r} d\vec{r'},$$

$$N=4; \quad \overline{F}_{2m}(\mathcal{E}_4) = \frac{1}{(2\pi\pi)^4} \int_{\vec{p}} d\vec{p}_i d\vec{p}_i d\vec{p}_i d\vec{r} d\vec{r'} d\vec{r'}.$$

$$(2.12)$$

with the normalized condition

$$\frac{\overline{Z}}{m}F_{\mathcal{L}m}(\mathcal{E}_{\mathcal{N}}) = 1.$$
(2.13)

The parameters are shown in table 1.

	Table 1 P	arameters			
N	cluster	r <sub>N</sub> (fm)	tw N(NeV)		
<b>e</b>			(for free cluster)		
2	d	1.96	8.1		
3	t	1.7	14.4		
3	3 <sub>He</sub>	1.88	11.7		
4	α	1.6	18.2		

24 The expressions of  $F_{\ell m}(\mathcal{E}_d)$  for d cluster are

$$\overline{F}_{20}(P) = \begin{cases} 1, & 2(P_{F} + \sqrt{E_{a}}m) < P \\ Q_{1}(\frac{1}{2}P - P_{F}) + Q_{2}(\frac{1}{2}P - P_{F}), & 2P_{F} < P < (\sqrt{E_{a}}m + P_{F}) \times 2 \\ Q_{2}(\sqrt{P_{F}^{2}} - \frac{1}{4}P^{2}), & 2\sqrt{P_{F}^{2}} - E_{a}m < P < 2P_{F} \\ 0, & P < 2\sqrt{P_{F}^{2}} - E_{a}m \end{cases}$$
(2.14)

$$\overline{F}_{1,1}(\underline{p}) = \begin{cases} 0, & 2-f_{\overline{p}} + 2\sqrt{k_{\overline{n}}} m < \underline{p} \\ 1 - Q_{1}(\frac{p}{2} - P_{\overline{p}}) - Q_{1}(\frac{p}{2} - P_{\overline{p}}), & 2-f_{\overline{p}} + 2\sqrt{k_{\overline{n}}} m < \underline{p} \\ 1 - 2Q_{1}(\sqrt{p_{\overline{n}}} - \frac{1}{4p})^{2}) + Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{1}(P_{\overline{p}} - \frac{p}{2}) \frac{2\sqrt{p_{\overline{p}}} - E_{\overline{n}}}{\sqrt{p_{\overline{p}}} - E_{\overline{n}}} < \underline{p} < 2/p_{\overline{p}} \\ 1 - 2Q_{1}(\sqrt{p_{\overline{n}}} - \frac{1}{4p})^{2}) - Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{1}(P_{\overline{p}} - \frac{p}{2}) \frac{2\sqrt{p_{\overline{p}}} - E_{\overline{n}}}{\sqrt{p_{\overline{p}}} - E_{\overline{n}}} < \underline{p} < 2/p_{\overline{p}} \\ 1 - 2Q_{1}(\sqrt{p_{\overline{p}}} - \frac{1}{4p})^{2}) - Q_{1}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} = 2\sqrt{k_{\overline{n}}} m < \underline{p} < 2/p_{\overline{p}} \\ 1 + Q_{1}(P_{\overline{p}} - \frac{1}{2p}) - Q_{1}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} < 2\sqrt{p_{\overline{p}}} \\ 0, & 1 < 2f_{\overline{p}} - 2\sqrt{k_{\overline{n}}} m \\ 0, & 1 < 2f_{\overline{p}} < 2\sqrt{p_{\overline{p}}} \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) + Q_{2}(\sqrt{p_{\overline{p}}} - \frac{1}{4p^{2}}) - Q_{3}(P_{\overline{p}} - \frac{p}{2}), & 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{k_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{k_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{k_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{k_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{E_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{E_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{E_{\overline{n}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{\overline{p}} - \frac{p}{2}) - Q_{2}(P_{\overline{p}} - \frac{p}{2}), & 2P_{\overline{p}} - 2\sqrt{p_{\overline{p}}} m < \underline{p} < 2\sqrt{p_{\overline{p}}^{2} - E_{\overline{n}}} m \\ Q_{1}(P_{1} - \frac{p}{2}) - Q_{2}(P_{1} - \frac{p}{2}) - Q_{2}(P_{1} - \frac{p}{2}) - Q_{2}(P_{1} - \frac{p}{2}) - Q_$$

with 
$$E_N = \frac{3}{2} \frac{1}{\pi} W_N$$
,  $y = \frac{\chi}{\sqrt{E_N m}}$ ,  
 $Q_1(\chi) = \frac{2}{3\pi} \left\{ 35in^{-1}(\chi) - 8\gamma (1 - \gamma^2)^{5/2} + 2\gamma (1 - \gamma^2)^{5/2} + 3\gamma (1 - \gamma^2)^{5/2} \right\}$ 
 $Q_2(\chi) = \frac{32\sqrt{E_N m}}{\pi \rho} \left\{ \frac{1}{5} \left( \frac{\rho^2}{4E_2 m} - \frac{2\xi_{\chi}}{E_{\chi}} + 1 \right) (1 - \gamma^2)^{5/2} - \frac{1}{7} (1 - \gamma^2)^{5/2} \right\}$ 
(2.15)

The relationship between P and  $\mathcal{E}_d$  is given by eq.(2.11). The expressions of formation factor for N=3 are

$$F_{30}^{(3)}(P) = \frac{27}{4\pi} \int_{3}^{\frac{1}{2}P-P_{\pi}} dp' p^{2} \left(\frac{4}{3}E_{3}m - p^{2}\right)^{\frac{3}{2}} \int_{0}^{1} d\cos\beta F_{20}(\tilde{p})$$

$$+ \int_{3}^{\sqrt{\frac{3}{2}}E_{3}m} dp' p^{2} \left(\frac{4}{3}E_{3}m - p^{2}\right)^{\frac{3}{2}} \int_{0}^{1} d\cos\beta F_{20}(\tilde{p}) \left(\tilde{p}\right) \left(\tilde{p}\right)$$

$$+ \int_{3}^{\sqrt{\frac{3}{2}}E_{3}m} dp' p^{2} \left(\frac{4}{3}E_{3}m - p^{2}\right)^{\frac{3}{2}} \int_{0}^{1} d\cos\beta F_{20}(\tilde{p}) \left(\tilde{p}\right) \left(\tilde{p}\right) \left(\tilde{p}\right) \left(\tilde{p}\right) \left(\tilde{p}\right)$$

$$\begin{split} \overline{F}_{21}^{(3)}(p) &= \frac{27}{4\pi(E_{3}m)^{3}} \left\{ \int_{-a}^{a} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \int_{-a}^{a} dcon\beta F_{11}(\vec{p}) \right. \tag{2.16} \\ & \left. + \int_{-a}^{A\frac{a}{3}} E_{3}m - p'^{2} \right]_{-a}^{3/2} \left[ \int_{-a}^{b} dcon\beta F_{11}(\vec{p}) + \int_{-a}^{a} dcon\beta F_{20}(\vec{p}) \right]_{-a}^{b} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left[ \int_{-a}^{b} dcon\beta F_{11}(\vec{p}) + \int_{-a}^{a} dcon\beta F_{20}(\vec{p}) \right]_{-a}^{b} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left[ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right]_{-a}^{b} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left\{ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{11}(\vec{p}) \right]_{-a}^{b} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left\{ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left\{ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left\{ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\} \right\} \\ & \left. + \int_{-a}^{A} dp' p'^{2} (\frac{a}{3}E_{3}m - p'^{2})^{3/2} \left\{ \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\} \\ & \left. + \int_{-a}^{A} dcon\beta F_{20}(\vec{p}) + \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\} \right\} \\ & \left. + \int_{-a}^{A} dp' p'^{2} \left( \frac{a}{3}E_{3}m - p'^{2} \right)^{3/2} \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\}$$

$$& \left. + \int_{-a}^{A} dp' p'^{2} \left( \frac{a}{3}E_{3}m - p'^{2} \right)^{3/2} \int_{-a}^{b} dcon\beta F_{20}(\vec{p}) \right\}$$

$$& \left. + \int_{-a}^{A} dcon\beta F_{20}(\vec{p}) \right\}$$

$$& \left. + \int_{-a}^{A} dp' p'^{2} dcon\beta F_{20}(\vec{p}) \right\}$$

$$& \left. + \int_{-a}^{A} dp' p'^{2} dcon\beta F_{20}(\vec{p}) \right\}$$

Here  $oldsymbol{eta}$  is the angle between P and p'.

The expression of formation factor for N=4(\$\alphi\$ particle\$) are  

$$\overline{f_{40}^{(a)}(P)} = \frac{2}{\pi (E_{4}m)^{a}} \int_{0}^{\sqrt{2E_{4}m}} dp' p^{p^{2}} (2E_{6}m - p^{r^{2}})^{3/2} \int_{0}^{\sqrt{2}} dcon\beta F_{20}(P_{*}) F_{30}(P_{*}) \\ F_{31}^{(a)}(P) = \frac{2}{\pi (E_{4}m)^{4}} \int_{0}^{\sqrt{2E_{4}m}} ap' p^{r^{2}} (2E_{6}m - p^{r^{2}})^{3/2} \\ \int_{0}^{\sqrt{2E_{4}m}} dp' p^{r^{2}} (2E_{6}m - p^{r^{2}})^{3/2} \\ \int_{0}^{\sqrt{2E_{4}m}} \sqrt{2E_{4}m} \\ f_{21}^{(a)}(P) = \frac{2}{\pi (E_{4}m)^{4}} \int_{0}^{\sqrt{2E_{4}m}} dp' ap^{r^{2}} (2E_{4}m - p^{r^{2}})^{3/2} \\ \left\{ \int_{-1}^{1} dcon\beta \left[ F_{21}(P_{*})F_{21}(P_{*}) + F_{11}(P_{*})F_{11}(P_{*}) + F_{22}(P_{*})F_{20}(P_{*}) \right] \right\},$$
(2.18)  

$$F_{32}^{(a)}(P) = \frac{2}{\pi (E_{4}m)^{4}} \int_{0}^{\sqrt{2E_{4}m}} dp' ap^{r^{2}} (2E_{4}m - p^{r^{2}})^{3/2} \\ \left\{ \int_{-1}^{1} dcon\beta \left[ F_{21}(P_{*})F_{21}(P_{*}) + F_{11}(P_{*})F_{11}(P_{*}) + F_{22}(P_{*})F_{20}(P_{*}) \right] \right\},$$
$$F_{13}^{(b)}(P) = \frac{2}{\pi (E_{4}m)^{4}} \int_{0}^{\sqrt{2E_{4}m}} dp' p^{r^{2}} (2E_{4}m - p^{r^{2}})^{3/2} \\ \left\{ \int_{-1}^{1} dcon\beta \left[ F_{21}(P_{*})F_{21}(P_{*}) + F_{22}(P_{*})F_{21}(P_{*}) \right] \right\}$$

$$F_{04}(2) = \frac{2}{\pi (E_{4}m)^{A}} \int_{0}^{\sqrt{2E_{4}m}} dp' p'^{2} (2E_{4}m - p'^{2})^{3/2} \int d(\sigma s \beta F_{01}(P_{1}) F_{02}(P_{1})),$$
with
$$P_{+} = \frac{1}{4} \frac{p^{2}}{p^{2}} + \frac{p}{p} (co \beta \beta,$$

$$P_{-} = \frac{1}{4} \frac{p^{2}}{p^{2}} + \frac{p}{p} (co \beta \beta.$$
(2.19)

The calculated results of cluster formation factors are shown in fig.1. It can be seen well that when the emitted charged particle energy is not so high, the pick-up process to form the cluster plays a important role, and occurs at the very begining of the equilibrium process, i.e. at the small exciton number state which has more high emission probability. Thus such pick-up process give a dominat contribution to the complex particle emission and the experimental data can be fitted well with this model.

### 3. Formulations of Emitted Particle Spectrum and Cross Section

We have calculated charged particle spectrum of  $n+^{54}Fe$  in order to see the validity of this model.

The compound system has the excitation energy as

$$E = \frac{M}{M+m} E_n + B_n (A+1) \approx \frac{A}{A+1} E_n + B_n (A+1). \tag{3.1}$$

Where  $E_n$  is the incident energy in L-system, A is the mass number of the target,  $B_n$  is the binding energy of the incident neutron in the compound system.

The life time master eqiation for first emission reads

$$- \delta_{nn_{\bullet}} = \lambda_{-}^{(n+2)} E J T^{(\nu)}(n+2) E J + \lambda_{+}^{(\nu)}(n-2) E J T^{(\nu)}(n-2) E J$$

$$- [\lambda_{+}^{(\nu)}(n, E) + \lambda_{-}^{(\nu)}(n, E) + W_{T}^{(\nu)}(n, E) ] T^{(\nu)}(n, E)$$
(3.2)

with initial exciton number  $n_{\sigma}$  for neutron induced reactions. We consider first and second emissions of n,p, ,d,t, He, for neutron induced structural material reactions.

The normalized condition is

$$\sum_{n} Z'''(n, Z) W_{T}'''(n, E) = 1$$
(3.3)

Table 2 shows the parameters related with  $n + {}^{54}Fe$  reaction.

Table 2. The spin and the binding energy of

## the emitted particles (in Mev)

	1	2	3	4	5	6
	n	p		d	t	He
	2	ł	0	1	ł	ł
	9.297	9.212	8.454	15.926	21.724	16.992
<sup>54</sup> Fe( <sup>55</sup> Fe-n)	13.318	8.853	8.418	18.684	22.961	19.734
<sup>54</sup> Mn( <sup>55</sup> Fe-p)	8.938	7.560	8.759	13.275	19.056	18.285
53 <sub>Mn</sub> (55 <sub>Fe-d</sub> )	12.055	6.561	9.156	16.375	19.379	20.398
52 <sub>Mn(</sub> 55 <sub>Fe-t)</sub>	10.534	6.544	8.656	13.581	20.324	17.678
52 <sub>Cr(</sub> 55 <sub>Fe-</sub> 3 <sub>He</sub>	)12.038	10.524	9•353	19.331	22.409	21.788
51 <sub>Cr(</sub> 55 <sub>Fe-</sub> )	9.261	9.510	8.941	16.628	21.926	17.892

From the physical point of view, the cluster will be constituted according to the arrangement of particles above and below the Fermi surface  $[\underline{l}, \underline{m}]$ . Actually, the m particles below Fermi surface do not come from the collision process. Thus, the increase of the hole number m to form the emitted cluster does not influence the change of exciton state density. By means of the detail balance princeple the emission rate for  $\underline{l}$  particles above Fermi surface can be expressed as

$$W_{\beta}^{g}(P,h,E,E_{\beta}) = \frac{2Z_{\beta}+I}{\pi^{2}h^{3}} \mathcal{U}_{\beta} \mathcal{E} \mathcal{O}_{In}^{P}(E,E_{\beta}) \mathcal{F}_{fm}(E_{\beta}) \mathcal{R}_{\beta}^{g}(P,h,E,E_{\beta})$$
(3.4)  
with 
$$(I) (P_{\alpha}P_{\beta} + E_{\beta}E_{\alpha} - E_{\beta})$$

$$R_{\beta}^{\mathcal{L}}(P,h, E, \mathcal{E}_{\beta}) = \frac{W(P-L, h, E-\mathcal{E}_{\beta} - \mathcal{B}_{\beta})}{W(P, h, E)}$$

Where  $I_{\beta}$  is the spin of emitted  $\beta$  particle,  $\omega$  is the exciton state density,  $\mathcal{O}_{\ell_{\alpha}}^{\beta}(E, \xi)$  is the inverse cross seation of emitted  $\beta$  particle with energy  $\xi_{\alpha}$  at compound system excitation energy E which can be

25

26 calculated from optical model,  $B_{\rho}$  is the binding energy of  $\beta$  particle in the system, which are shown in table 2. Here the renormalized Williams formula is employed for the exciton state density.

The emission rate for all case of f, m reads

$$W_{\beta}(P,h,E,\mathcal{E}_{\beta}) = \frac{\overline{Z}}{\mathcal{L}(\beta)} W_{\beta}^{\mathcal{L}}(P,h,E,\mathcal{E}_{\beta})$$
(3.5)

Here  $\mathcal{L}(\beta)$  stands for sum over all of the possible  $\mathcal{J}$  values. The total emission rate is

$$W_{\tau}(p,h,E) = \sum_{\beta} \sum_{\substack{B \ P,h}} \int W_{\beta}^{P}(p,h,E,\xi_{\beta}) d\xi_{\beta}$$

$$= \sum_{\substack{B \ P,h}} \sum_{\substack{A \ P,h}} W_{\beta}^{P}(p,h,E).$$
(3.6)

For  $\gamma$ -ray emission( $\beta$ =7), the Weisscopf strong coupling model has been adopted.<sup>(6)</sup>

After first parti le emission with energy  $\mathcal{E}_{\beta}$ , the residual excitation energy is

$$\overline{E_{\beta}}' = \overline{E} - \overline{E_{\beta}} - \overline{B_{\beta}(\theta + 1)}$$
(3.7)

Taking into account the second emission process, the master equiation for residual system takes the form of

$$\frac{\partial}{\partial t} P_{\pm}^{(a)}(p, h, E_{\beta}', t) = \lambda_{\pm}^{(a)}(p-1, h-1) P^{(a)}(p-1, h-1, E_{\beta}', t) + \lambda_{\pm}^{(a)}(p+1, h+1) P^{(a)}(h+1, E_{\beta}', t)$$

$$(3.8)$$

$$(3.8)$$

$$+ \omega_{\beta}^{(a)}(p+1, h, E, E_{\beta}) P^{(a)}(p+2, h, E_{\beta}', t)$$

with initial condition as  $p^{(\prime)}(\rho,h,E',t=0)=0$ 

and 
$$p^{(3)}(P,h,E',t \rightarrow m) = 0.$$
 (3.9)

The life time master equiation of eq.(3.8) reads

$$- W_{\beta}^{\ell}(p+l,h,E, \Sigma_{\beta}) T^{(\prime)}(p+l,h,E)$$

$$= \lambda_{-}^{(\mu)}(p+l,h+l) T_{\lambda}^{(\mu)}(p+l,h+l,E_{\beta}^{\prime}) + \lambda_{+}^{(\mu)}(p-l,h-l) T_{\lambda}^{(\mu)}(p-l,h-l,E_{\beta}^{\prime})$$

$$- \left[ \lambda_{+}^{(\mu)}(p,h) + \lambda_{-}^{(\mu)}(p,h) + W_{\gamma}^{(\mu)}(p,h,E_{\beta}^{\prime}) \right] T_{\lambda}^{(\mu)}(p,h,E_{\beta}^{\prime}),$$
(3.10)

Summing over exciton state one gets

$$\frac{\overline{Z}}{P,h} W_{p}^{\rho}(P+l,h,E,E_{p}) \overline{C}_{l}^{(\nu)}(P+l,h,E)$$

$$= \frac{\overline{Z}}{P,h} W_{T}^{(\nu)}(P,h,E_{p}') \overline{C}_{l}^{(\nu)}(P,h,E_{p}')$$
(3.11)

The normalized condition can be obtained in the followed way

$$\frac{\overline{Z}}{2}\int \overline{Z}W_{T}^{(L)}(P,h,E_{p}')T_{X}^{(L)}(P,h,E_{p}') dE_{p} = 1,$$
(3.12)

The double energy spectrum of two particle emissions with energy  $\mathcal{E}_{\rho}$  and  $\mathcal{E}_{r}$ , respectively, is given by

$$\frac{d^2 \mathcal{O}}{d\epsilon_{p} d\epsilon_{p}} = \mathcal{O}_{\mathbf{A}} \sum_{\mathcal{L}} Z \mathcal{T}_{\boldsymbol{\rho}}^{(s)}(\boldsymbol{p}, \boldsymbol{h}, \boldsymbol{E}_{\boldsymbol{\rho}}') \boldsymbol{\omega}_{\boldsymbol{\delta}}^{(s)}(\boldsymbol{p}, \boldsymbol{h}, \boldsymbol{E}_{\boldsymbol{\rho}}', \boldsymbol{\delta}\boldsymbol{\delta})$$
(3.13)

With the normalization condition(3.12), one can easily get

$$\frac{\sum}{\beta S} \iint \frac{d^2 \sigma}{dS_{\beta} dS_{\beta}} dS_{\beta} dS = 1$$
(3.14)

For different first particle emission,  $B_{\beta}$  as well  $(\chi,m]$  (at same  $B_{\beta}$ ) is diffrent. Thus we have to solve master equiations one by one for second emission process, which are independent each other.

For  $\beta$  or  $\mathcal{S}=7$  process, the spectra are

$$\frac{d\sigma}{d\epsilon_{\beta}} = \int \frac{d^{2}\sigma}{d\epsilon_{\beta} d\epsilon_{\gamma}} d\epsilon_{\gamma} = \sigma_{a} \sum_{I(\beta)} \sum_{P,h} \overline{\zeta} \tau_{I}^{(\mu)}(P,h, \epsilon_{\beta}) W_{\gamma}^{(\mu)}(P,h, \epsilon_{\beta})$$
(3.15)  
$$\frac{d\sigma}{d\epsilon_{\delta}} = \int \frac{d^{2}\sigma}{d\epsilon_{\beta} d\epsilon_{\delta}} d\epsilon_{\beta} = \sigma_{a} \int_{\rho} \sum_{P,h} \overline{\zeta} \tau^{(\mu)}(P,h, \epsilon-\epsilon_{\gamma}\epsilon_{\delta}) d\epsilon_{\gamma}$$
(3.15)

Thus the cross section of one particle emission process can be written as

$$\begin{aligned}
\mathcal{O}(n,\beta) &= \sigma_{n} \sum_{k(\beta)} \sum_{k,h} \mathcal{T}_{k}^{(a)}(P,h, E_{\beta}') W_{7}^{(a)}(P,h, E_{\beta}') \\
&= \mathcal{E} - \mathcal{E}_{\beta} \\
&= \mathcal{E} - \mathcal{E} - \mathcal{E}_{\beta} \\
&= \mathcal{E} - \mathcal{E} - \mathcal{E} \\
&= \mathcal{E} - \mathcal{E} - \mathcal{E} \\
&= \mathcal{$$

In fact, for  $\beta = 7, \delta = 1, 2, 3, 4, 5, 6$  process the results are quite small (<1mb) to be neglected.

The normalized spectrum is

$$\overline{F}_{\beta}(\underline{s}_{\beta}) = \left[\frac{d\sigma}{d\underline{s}_{\beta}}(n,\beta r) + \frac{d\sigma}{d\underline{s}_{\beta}}(n,r\beta)\right] / \sigma(n,\beta).$$
(3.17)

We also have  $\mathcal{O}(n,r)$  for  $\beta = 5=7$  as

$$\overline{G(n, r)} = \iint \frac{d^{2}\overline{G}}{d\overline{z}_{7} A\overline{z}_{7}} d\overline{z}_{7} d\overline{z}_{7}^{\prime} (p, h, \overline{z}) W_{7}^{\prime \prime \prime}(p, h, \overline{z}-\overline{z}) d\overline{z} \qquad (3.18)$$

The spectra for  $\beta$ ,  $\delta$  +7 are

$$\frac{d\sigma}{dE_{\beta}} = \int \frac{d^{2}\sigma}{dE_{\beta} dE_{\delta}} dE_{\delta} = \sigma_{A} \sum_{l(\beta)} \sum_{l,h} E_{A}^{(a)}(p,h,E_{\beta}) W_{\delta}^{(a)}(p,h,E_{\beta})$$
(3.19)

$$\frac{dO}{d\Sigma_{5}} = \int \frac{d^{2}O}{d\Sigma_{\beta} d\Sigma_{5}} d\Sigma_{\rho} = O_{A} \int \sum_{\mathcal{L}(\rho)} \sum_{\mathcal$$

Here  ${
m N}_{oldsymbol{eta}}$  is the mass number of the first emitted particle .

The cross section for two particle emissions is given by

$$\begin{aligned}
\sigma(n, \beta \delta) &= \iint \frac{d^2 \sigma}{d \xi_{\beta} d \xi_{\delta}} d \xi_{\beta} d \xi_{\delta} \\
&= \sigma_{A} \int_{0}^{\xi_{B}} \frac{\overline{z}}{z} \, \overline{z} \, \mathcal{I}_{a}^{(2)}(\rho, h, \overline{z}_{\beta}') \, \mathcal{W}_{\delta}^{(2)}(\rho, h, \overline{z}_{\beta}') d \xi_{\beta} . \end{aligned} \tag{3.21}$$

The normalized spectrum for (n, 2n) reaction( $\beta = \delta = 1$ ) takes

$$\overline{F}_{2n}(z) = \frac{1}{2G(n,2n)} \left( \frac{\alpha G}{\alpha S \rho} \right|_{\rho=1} + \frac{\alpha G}{\alpha S \sigma} \left|_{S=1} \right].$$
(3.22)

The parameter of the internal transition K takes the value of K=400 MeV<sup>3</sup>. The pair correlation parameters  $\Delta$  (A.Z) are the fit parameters. Lack of the experimental data on some reaction channels, we set $\Delta$ =0 temporarily except the reaction channels of (n,p) and (n, $\alpha$ ) in which  $\Delta$  (<sup>54</sup>Mn)=-0.75MeV and (<sup>54</sup>Fe)=1.2MeV are taken to fit the data. The calculated results of n+ <sup>54</sup>Fe are shown in Fig.2. The contributions from  $F_{lm}$  ( $\mathcal{E}_{\alpha}$ ) in the (n, $\alpha$ ) reaction are shown in Fig.3,4,5 for the incident reutron energies of En=12,16,20, respectively. The results indicute that the dominant pickup components are from l=1 and 2, which are corresponds to three and two particle pickup-type reaction. It turns out that the previous calculations, in which the particle emission only starts at the particle number  $P \ge 4$ , always produce much smaller composite particle spectra in absolute value than the data. In our work the degree of fitting to the data of  $\alpha$  -outgoing energy spectra is excellent without any adjuctive parmeter. We belive that the pickup - type machanism mast be taken into account for composite particle **4**missions.

#### Discussion

The UCP model presents a clear physical picture. The pre-equilibrium process transites into the equilibrium process smoothly instead of the combination of two models. The formulas are straightforward and the number of the conjuctable parameters in the UCP model is less than that in the combination model.

There are some problems remained in the UCP model. One is the spin population factor f(n,E,I) which counts the contribution of spin and angular momentum. In present paper we set f=1 unless we learn the exact effective expression. Another is the determination of the value of the parameters in the formation factors of the cluster for instance, the value of the Fermi energy of single particle  $\boldsymbol{\xi}_{f}$ . In a uniformed level model the value of  $\boldsymbol{\xi}_{f}$  should differ from that of the shell model and other models, and the oscillator parameter  $\boldsymbol{\pi}$  we should also be different from that of a free cluster. Under reasonable physical conditions they can be treated as the conjuctable parameter.

The enhansment factor is exclusived in the UCP model because the formation factors are taken into account. Based on the framework worked out by now the code of the calculation of the double differential cross section will be disigned with the consideration of the Fermi motion, Pauli principle, and the energy correlation. 28 In addition, the code for transition from C.M. system to the Lab. system of the formulas mentioned above ready already.

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FIG. 1. The normalized formation factors Fim



Incident Neutron Energy (MeV)

FIG. 2.



Reaction Spectrum (mb/MeV)



FIG. 4.

23





#### Toward an Improved Multi-step Direct Multi-step Compound Reaction Model

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#### ABSTRACT

A multi-step direct multi-step compound model free of the criticisms suffered by that of Feshbach, Kerman and Roonin is defined in terms of the statistical hypotheses made about the interaction matrix elements. The model is briefly described and discussed. Also described are our unsuccessful attempts to parametrize the level and transition strength densities needed in pre-equilibrium calculations in terms of their moments.

#### 1.0 INTRODUCTION

In the last decade, an intense effort has been made to obtain a consistent quantum mechanical description of preequilibrium reactions. This has been motivated in great part by the growing body of experimental cross section data, differential in energy and angle, which has been obtained over the same period. The early pre-equilibrium models (1), using emission rates based on the Weisskopf model, were able to describe the energy spectra observed but were not prepared to deal with their forward peaked angular distributions. More recent versions of one of these , the exciton model, have succeeded in describing well the experimental angular distributions (2,3). The pre-equilibrium and Hauser-Feshbach equilbrium compound emission have also been unified within this model through the inclusion of the effects of angular momentum in the emission rates (3). Despite their successes however, these models remain semiclassical ones based on hypotheses which are intuitively reasonable but difficult to evaluate or improve.

The first major step towards a quantum mechanical model of pre-equilibrium reactions was taken by Agassi, Weidenmuller and Mantzouranis (AWM) (4). Using well defined hypotheses on the statistical nature of the matrix elements coupling con-

figurations, they obtained a unified model of preequilibrium and equilibrium reactions. Their hypotheses however yield angular distributions symmetric about  $90^{\circ}$  and can only describe the multi-step compound part of the reaction.

A quantum mechanical model providing the observed anisotropy was developed shortly thereafter by Tamura and Udagawa (TU) (5,6). Applying statistical hypotheses similar to those of AWM to the states excited in direct reactions, they obtained a good description of the multi-step direct component of the pre-equilibrium reaction.

One of the first works to attempt to unite the direct and compound processes in one formalism was that of Feshbach, Kerman and Koonin (FKK) (7). Although their model has been used successfully to describe a large body of experimental data (8), it has also justly suffered many criticisms. Their model of the multi-step compound component makes use of a "never come back" hypothesis which prohibits the unified description of the pre-equilibrium and equilibrium contributions. The latter must be included by hand. Several authors (9,10) have noted that the multi-step direct component cannot be written in terms of DWBA matrix elements as done by FKK. Feshbach claims to have shown that this can in fact be done (11). The fact that all successful comparisons with experimental data have been made using DWBA matrix elements certainly provides strong motivation for such an at-However, Udagawa, Low and Tamura have pointed out tempt. other approximations in the model's multi-step direct component which would still leave its accuracy in doubt (10).

Here, we will draw on the works of the Heidelberg (4,12) and University of Texas (5,6) groups to show how the FRR model can be modified so as to satisfy the criticisms above. We will then discuss our not so successful attempts at parametrizing the level densities and transition strength densities necessary for its use.

#### 2.0 AN IMPROVED MULTI-STEP DIRECT MULTI-STEP COMPOUND MODEL

We can improve the multi-step direct multi-step compound model of FKK by modifying the statistical hypotheses on which it is based. We will use hypotheses consistent with those of AWM and of TU. The multi-step direct reaction model of deeply inelastic heavy ion collisions developed by Agassi, Ko and Weidenmuller (12) serves as a useful guide in restating the statistical hypotheses used by TU in terms of the interaction matrix elements. In particular, we note their emphasis of the requirement that all statistical hypotheses be made in terms of reduced matrix elements in order to conserve angular momentum.

As in the FKK model, we divide the space of states to be considered into a part in which all particles are in bound single particle states and another in which one and only one of these particles is in a continuum state. We label these by C (for compound) and D (for direct) respectively. We take as statistical hypotheses on the reduced matrix elements the following:

For the bound state to bound state interaction,  $\overline{V_{e}V_{e}}$ ,

$$\frac{(Y, \|N^{TE}\|Y', )(X_{2}'\|N^{TE}\|Y')}{= S_{Y,Y_{2}} S_{TT'} S_{TT'}}$$

$$= S_{Y,Y_{2}} S_{Y,Y_{2}'} S_{TT'} S_{TT'}$$

$$\times (Y, \|N^{TE}\|Y')(Y', \|N^{TE}\|Y')$$

- For the continuum to bound state interaction,  $\overline{V_{v}V_{v}}$ ,

$$(c, I, (s, e, ) 1, || V^{T \pi} || Y, ) (Y_{2} || V^{T, \pi'} || c_{2} I_{2} (s, e_{2}) 1_{2})$$

$$= \delta_{x, x_{2}} \delta_{-1} c_{2} \delta_{T, I_{2}} \delta_{-1} s_{2} \delta_{-1} s_{2}$$

- For the continuum to continuum interaction,  $\overline{\mathbf{v}}_{\mathbf{v}}$ 

$$(c, I, (s, e, i), || N^{TR} || c, I, (s, e, i), i') (c_{\lambda}' I_{\lambda}'(s, c_{\lambda}'))_{\lambda}' || N^{T'T'} || c_{2} I_{\lambda}(s, e_{\lambda}) (L)$$

$$= \delta_{c, c_{\lambda}} S_{c, c_{\lambda}}' S_{I, I_{\lambda}} \delta_{I, I_{\lambda}} \delta_{s, s_{\lambda}} \delta_{s, s_{\lambda}} \delta_{s, s_{\lambda}}'$$

\* (c, I, (s, e,)1, || NIR || c,'I.'(s, e, i)1,')(c,'I,'(s, l'2)12' || NI'R' || c, I, (s, l'2)12)

with all other possible pairs averaging to zero. In summary, we suppose that the average coupling is non-zero only for pairs of interactions that couple the same continuum channels and/or bound states.

Let us now briefly discuss the pre-equilibrium model which we obtain using these hypotheses. We start with the Born expansion of the Lippmann-Schwinger equation for the Green's functions.

$$\begin{pmatrix} G_{cc}^{\pm} & G_{ca}^{\pm} \\ G_{oc}^{\pm} & G_{oa}^{\pm} \end{pmatrix}^{\pm} \begin{pmatrix} G_{oc}^{\pm} & O \\ O & G_{oa}^{\pm} \end{pmatrix}^{\pm} \begin{pmatrix} G_{oc}^{\pm} & O \\ O & G_{oa}^{\pm} \end{pmatrix} \begin{pmatrix} V_{cc} & V_{cb} \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ O & G_{ca}^{\pm} \end{pmatrix} \\ + \begin{pmatrix} G_{oc}^{\pm} & O \\ O & G_{ob}^{\pm} \end{pmatrix} \begin{pmatrix} V_{cc} & V_{cb} \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ O & G_{ob}^{\pm} \end{pmatrix} \begin{pmatrix} V_{cc} & V_{cb} \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O \\ V_{ac} & V_{ab} \end{pmatrix} \begin{pmatrix} G_{oc}^{\pm} & O$$

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Since the terms in the expansion which couple continuum to bound states involve an odd number of like interactions, they will be zero on the average.

We obtain equations for the average continuum and bound state components of the Green's function by keeping the lowest order terms in the asymptotic expansion of their average as described in the work of the Heidelberg group. We will use their notation of a bar joining two matrix elements to denote the average.

For the average continuum state Green's function, we obtain

$$G_{s}^{T} = G_{so}^{T} + G_{ss}^{T} U^{T} G_{s}^{T}$$

where the optical potential, given by

depends again on the average Green's functions. This optical potential is nonlocal and generally quite complicated, depending on the energy, excitation energy, angular momenta and configuration. To our knowledge, only its ground state elements have been studied (13).

We obtain a similar Lippmann-Schwinger equation for the average continuum wavefunction

$$|\Psi^{\pm}\rangle = |\phi^{\pm}\rangle + G_{\bullet,\bullet}^{\pm} U^{\pm}|\Psi^{\pm}\rangle$$

which we can write in differential form as

$$\left(\mathbf{E}-\mathbf{T}-\mathbf{\varepsilon}_{\bullet}-\mathbf{V}_{\bullet\bullet}-\mathbf{U}_{\bullet}^{\pm}\right)|\mathcal{Y}_{\bullet}^{\pm}\rangle=0$$

where  $\mathcal{E}_{v}$  is the channel excitation energy and  $V_{vv}$  is the initial distorting potential which we take to be real.

The average bound state Green's function is determined by the equation

$$G_{c}^{\pm} = G_{oc}^{\pm} + G_{oc}^{\pm} \left( \Delta = \frac{1}{2} \left( \Gamma^{\dagger} + \Gamma^{\psi} \right) \right) G_{c}^{\pm}$$

where the shift factor and "escape" width are determined by

$$\Delta \mp \frac{1}{2} \Gamma^{\uparrow} = V_{co} G_{o}^{\pm} V_{oc}$$

32

while the spreading width is given by

To calculate average cross sections, we first express them in terms of the Born series expansion of the transition matrix.

$$\overline{\nabla z_i} = \overline{\langle \phi_z^2 | T | \phi_i^* \rangle \langle \phi_i^* | T^\dagger | \phi_z^* \rangle}$$
$$= \overline{\langle \phi_z^2 | v_1 v_G^* v_1 \cdots | \phi_i^* \rangle \langle \phi_i^* | v_1 v_G^* v_1 \cdots | \phi_z^* \rangle}$$

Beside the average shape elastic cross section, we find in general contributions from multi-step direct and multi-step compound processes.

The average shape elastic cross section is determined by the average transition matrix.

$$\overline{v_{ie}} = |\langle \phi^{-}|\overline{\tau}|\phi^{+}\rangle|^{2}$$
  
=  $|\langle \phi^{-}|u^{+}|\psi^{+}\rangle|^{2}$ 

The multi-step direct contribution can be written as

$$(\sigma_{0})_{\xi_{i}} = \rho_{\xi} \langle Y_{\xi}^{-} | \overline{v_{00}} | Y_{i}^{*} \rangle \langle Y_{i}^{+} | \overline{v_{00}} | Y_{\xi}^{-} \rangle$$

$$(\sigma_{0})_{\xi_{i}} = \rho_{\xi} \langle Y_{\xi}^{-} | \overline{v_{00}} | Y_{i}^{*} \rangle \langle Y_{i}^{+} | \overline{v_{00}} | G_{0}^{-} \overline{v_{00}} | Y_{\xi}^{-} \rangle$$

The first term in this expansion is the one-step DWBA while the second is the two-step process (neglecting any nonorthogonality terms) so that the two together reproduce the model of TU. There are, of course, higher order terms that could be included although care should be taken with nonorthogonality terms that also might be necessary.

In the multi-step compound contribution to the cross section, the formation of the compound nucleus and the posterior particle emission are described by the factors

while the transitions between classes of states in the compound nucleus are determined by the matrix  $\widetilde{\mathcal{T}}$  where

$$(\overline{\pi}^{-1})_{\alpha\beta} = \delta_{\alpha\beta} 2\pi p_{\alpha} (\Gamma_{\alpha}^{\dagger} + \Gamma_{\alpha}^{\dagger}) - \overline{T}_{\alpha\beta}^{\dagger} - \overline{T}_{\alpha\beta}^{\dagger}$$

Here, the external mixing matrix is given by  $T_{\lambda\beta}^{\uparrow} = 2\pi \rho_{\lambda} \langle \lambda | V_{co} G_{0}^{+} V_{0c} | \beta \rangle 2\pi \rho_{\lambda} \langle \beta | V_{co} G_{0}^{-} V_{0c} | \kappa \rangle$   $+ 2\pi \rho_{c} \langle \lambda | V_{co} G_{0}^{+} V_{0A} G_{0}^{-} V_{0c} | \beta \rangle 2\pi \rho_{\lambda} \langle \beta | V_{co} G_{0}^{-} V_{0A} G_{0}^{-} V_{0c} | \kappa \rangle$   $+ 2\pi \rho_{c} \langle \lambda | V_{co} G_{0}^{+} V_{0A} G_{0}^{-} V_{0c} | \beta \rangle 2\pi \rho_{\lambda} \langle \beta | V_{co} G_{0}^{-} V_{0A} G_{0}^{-} V_{0c} | \kappa \rangle$ 

while the internal one is

33

4 . . . . .

We note that the multi-step compound component depends on the continuum-continuum interaction which modifies the formation/emission factors, the external transition matrix and the escape widths. It is easily seen however that these modifications do not effect the symmetry about 90° of the compound angular distribution. This symmetry is a result of the statistical hypothesis on the continuum to bound state interaction which requires that partial waves differing in total angular momentum or parity contribute incoherently to the cross section.

In the limit in which the continuum to continuum interaction goes to zero, the multi-step compound component almost reduces to the AWM expression for the cross section. The only difference is the elastic enhancement factor which is missing here. This reflects a deficiency in our statistical hypotheses which do not yet contain all of the symmetry to be expected. We are studying the extension of the statistical hypotheses necessary to include this symmetry, although we expect the resulting modifications to have little effect at the energies at which pre-equilibrium reactions are important.

The statistical hypotheses we have given thus define a preequilibrium model which yields cross sections having a multi-step direct component equal to that of TU and a unified multi-step compound component similar to the one obtained by AWM. The model also specifies the average optical potentials, Green's functions and wave functions requiring only the average interaction matrix elements as input parameters.

We admit that the model is exceedingly complex, even more so than the original multi-step model of FKK. Given present computational possibilities, it will be necessary to approximate it in some manner before it can be usefully applied. As it stands however, it could prove useful as a context within which we can better understand and evaluate the approximations and models which we use.

#### 3.0 A MOMENT METHOD APPROXIMATION OF LEVEL AND TRANSITION STRENGTH DENSITIES

The most important quantities which enter pre-equilibrium calculations are the average interaction matrix elements and the level densities. An alternative description uses the appropriate product of the two, the density of interaction matrix elements, which we will call the transition strength density.

Combinatorial methods can calculate densities to within the accuracy of the set of single particle states and the residual interaction used. Such calculations become prohibitive for large energies and/or complex configurations however. We have thus studied the possibility of using a simple moment method to reproduce the average trend of combinatorial calculations.

#### 3.1 LEVEL DENSITIES

We will illustrate the moment method calculation of level densities with a simple case involving one type of particle and hole. We will assume that we have N particle states and N hole states and will write their energies as positive ones with respect to the Fermi energy.

We first define an appropriately unnormalized one-body density operator for the system.

$$F_{0}(p, x) = \frac{N_{p}}{N_{1}} (a_{1}a_{1}^{\dagger} + a_{1}^{\dagger}a_{1} \times p e^{\beta x_{1} - x m_{1}})$$

$$\times \frac{N_{1}}{N_{1}} (a_{1}^{\dagger}a_{1} + a_{3}a_{1}^{\dagger} \times p e^{\beta x_{1} - x m_{3}})$$

We note that when  $\beta \rightarrow \infty$ , for fixed  $\checkmark$ , this becomes the density operator for the independent particle ground state. We obtain the partition function by taking the trace of this operator.

$$Z(p,x) = Tr[F_{\bullet}(p,x)]$$

$$= \frac{M_{\bullet}}{7L}(1+x_{e}e^{px_{i}-x_{a}x_{i}}) \frac{M_{a}}{7L}(1+x_{e}e^{px_{i}-x_{a}x_{i}})$$

$$= \frac{M_{\bullet}}{1+1}$$

A power expansion in the factors  $x_{i}$  and  $x_{i}$ , a device first used by Bloch (14), then permits us to identify the partition function of each configuration.
$$Z(p,x) = \sum_{p,m} (x_p)^p (x_m)^m Z(p,m;p,x)$$

The density of states could be obtained by performing the inverse Laplace transform of the partition function.

$$p(p,h;U,M) = \frac{1}{(2\pi i)^2} \int_{0}^{0} dp \int_{0}^{0} dx = (p,h;p,r) e^{AU \cdot rM}$$

In terms of a configuration's partition function, we can calculate its moments using

$$\langle U^{1}M^{\kappa}\rangle_{P_{N}} = \frac{1}{N_{P_{N}}} \left(\frac{-\partial}{\partial A}\right)^{1} \left(\frac{-\partial}{\partial X}\right)^{\kappa} Z(P,N;A,X) \Big|_{A=X=0}$$

where

35

It turns out, however, to be easier to calculate the moments for all configurations at the same time using

$$\left(-\frac{\partial}{\partial \beta}\right)^{4}\left(-\frac{\partial}{\partial x}\right)^{2} Z(\beta, x)\Big|_{A=x=0} = \sum_{h,n} (x_{h})^{h} (x_{n})^{n} M_{h_{n}} \langle U^{3} M^{n} \rangle_{h_{n}}$$

For example, we have

$$Z(\beta, \gamma)\Big|_{\beta=\gamma=0} = (1+\chi_{\beta})^{N_{p}} (1+\chi_{\gamma})^{N_{q}}$$
$$= \sum_{f,\chi} (\chi_{\beta})^{f} (\chi_{\gamma})^{\chi} \binom{N_{p}}{p} \binom{N_{q}}{m}$$
$$= \sum_{f,\chi} (\chi_{\gamma})^{f} (\chi_{\gamma})^{\chi} N_{f\chi}$$

so that the number of states with p particles and h holes is

$$N_{\mu n} = \begin{pmatrix} N_{\mu} \\ \mu \end{pmatrix} \begin{pmatrix} N_{\mu} \\ n \end{pmatrix}$$

Likewise,

$$= \sum_{\substack{k \in \mathbb{N} \\ k \in \mathbb{N}}} (\chi_{k})^{k} (\chi_{k})^{k} = \sum_{\substack{k \in \mathbb{N} \\ k \in \mathbb{N}}} (\chi_{k})^{k} (\chi_{k})^{k} \left[ \binom{N_{k}-1}{k} \binom{N_{k}}{k} (\chi_{k})^{k} ($$

.

so that the centroid in energy of the  ${\bf p}$  particle  ${\bf h}$  hole configuration is

where  $\langle i \rangle_{i}$  and  $\langle i \rangle_{i}$  are the average energies of the single particle and single hole states, respectively.

Other low moments of interest are the variance in energy

$$\langle U^{2} \rangle_{p_{N}} - \langle U \rangle_{p_{N}}^{2} = \frac{p(N_{p}-p)}{N_{p}-1} (\langle \varepsilon^{2} \rangle_{p} - \langle \varepsilon \rangle_{p}^{2}) + \frac{h(N_{n}-h)}{N_{n}-1} (\langle \varepsilon^{2} \rangle_{n} - \langle \varepsilon \rangle_{n}^{2})$$

and the variance of the spin projection, the spin cutoff factor,

$$\langle M^{2} \rangle_{p_{M}} - \langle M \rangle_{p_{M}}^{2} = \frac{2(N_{p} - p)}{N_{p} - 1} (\langle m^{2} \rangle_{p} - \langle m^{2} \rangle_{p}) + \frac{N(N_{n} - N)}{N_{n} - 1} (\langle m^{2} \rangle_{n} - \langle m^{2} \rangle_{n})$$

36

The reconstruction of the density is most easily performed in terms of the cumulants rather than the moments. These are defined as

$$(K_{1x})_{pu} = \left(-\frac{\partial}{\partial p}\right)^{1} \left(-\frac{\partial}{\partial x}\right)^{x} ln \neq (p, n; p, x) | p = x = 0$$

and are simple polynomial functions of the moments.

We calculate the cumulants through sixth order in  $\beta$  and  $\gamma$ and approximate the configuration partition function as

$$Z(p,n;p,x) = exp\left[\sum_{j:x_{1}b} (x_{j}x)_{j} + \frac{(-x)^{2}}{2!} (\frac{-x}{2!}\right]^{k}$$

We can then write the density of states as a derivative expansion about a Gaussian,

$$p(\mu, h; U, M) = \frac{N_{AM}}{2\pi \sqrt{4et K_{PL}}} exp\left[\sum_{3 \leq j \neq k \leq k} \frac{1}{j! k!} \frac{1}{k!} \frac{(K_{Jk})_{kl} (\frac{\partial}{\partial U})^{(-\partial)k}}{(\frac{\partial}{\partial M})}\right]$$

$$x exp\left[-(U - \langle U \rangle_{Ph})^{M} - \langle M \rangle_{Ph}\right] \frac{1}{2K_{PL}} \left(\frac{U - \langle U \rangle_{PL}}{M - \langle M \rangle_{Ph}}\right)\right]$$

where

$$\widetilde{K}_{\rho n} = \begin{pmatrix} (K_{20})_{\rho n} & (K_{11})_{\rho n} \\ (K_{10})_{\rho n} & (K_{02})_{\rho n} \end{pmatrix} = \begin{pmatrix} \langle U^{2} \rangle_{\rho n} - \langle U \rangle_{\rho n}^{2} & \langle U^{m} \rangle_{\rho n} - \langle U \rangle_{\rho n} \\ \langle U^{m} \rangle_{\rho n} - \langle U \rangle_{\rho n}^{2} & \langle U^{m} \rangle_{\rho n} - \langle U \rangle_{\rho n}^{2} \end{pmatrix}$$

We expand the exponential derivative keeping terms through sixth order. Finally, we obtain the level density using Bethe's difference formula.

$$p(p,n;U,T) = p(p,n;U,M=T) - p(p,n;U,M=T+1)$$

In the calculations performed, we have distinguished between protons and neutrons permitting independent particle and hole states for each. As the cumulants of the state densities for noninteracting particles are additive, the generalization to this case is trivial.

We have compared the moment method densities with combinatorial ones obtained using the same sets of single particle states. Although protons and neutrons were distinguished in the calculations, this distinction was not investigated. We have compared densities summed over all configurations with the same number of particles and holes.

In Figures 1 and 2, we show two examples of the relatively good agreement obtained for the density of four particle two hole levels in <sup>92</sup>Zr. Similar results were obtained for other values of the angular momentum. We note however that the oscillations in the combinatorial densities due to shell effects are not reproduced by the moment method results.

We would expect the shell effects to become less important for more complex configurations. Indeed, as we can see in Figure 3, the combinatorial total level density of five particle three hole states in <sup>12</sup>2r is much smoother than the four particle two hole one. However, we encounter here the principal drawback of the moment method. It can describe the energy dependence of the density only within the first few standard deviations of the centroid. Although the density falls about four orders of magnitude from its centroid value in this range, we can see from the figure that the error is still extremely large. Similar results, using up to 18 moments, have been reported recently by Jacquemin and Kataria (15). We thus cannot hope to solve the problem by simply extending the expansion to include higher moments.

#### 3.2 TRANSITION STRENGTH DENSITIES

We have also applied the moment method to the calculation of the average spectroscopic amplitudes to be used in the DWBA calculation of one-step direct reactions. Following TU we assume a Wigner form for the residual interaction and write its reduced matrix elements as

$$\sum_{k} (-1)^{T-1, -T_{k}} \frac{5^{L_{k}-L_{k}-\ell}}{\sqrt{4\pi}} (\hat{k}, \hat{j}, \hat{s}, \hat{T}, \hat{f}_{k}, \hat{L}^{2}(\ell_{k}, 0, 0) \ell_{k} d\delta)$$

~

$$\times W(1_n I_n 1_c I_c; Ie) \begin{cases} l & s & s \\ e & o & l \\ l & s & 1 \end{cases} \beta_l d_l$$

We use a single form factor f(r), proportional to the radial derivative of the optical potential, for all angular momentum transfers and all excitation energies.

As we will look only at the one-step excitation from the ground state, we write the spectroscopic amplitudes as

$$d_{l}^{BC} = d_{l}^{BO} = d_{l}^{B}$$

To be consistent with the statistical hypotheses discussed earlier, we must have



The total one-step angular distribution will then take the form

$$\frac{d\tau''}{dr} (E_x, \mathcal{R}) dE_x = \sum_{L} \beta_L^2 \left( \frac{d\tau}{dL} \right)^2 \frac{d\tau}{dr} (E_x, \mathcal{R})$$

As a single application of the residual interaction will only excite one particle one hole states,

$$|B\rangle = |\Sigma_{P} + \varepsilon_{n}| (1/1-1) Cm\rangle$$

the necessary squared spectroscopic amplitudes are simply

$$\left( d_{L}^{L} \right)^{2} = \left| \left( \int_{P} ||_{j}^{L} Y_{L} || \int_{n} ||_{2}^{2} \right)^{2} \\ = \frac{1}{4\pi} \hat{\ell}_{s}^{2} \hat{\ell}_{s}^{2} \hat{\ell}_{s}^{2} \hat{\ell}_{s}^{2} \left( \begin{pmatrix} L, L, L \\ 0 & 0 \end{pmatrix}^{2} W(\ell_{s}), \ell_{n}) \right|^{2} \right|^{2}$$

In general, to calculate moments of the distribution of spectroscopic amplitudes, we would start with a partition function

$$Z(p,r;p',r') = Tr[OF_{e}(p,r)O^{\dagger}F_{e}(p',r')]$$

where  $F_{\alpha}$  is the one body density operator described earlier and  $\eth$  is the appropriate transition operator. The function 2 now has two pairs of arguments, referring to the initial and final states respectively. For arbitrary configurations, the calculation of such a partition function is an extremely difficult problem. Fortunately, it simplifies considerably in the case of interest mere. Because we specify the angular momentum transferred and the initial state, the number of arguments reduces to one.

$$Z_{k}(p) = T_{r} \left[ \mathcal{O}_{k} F_{o}(p) \mathcal{O}_{k}^{\dagger} \right]$$

We can then calculate the moments as before.

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We have used the moment method to calculate the density of spectroscopic amplitudes in <sup>56</sup>Ni. The same set of single particle states, shown in Figure 4, were used for protons and neutrons. The resulting one particle one hole spectrum and the allowed angular momentum transfers are also shown there. We note that, because of the Wigner form assumed for the residual interaction, only natural parity transitions are possible.

We have used the resulting spectroscopic densities to calculate the energy-angular distributions for <sup>56</sup> Fe at 14.6 and 25.7 MeV. We introduced two free parameters,  $\beta_{+}^{2}$  and  $\beta_{-}^{2}$ , which multiplied the contributions to the angular distribution of even and odd transferred angular momenta, respectively. These were adjusted to obtain the best fit to the data at 25.7 MeV (16). The strength density so obtained ( $\beta_{T}^{2}$ times the spectroscopic density) can be seen in Figure 5.

The fit to the 25.7 MeV data can be seen in Figure 6. In Figure 7, we show the results obtained at 14.7 MeV, where the same parameters,  $\beta_{\pm}^{A}$  and  $\beta_{\pm}^{A}$ , have been used but an isotropic Hauser-Feshbach component has been added at the higher energy losses. We see that the resulting fits are not at all good. Comparing the results at the two energies however, we find the poorness of fit, at a given excitation energy, to be about the same for the two. A look at the combinatorial spectroscopic distribution suggests that it could better reproduce the experimental cross sections. The moment method has failed here because it cannot reproduce the structure of the combinatorial density but only its global trend.

We thus conclude that the moment method will not provide an immediate solution to the problem of precision in level and transition strength densities. The combinatorial method could provide the necessary precision for simple configurations or at low energy. In some cases, such as that of the one particle one hole transition strength, even more precise methods could be warranted (6,18). Such methods cannot offer a complete solution to the problem however. They are too time consuming to be practical for the calculation of densities involving complex configurations. We believe that the moment method could still provide a partial solution in these cases (19). It will be necessary though to supplement it with other approximate expressions in order to describe these densities over the entire energy range.

#### 4.0 CONCLUSIONS

We have given statistical hypotheses on the interaction matrix elements which define a multi-step direct multi-step compound pre-equilibrium model. The model specifies the average optical potentials, Green's functions, wave functions and cross sections in terms of the average matrix elements. The resulting cross sections have the multi-step direct component of TU and a multi-step compound component similar to that of AWM. As it stands, the model is too complex to be useful for practical calculations but it can furnish a context within which more approximate models could be understood and evaluated.

The most important quantities which enter pre-equilibrium calculations are the average matrix elements and the level densities or, alternatively, the transition strength densities. We have studied the possibility of using the moment method as a means of efficiently parametrizing these and found it to be generally unsuccessful. The method does not succeed in reproducing the structure observed in densities involving simple configurations and, for more complex ones, can describe the densities only near their energy centroids. We have not completely discarded the method however but continue to look for some combination of methods (combinatorial, moment and others) which could provide a good approximation to the necessary densities.

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Fig. 1 Comparison of the density of 4 particle 2 hole levels of spin 0 in <sup>42</sup>2r calculated using the combinatorial method (histogram) and the moment method (smooth curve).



Fig. 2 Comparison of the density of 4 particle 2 hole levels of spin 10 in <sup>92</sup>Zr calculated using the combinatorial method (histogram) and the moment method (smooth curve).



Fig. 3 Comparison of the density of all 5 particle 3 hole levels in <sup>f1</sup>Zr calculated using the combinatorial method (histogram) and the moment method (smooth curve).



Fig. 4 Neutron (and proton) single particle levels used for  $\pi$ Ni, the resulting 1 particle 1 hole spectrum and possible transferred angular momenta.

Fig. 5 Transition strength densities obtained for <sup>5</sup> Fe based on the moment method spectroscopic amplitude distribution of <sup>56</sup>Ni.



Fig. 6 Comparison of the calculated one-step DWBA angular distributions to the experimental data at 25.7 MeV (ref. 16).



Fig. 7 Comparison of the calculated one-step DWBA angular distributions to the experimental data at 14.6 MeV (ref. 17).

# SESSION

# EXITON, HYBRID, UNIFIED PRE-EQUILIBRIUM MODELS

Count of p-h configurations by combinatorial method in the frame of BCS theory

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#### Abstract

A microscopic approach is described for the calculation of exciton level densities based on combinatorial method for the determination of the various configurations generated according to a given shell model spectrum of single particle levels. The total configuration energies are determined in the frame of BCS theory.

The method allows for the spin and parity distribution and can be used indifferently both for spherical and deformed nuclei.

We confine ourselves mainly to the results for aluminium to be used in preequilibrium calculations.

#### Introduction

47

The main deficiencies of usually adopted exciton level density formulae are known. They mainly depend on the underlying statistical assumptions which fail in particular at lower excitation energies and exciton numbers. In order to avoid this type of difficulty we included the details of the nuclear structure using a microscopic approach.

Accordingly in this paper we describe an attempt to deal with our problem in terms of combinatorial calculations applied to a shell model basis of single particle states. The total configuration energy being estimated in the frame of the BCS theory. The model

We used combinatorial calculations to determine the number of configurations which can be generated at a given excitation energy starting from a given shell model spectrum of single particle sates (sps). In order to account for the pairing interaction BCS theory was used.

The great flexibility of the method allowed us to determine for fixed exciton numbers of both neutron and proton type, the exciton level density, the distribution of levels according to the spin projection and the parity distribution.

For spherical nuclei we used shell model single particle levels (spl) and for deformed nuclei we used Nilsson model sps.

The pairing force was introduced as a residual interaction in the frame of the BCS with use of the blocking method.

To determine the parameter G of the pairing interaction strength, we iterated over the solution of the BCS equations for the state with the lowest energy until a G-value reproducing the experimental pairing energies as given in /1/ was found.

We treated protons and neutrons separately and assumed no interaction between neutron and proton gasses.

The method adopted is the same already illustrated in ref. 1, where we investigated the dependence on energy and exciton number of the spin cut-off parameter. In this paper we want to show that the method is useful also to investigate pairing effect for even and odd systems and parity distributions.

In what it follows we indicate the configuration type with 4 digits corresponding to p-h configurations for neutrons and protons respectively.

More details will be found in refs. 2, 3 and 4.

#### Results and discussion

Deformation effects. Calculations using shell model approach without BCS are shown in fig. 1. As one can see, the gaps in shell model sps spectrum are propagated to the energy behaviour of the density of exciton states and to that of the spin cut-off parameter, giving place to fluctuations characterized by large deeps more pronounced at lower exciton numbers and at lower excitations. This typical nuclear structure effect cannot be accounted for in the frame of the usual statistical approaches like the Williams' formula /6/.

For a deformed nucleus it is more appropriate to use (sps) according to Nilsson model. The effect of deformation is to remove degeneracies in spl producing in the state density a more uniform distribution as one can see in fig. 1.

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Use of sps instead of spl has consequences also on the minimum configuration energy. Since the effect of introducing deformation is to split spl, thresholds are generally lowered as shown in fig. 2.

Obviously, similar consequences are observed also in the behaviour of the spin cut-off parameter, see fig. 3

<u>Pairing effects.</u> One result of introducing the pairing interaction is to decrease the total configuration energy. The difference between the total energy of a system of free nucleons and the energy calculated with the pairing interaction is called the condensation energy.

For a given configuration type in even systems, the condensation energy has its maximum value for the groud state and decreases for excited states.

One consequence of this property is that the excitation energy of an even system with the pairing interaction will always be greater than that of the system without.

For an odd system this is not always true. It is possible that the condensation energy for the ground state be lower than that of an excited one. This can occur when the unpaired nucleon blocks an orbital important for the pairing correlation. Thus the excitation energy of an odd system with inclusion of the pairing interaction E(BCS), can be lower than that without pairing E, making the difference E(BCS)-E negative.

An example of the spectrum of the energy shifts for an odd system can be seen in fig. 4, where one can note both positive and negative energy shifts. On the contrary, in the lower part of fig. 4 we see an example of an even system, where only positive shifts are possible.

Since the effect of the pairing interaction is to shift the energy spectrum of the state density a first possible consequence is to change the configuration thresholds, as shown in fig. 5.

In addition the shifts in the spectrum which result from the pairing interaction can change the location and the size of the gaps changing the fluctuations in the state density see fig. 5.

All the mentioned consequences of the inclusion of the pairing interaction are also observed in the spin cut-off as shown in fig. 6. In particular, the trend of the spin cutoff parameter with energy generally fluctuates about a more or less costant value, see fig. 7. Fluctuations become more pronounced at lower excitation energy and for configurations with lower exciton numbers as it is clearly seen from the comparison of figs. 6 and 7.

For lighter nuclei and lower configurations it is not easy to establish a general behaviour for the spin cut-off with excitation energy. We note however that at high excitation energy, the spin cut-off increases with energy. This happens because the single particle states with higher spins are becoming available with increasing E. At sufficiently high energies the spin cut-off tends to a costant value that depends on the nucleus and on the exciton configuration.

<u>Parity distribution.</u> The method adopted allows for the determination of the parity distribution as well. In fig. 8 one can see the parity distribution using the sps from ref. 9 and BCS theory.

We note that, as expected from statistical considerations, the nuclear states tend to be equally distributed between the two parities at higher excitation energies and for configurations with higher exciton numbers. However, at lower excitation energies and for configurations with low exciton numbers the nuclear structure greatly influences the parity distribution inducing strong fluctuations, which are more pronounced for lighter nuclei as can be seen in fig. 8.

#### Conclusions

On a theoretical basis substantial differences are expected between the results of Williams' formulation and our combinatorial calculations. The effect of the nuclear structure typical of a sps spectrum cannot be accounted for by any statistical approach. Such an effect can be very dramatic for configurations with lower exciton number. For instance in fig. 5, for 1 exciton configuration, Williams' formula yields a constant level density given by the sps density g=2/13 /7/.

Also the gaps present in our microscopic calculations are not reproduced by Williams' formula.

Another severe difficulty in using Williams' approach comes from the necessity of introducing the appropriate ndependent excitation energy threshold i.e. the minimum energy needed to excite a given n-exciton configuration. In terms of our approach the latter is automatically given as the sum of the shell gap and the pairing gap.

In addition our calculations, soon above threshold, exhibit a sharp increase with energy, while according to Williams' formula the level density curve rise up more slowly, see fig. 9.

A draw back is that our calculations appear to be very sensitive to the adopted shell model basis. This implies detailed analyses of the nuclear structure properties in order to determine the best sps spectrum. As an example, using Seeger and Howard /8/ or Nix-Moller /9/ the structure can be very different with deeps remarkably displaced from one to another, see fig. 10

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Fig.l State densities for lp-lh neutron configurations in 170Er calculated without pairing in the space of sps by ref. 8.



Fig.2 State sensity for lp-lh proton configurations in 49Ti calculated without pairing in the space of spherical (upper part) and deformed (lower part) shell-model sps.



Fig.3 Spin cut-off parameter for 1p-1h neutron states in 170Er calculated in the space of spherical (upper part) and deformed (lower part) shell-model sps.



Fig.4 Spectra and energy shifts induced by pairing interaction in the excitation energy of the states for 2p-lh proton and lp-lh neutron configurations in 27A1.



Fig.5 State densities for 1p-0h proton and 1p-1h neutron configurations in 27Al calculated with and without pairing interaction taken into account.

Fig.6 Spin cut-off parameter for lp-lh neutron states in 27Al calculated with and without pairing interaction taken into account.



Fig.7 Spin cut-off parameter for lp-lh neutron as well as for lp-lh neutron and lp-lh proton configurations in 56Fe, calculated in the space of spherical shell model orbitals. Solid hystograms represent calculations with pairing interaction taken into account. The dashed hystograms represent calculations without pairing, shifted to make thresholds of both curves to coincide.



Fig.8 The fraction of states with positive parity calculated for 1p-1h neutron configurations in 170Er and 27A1.



Fig.9 The ratio of the lp-lh neutron configuration state densities in 27Al to the 2p-lh neutron configuration densities in 28Al calculated in the space of sps by ref. 8 (dashed-dotted hystogram) and ref. 9 (solid hystogram). The dashed line represents the prediction from Williams' formula.



Fig.10 State densities for 2p-2h neutron configurations in 48Ti as well as 2p-2h neutron and 2p-2h proton configurations in 58Ni calculated in the space of spherical shell model sps compared with the predictions of the formula by Williams. Single particle state density parameter g and energy shift S, used in the formula are indicated in the figure.

# Single Particle Effects in Precompound Decay Reactions

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# 1. Introduction

Precompound decay models generally rely on use of a partial state density (PSD) formula which is generated using an assumed equidistantly spaced set of single particle levels. We expect this to be a reasonable assumption for mid-shell nuclei; however it has been demonstrated <sup>1,2</sup> that quite large errors may be introduced by making the equidistant spacing assumption for nuclei which have neutron or proton numbers near or at major shell closures. In this work we wish to review the simple qualitative considerations of those deviations expected for near closed shell nuclei, compare these expectations with experimental results, and then begin steps to implement use of partial state densities calculated with more realistic sets of single particle levels in precompound decay calculations. We will do this for the case of Zr targets.

# 2. Qualitative Considerations

A (p,n) precompound reaction should result primarily from neutron emission from a three quasiparticle configuration characterized by a pnn<sup>-1</sup> description, leaving a residual nucleus of pn<sup>-1</sup> character. Consider the shell model representation of the target nuclei 90.91.92.94 Zr in Figure 1. where the neutron levels are represented<sup>3</sup>. Consider a (p,n) reaction on these targets. In the case of <sup>90</sup>Zr, any one of ten  $(g_{9/2})$  neutrons may be ejected to give a ground state product. For slightly more energy, 8 neutrons  $(P_{1/2}, f_{5/2})$  may be ejected. We therefore expect the precompound  ${}^{90}Zr(p,n)$  spectra to start with a large ground state cross section, and continue to higher residual excitations with high cross sections.

54

For the <sup>91</sup>Zr(p,n) reaction, we can only populate the ground state if the single  $d_{5/2}$  neutron is ejected. If this is not the case, there is a 4 MeV gap in order to eject one of the ten  $g_{g/2}$  neutrons. We could therefore expect a small ground state peak, a large gap, followed by a spectrum which otherwise resembled that of <sup>90</sup>Zr(p,n).

For  $^{92,94}Zr(p,n)$  we would expect larger ground state transitions than for  $^{91}Zr(p,n)$ . Because nuclear deformation should increase with increasing neutron number, we might expect the 4 MeV gap to decrease for the heavier target isotopes.

In Figure 2 we show experimental (p,n) spectra from these four target isotopes compared with geometry dependent hybrid model calculations<sup>4</sup>. The qualitative expectations discussed above are observed, and it is seen that the GDH model precompound calculations with equidistant level spacings (ESM) are unable to reproduce the nuclear structure effects noted. This is not the case for mid-shell nuclei, as is shown in Figure 3. We therefore wish to replace the ESM densities with values calculated using shell model single particle orbitals. The method used to do this was by use of recursion relationships, as originally programmed by Williams, and later modified by Albrecht and by Grimes.<sup>1,2,5,6</sup> A brief description of the method used is given below, much quoted directly from (3).

## 3. Calculation of Few Quasiparticle Densities

The few exciton state densities  $\omega(Q,N)$  for N similar fermions above the Fermi energy with a total excitation energy Q are calculated from a set of single particle energies  $c = E_i - E_F$  measured with respect to the target Fermi energy<sup>2</sup>  $E_F$  using the recursion relation<sup>1</sup>

$$\omega_{i}(Q,N) = \omega_{i-1}(Q,N) + \omega_{i-1}(Q-c_{i},N-1).$$
(1)

The recursion index i refers to the ith single particle energy. The state density  $\omega(U,N_{\rm H})$  for  $N_{\rm H}$  holes that share the excitation energy U can be similarly calculated. The recursion converges rapidly. Results are then folded to give the particle-hole state density  $\omega(Q,N,N_{\rm H})$ :

$$\omega(Q,N,N_{H}) = \sum_{\substack{V=0}}^{Q} \omega(U,N)\omega(Q-U,N_{H}).$$
(2)

If both kinds of nucleons share the excitation energy  $E^*$ , an equivalent calculation based on the corresponding set of single particle levels gives  $\omega(0, 2, Z_{\rm H})$ . Folding of both results yields the final partial state density,

These densities are defined by energy only; no information is maintained on the angular momentum distribution; this is one possible shortcoming of the present approach. Work by Reffo and his collaborators offers the possibility to remedy this situation.

The subroutines used presently allow a choice of any of three sets of internally generated single particle levels, or the option of reading in an arbitrary set of levels. The internally generated single particle sets are those due to Nilsson, <sup>7</sup> Seeger-Howard<sup>8</sup> and Seeger-Perisho.<sup>9</sup> A BCS pairing treatment is used, <sup>10</sup> and the nuclear deformation is an input parameter. For pairing in this work we use  $\delta = 11/\sqrt{A}$ , unless otherwise noted. The final state densities are averaged over a Gaussian averaging function which approximates various causes of level broadening, as well as facilitating comparisons with data which are broadened due to experimental resolution.

# 4. Implementation of Few Quasiparticle Densities into Code ALICE

Figure 2 shows that the contribution of the 3 quasiparticle decay dominates the high kinetic energy region of the spectra. We therefore will use 'realistic' partial state densities only for the two and three quasiparticle configurations in our hybrid model precompound decay calculation, using the equidistant spacing model for higher order terms.

Before proceeding further, let us summarize some of the difficulties in the calculation:

 The calculation considers only the energies of the single particle levels: however, each residual interaction and coupling of the angular momenta of unpaired particles should yield different level energies rather than the degenerate results assumed in our codes.

7

- 2. The targets used, due to being closed shell or near closed shell in nature, involve single particle orbitals which may have very large ranges of angular momenta to which they may couple. The reaction kinematics may strongly select against population of some of these levels due to the kinematically allowed orbital angular momentum transfers. These restrictions are not considered (as yet) in our codes for generating few quasiparticle densities.
- Positions calculated for excited single particle levels will be even more sensitive to details of the shape of the assumed potential well than for lower lying orbitals.
- 4. As particle orbitals become unbound, the shell model levels become questionable in meaning; the centrifugal barrier, and for protons the Coulomb barrier may mitigate this point for a few MeV. (for 90,91,92,94 Nb, the proton binding energies are 5.2, 5.8, 6.0, and 6.8 MeV, respectively.)
- As the single particle energies increase the lifetime decreases, and the natural width due to the Heisenberg principle increases.

Similarly, the spreading width will change. We might therefore expect that the constant averaging width of our calculation might better be replaced by an energy dependent function.

With these caveats in mind, our first goal is to get some improvement over results using ESM. We may then concentrate attention on improving the treatment of the partial state densities for some of the objections noted above.

For neutron induced reactions we compute the following PSD tables:  $nnn^{-1}$ ,  $npp^{-1}$ ,  $nn^{-1}$ ,  $pp^{-1}$ , and  $np^{-1}$ . For proton induced reactions we compute  $ppp^{-1}$ ,  $pnn^{-1}$ ,  $pp^{-1}$ ,  $pn^{-1}$ , and  $nn^{-1}$ . These results are calculated for excitation energies up to 20 MeV. Above that energy the 'values at 20 MeV are extrapolated using the ESM energy dependence for each exciton number. The expressions used for the decay of the three quasiparticle states are given by the following:

for n,n'

$$\frac{d\sigma}{dE} = \sigma_{R} \left[ \frac{0.5\rho(nn^{-1}U)}{\rho(n^{2}n^{-1}E)} + \frac{0.75\rho(pp^{-1}U)}{\rho(pnp^{-1}E)} \right] \left[ \frac{\lambda_{c}(E)}{\lambda_{c}(E) + \lambda_{c}(E)} \right]$$

where the second set of square brackets represents the fraction of the nucleons at energy c which are emitted;

for (n,p), we use

$$\frac{d\sigma}{dE} = a_{R}\left[\frac{0.75\rho(np^{-1}U)}{\rho(pp_{h}^{-1}E)}\right]\left[\frac{\lambda_{c}(E)}{\lambda_{c}(E)+\lambda(E)}\right]$$

for (p,n) we use

$$\frac{d\sigma}{dE} = \sigma_{R} \left[ \frac{0.75\rho(pn^{-1}U)}{\rho(pn^{-1}n,E)} \right] \left[ \frac{\lambda_{c}(E)}{\lambda_{c}(E) + \lambda_{c}(E)} \right]$$

.56 and for p,p',

 $\frac{d\alpha}{d\xi} = \sigma_{\mathsf{R}} \left[ \frac{0.75\rho(\mathsf{nn}^{-1},\mathsf{U})}{\rho(\mathsf{pp}^{-1}\mathsf{n},\xi)} + \frac{0.5\rho(\mathsf{pp}^{-1},\mathsf{U})}{\rho(\mathsf{p}^{2}\rho^{-1},\xi)} \right] \left[ \frac{\lambda_{\mathsf{c}}(\xi)}{\lambda_{\mathsf{c}}(\xi) + \lambda(\xi)} \right]$ 

## 5. Results and Discussion

We present results of these calculations using single particle sets due to Seeger-Howard<sup>8</sup> and to Seeger-Perisho<sup>9</sup> in figures 3-13. Several values of the nuclear deformation parameter between 0 and 0.2 have been used to illustrate the sensitivity of results to this parameter.

We find some success in reproducing the structure effects on precompound spectra. The overall quality of fit is probably superior to the results of using ESM in Figure 2: The precompound routine in ALICE<sup>11</sup> has been revised to generate and use realistic partial state densities for the leading (3 exciton) term.

There is great room for improvement of these results. One goal for the future is an improved set of single particle levels. A candidate to be tried is a recent set due to P. Moller.<sup>12</sup> A next step would be use of PSD results with explicit dependence on angular momentum.<sup>13</sup> Finally, we must give consideration to using known low lying excited states to overcome the inevitable inability to predict these levels accurately via Nilsson type calculations.

Much work remains to be done in this area. We feel that these preliminary results are encouraging, and that further work is justified.

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10<sup>2</sup> 25 MeV ℓp, xn} <sup>90</sup> Zr 18 MeV 10<sup>1</sup> 10<sup>2</sup> <sup>91</sup>Zr 10<sup>1</sup> 100 do/de {mb/MeV} 10<sup>2</sup> WĄ. <sup>92</sup>Zr 101 10<sup>0</sup> 10<sup>2</sup> <sup>94</sup> Zr 10<sup>1</sup> 10<sup>0</sup> 10-6 22 10 18 14 6 10 14 18 Neutron energy (MeV)

Figure 1: Schematic single particle level schemes for several stable Zr isptopes based on the levels due to Seeger and Howard (Ref. 8). Occupation of the 2d<sub>5/2</sub> levels by neutrons is indicated by closed circles; level splitting due to several deformation parameters 4 is shown. figure 2: Calculated and experimental (p,xn) spectra for proton energies of 18 and 25 MeV on targets of 90,91,92,94 Zr. Solid points represent the experimental angle integrated data corrected for background and for isotopic impurities. The solid curves are results of the geometry dependent hybrid model plus evaporation model calculations. The dotted curves are the contribution of the first  $(n_0-3)$  exciton number to the total calculated neutron spectra. Arrows represent end point energies. Data are from Ref. 3.





Figure 3: Calculated and experimental results for <sup>159</sup>Tb(p,n). The solid curve is the (lþ)(ln)<sup>-1</sup> two quasiparticle density for <sup>159</sup>Dy with a=0.31 plotted as levels per 100 keV. Open points joined by line segments are the experimental angle integrated spectrum for 25 MeV proton energy. The dashed curve is the result of the geometry dependent hybrid model (GDH). The GDH and experimental results are plotted as mb/MeV vs. residual excitation. Data are from Ref. 3: Figures 4-14: The heavy dots connected by a line represent the experimentally measured angle integrated (p,n) spectra on 90,91,92,94 Zr with 25 MeV incident protons.<sup>3</sup> The dotted lines represent the spectra calculated as described in the text, using single particle levels due to Seeger and Howard (S-H) or Seeger and Perisho (S-P), with deformation parameter  $\delta$  as indicated.



FIGURE 4.







61

# EFFECTS OF ANGULAR-MOMENTUM CONSERVATION IN

### UNIFIED PRE-EQUILIBRIUM AND EQUILIBRIUM REACTION MODELS

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# ABSTRACT

The master-equation theory of precompound and compound nuclear decay is generalized to the inclusion of the conservation of angular momentum. It is demonstrated that the constructed model contains the Hauser-Feshbach, Weisskopf-Ewing as well as standard exciton models as limiting cases. This unified pre-equilibrium/Hauser-Feshbach model, which may be considered as a practicable version of the quantum-statistical, so-called AWM theory of Agassi et al., has been computationally optimized, such that the related numerical effort has become comparable to or less than that of a standard Hauser-Feshbach calculation. With this unified model the nature and importance of some spin effects in pre-equilibrium reactions has been investigated. The main conclusion from numerical calculations is that the standard precompound-model results are close to those of the angular-momentum conserving model, implying that the popular semi-classical models are quite reliable in this respect from a practical point of view.

# 1. INTRODUCTION

Semi-phenomenological models for pre-equilibrium decay, notably the exciton and hybrid models, are globally successful in predicting emission cross-sections and spectra at bombarding energies above about 10 MeV [1,2]. These models do not consider, however, the spin and parity conservation laws and disregard information conerning angular momentum altogether. In this respect their status is similar to that of the Weisskopf-

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Ewing model, rather than to the Hauser-Feshbach model. There exist more basic quantum-statistical theories of precompound reactions [3-6] to which the above comments do not apply, but these are hardly amenable for practical use. An exception is the multi-step model of Feshbach et al. [4], but even this model is quite complicated, whereby for practical application it has to adopt several additional simplifications.

A common procedure for applied purposes is to introduce a separate (phenomenological) pre-equilibrium correction into Hauser-Feshbach model codes. It has been pointed out [7] that such an approach is ad hoc and will lead to inconsistencies. A similar remark applies to the model of Fu [8], who proposed to use the spin population of exciton states at equilibrium also for the pre-equilibrium region.

It is therefore not surprizing that not very much is known about the nature and importance of spin effects in pre-equilibrium reactions. It is certainly of interest to investigate this problem, if only to gain some insight into the reliability of existing pre-equilibrium models in this regard. Furthermore, knowledge about the spin population of exciton states during equilibration is needed in considering the de-excitation to discrete levels.

The present paper is an attempt to address the question of the introduction and the assessment of angular-momentum effects in pre-equilibrium reaction models. In addition to the results of quantum-theoretical studies [3,4], it builds upon earlier, partial, investigations by Reffo et al. [9,10] and preliminary studies by Gruppelaar et al. [7,11] and Fu [8,12]. Some of the results presented here have been reported in a letter [13].

Section 2 of this paper develops our model for unified pre-equilibrium and equilibrium reaction calculations with conservation of angular momentum. The framework chosen is that of the master-equation approach [3,14], within which it is shown that a unified pre-equilibrium/Hauser-Feshbach model can be constructed. In Sec. 3 it is proved that this unified model contains the Hauser-Feshbach, Weisskopf-Ewing as well as the standard exciton models as limiting cases. Section 4 outlines the computational procedures, which have been designed such that the model is easy and practical to use (the computational effort being not greater or even less than that of a normal Hauser-Feshbach calculation) and it still satisfies a set of consistency rules discussed in the earlier part of the paper. Numerical results and their physical interpretation are the subject of Sec. 5. Section 6 summarizes our conclusions concerning the effects of angularmomentum conservation in precompound decay.

### 2. THE SPIN-DEPENDENT MASTER EQUATION AND ITS SOLUTION

The different versions of the pre-equilibrium exciton model [1,2] can all be derived from a Pauli master equation describing the temporal evolution of the occupation probabilities q(n,t) of the nuclear exciton states n. The master equation of the standard exciton model reads [14]:

$$dq(n,t)/dt = \lambda_{+}(n-2)q(n-2,t)+\lambda_{-}(n+2)q(n+2,t)-[\lambda_{+}(n)+\lambda_{-}(n)+W_{t}(n)]q(n,t),$$
(1)

where  $\lambda_{\pm}(n)$  and  $W_{\pm}(n)$  are the internal transition and total emission rates. Average emission cross-sections are calculated from:

$$\frac{d\sigma}{d\varepsilon}(a,b) = \sigma_a \sum_n^{\Sigma} W_b(n,\varepsilon)\tau(n).$$
<sup>(2)</sup>

Here, a and b stand for the projectile and ejectile and  $\sigma_a$  is the total composite-formation cross section. The mean lifetimes  $\tau(n) = \int_{0}^{0} q(n,t) dt$  are obtained from Eq.(1) integrated over time [3]:

$$-q(n,t=0) = \lambda_{+}(n-2)\tau(n-2)+\lambda_{-}(n+2)\tau(n+2)-[\lambda_{+}(n)+\lambda_{-}(n)+W_{+}(n)]\tau(n), \quad (3)$$

for which exact analytical solutions [15] and very fast computational schemes [16] exist. We note that the above formula yields both the preequilibrium and equilibrium contributions to the nuclear reaction. Agassi et al. [3] and Bunakov [17] have developed a quantum-mechanical foundation with regard to the above (phenomenological) master-equation approach to precompound decay, by connecting it with a microscopic random-matrix model of the nuclear Hamiltonian [3] and by considering the nucleus as a finite open system [17]. Below we set out to generalize the master-equation approach to the conservation of angular momentum. First, we observe that during the equilibration process of the composite nucleus the transitions within the system may not change the spin J and parity  $\mathbb{N}$  of the composite nucleus. Since it is this process that is described by the master equation, it is obvious that the generalization of the master equation to spin effects is obtained by simply subjoining indices J and N to the above equations.

Thus, the angular-momentum conserving precompound model is expressed by:

$$dq^{J\Pi}(n,t)/dt = \lambda_{+}^{J\Pi}(n-2)q^{J\Pi}(n-2,t) + \lambda_{-}^{J\Pi}(n+2)q^{J\Pi}(n+2,t)$$
$$-[\lambda_{+}^{J\Pi}(n) + \lambda_{-}^{J\Pi}(n) + W_{t}^{J\Pi}(n)]q^{J\Pi}(n,t), \qquad (4)$$

whence one obtains from integration over time:

$$-q^{J\Pi}(n,t=0) = \lambda_{+}^{J\Pi}(n-2)\tau^{J\Pi}(n-2) + \lambda_{-}^{J\Pi}(n+2)\tau^{J\Pi}(n+2) - [\lambda_{+}^{J\Pi}(n) + \lambda_{-}^{J\Pi}(n) + W_{t}^{J\Pi}(n)]\tau^{J\Pi}(n), \qquad (5)$$

and the average emission cross-sections are given by:

$$\frac{d\sigma}{d\epsilon}(\mathbf{a},\mathbf{b}) = \sigma_{\mathbf{a}} \sum_{J\Pi} \sum_{n} W_{\mathbf{b}}^{J\Pi}(\mathbf{n},\epsilon) \tau^{J\Pi}(\mathbf{n}), \qquad (6)$$
with  $\sigma_{\mathbf{a}} = \sum_{J\Pi} \sigma_{\mathbf{a}}^{J\Pi}$ .

Next, one needs to know the emission and internal transition rates as a function of J and  $\Pi$ . The emission rates can be written as:

$$W_{\mathbf{b}}^{\mathbf{J}\Pi}(\mathbf{n},\boldsymbol{\epsilon}) = \frac{1}{2\pi\hbar} \sum_{\mathbf{l}',\mathbf{l}',\mathbf{j}',\Pi} T_{\boldsymbol{\ell}',\mathbf{j}'}^{\mathbf{b}}(\boldsymbol{\epsilon}) \rho_{\mathbf{b}}(\mathbf{n}-\mathbf{b},\mathbf{l}',\Pi',\mathbf{E}') Q_{\mathbf{b}}(\mathbf{n}) / \rho_{\mathbf{c}}(\mathbf{n},\mathbf{J},\Pi,\mathbf{E}). \quad (7)$$

Here,  $\rho_b$  and  $\rho_c$  indicate the residual and composite nuclear-level densities. T designates the transmission coefficient, I' and T' denote the spin and parity of the residual nucleus and  $\ell$ ' and j' stand for the orbital angular momentum and the channel spin of the emitted particle b.  $Q_b(n)$  is a factor accounting for the memory of the projectile type by the nuclear system during the pre-equilibrium stages [18]; it is unity at equi-

librium. We remark that in the derivation of Eq. (7) no improper use of detailed balance is implied; an energy average over final states has been introduced, however. The internal transition rates can formally be obtained from Fermi's golden rule:

$$\lambda_{\pm}^{J\Pi}(n) = \frac{2\pi}{\hbar} \langle M_{J\Pi}^2 \rangle \rho_f(n\pm 2, J, \Pi) . \qquad (8)$$

In order to solve Eq. (5) for the mean lifetimes  $\tau^{J\Pi}(n)$  we further need an expression for the initial condition. It is evidently given by:

$$q^{J\Pi}(n,t=0) = \frac{\sigma_{a}^{J\Pi}}{\sigma_{a}} q(n,t=0), \qquad (9)$$

where q(n,t=0) is identical to the initial condition for the standard master equation, being equal to  $\delta_{n,n_0}$  for the first emission.

Equations (4)-(9) constitute a complete master-equation model for compound and precompound decay with conservation of angular momentum. As it stands now, however, it will also be quite involved for practical use, since for each J and R a different set of coupled equations must be solved. Moreover, the angular-momentum structure of the averaged squared matrix element in Eq. (8) is not clear beforehand. Like in Ref. [4], a precise calculation will involve complicated angular-momentum coupling expressions. The discussion of these computational questions will be deferred to Sec. 4, where we will suggest some approximate, time-saving, but still physically plausible procedures.

Finally, we want to point out that the angular-momentum conserving masterequation model as developed here can be rewritten in a form that closely resembles the Hauser-Feshbach formula. Equation (5) is a probability-balance equation, very similar to the one derived in Ref. [3]. Summing it over all exciton states and inserting Eq. (9), it follows that:

$$\sum_{n} W_{t}^{J\Pi}(n) \tau^{J\Pi}(n) = \sigma_{a}^{J\Pi} / \sigma_{a}, \qquad (10)$$

63

64 which is nothing else than the law of probability conservation. As a consequence, the cross-section formula (6) may be written in the equivalent form:

$$\frac{d\sigma}{d\varepsilon} (a,b) = \sum_{J\pi} \sigma_{a}^{J\pi} \frac{\sum_{n} W_{b}^{J\pi}(n,\varepsilon) \tau^{J\pi}(n)}{\sum_{n'} W_{t}^{J\pi}(n') \tau^{J\pi}(n')} .$$
(11)

Upon writing out Eq. (11) with the aid of Eq. (7), we find:

$$\frac{d\sigma}{d\epsilon} (a,b) = \pi \pi^{2} \sum_{J\pi} \frac{(2J+1)}{(2s+1)(2I+1)} \sum_{\ell j} T_{\ell j}^{a}(E) \times \frac{\sum_{I'\ell' j'\pi';n} T_{\ell'j'}^{b}(\epsilon)\rho_{b}(n-b,I',\pi',E')\tau^{J\pi}(n)Q_{b}(n)/\rho_{c}(n,J,\pi,E)}{\sum_{I''\ell''j'\pi';n'b'} \int d\epsilon' T_{\ell''j''}^{b''}(\epsilon')\rho_{b}(n'-b',I'',\pi'',E'')\tau^{J\pi}(n')Q_{b}(n')/\rho_{c}(n',J,\pi,E)}.$$
(12)

Equation (12) is equivalent to Eq. (2). It is seen that this expression for the combined pre-equilibrium and equilibrium emission cros-sections is formally obtained from the usual Hauser-Feshbach expression by the replacement:

$$\rho_{\mathbf{b}}(\mathbf{I}', \mathbf{\pi}', \mathbf{E}') \rightarrow \sum_{\mathbf{n}} \rho_{\mathbf{b}}(\mathbf{n}-\mathbf{b}, \mathbf{I}', \mathbf{\pi}', \mathbf{E}') \tau^{\mathbf{J}\mathbf{\pi}}(\mathbf{n}) Q_{\mathbf{b}}(\mathbf{n}) / \rho_{\mathbf{c}}(\mathbf{n}, \mathbf{J}, \mathbf{\pi}, \mathbf{E}).$$
(13)

Hence, the model constructed in this section may be viewed as a unified precompound/Hauser-Feshbach model. This will be further elucidated in the next section. In addition, the above discussion has made clear that our angular-momentum conserving master-equation model may be interpreted as a practicable version of the AWM theory of Agassi et al. [3].

# 3. THE HAUSER-FESHBACH, WEISSKOPF-EWING AND STANDARD EXCITON MODELS AS LIMITING CASES OF THE UNIFIED MODEL

Pre-equilibrium models are intuitively expected to include the Hauser-Feshbach cross-section, derived from standard statistical compoundnucleus theory, as their equilibrium component. This can transparently be demonstrated for the master-equation model developed in the previous section. At equilibrium the exciton-state occupation probabilities are directly related to the available phase space:

$$q^{J\Pi}(n,eq.) = \frac{\sigma_{a}^{J\Pi}}{\sigma_{a}} \frac{\rho_{c}(n,J,\pi,E)}{\rho_{c}(J,\pi,E)},$$
(14)

with  $\rho_c(J,\Pi,E) = \sum_n \rho_c(n,J,\Pi,E)$ . Eq. (14) also corresponds to the stationary solution of the spin-dependent master equation (4) (with, of course, the emission set equal to zero). Further,  $Q_b(n) = 1$  at equilibrium and the mean lifetimes are taken proportional to Eq. (14). (From an exact standpoint there will be slight numerical deviations, since the Hauser-Feshbach and Weisskopf-Ewing models explain nuclear decay with the presupposition that there is strict equilibrium. This inconsistency is not present in the dynamic master-equation approach: only a quasi-equilibrium can occur in dissipative systems.) Inserting the above equilibrium conditions into the generalized cross-section expression (12), we immediately obtain the usual Hauser-Feshbach formula.

It is well known [19] that the Weisskopf-Ewing model can be derived from the Hauser-Feshbach formula by means of the assumptions:

$$\rho_{\rm b}({\rm I}',{\rm R}',{\rm E}') = (2{\rm I}'+1) \omega_{\rm b}({\rm E}'), \qquad (15.a)$$

 $\boldsymbol{\omega}_{_{\mathbf{h}}}(\mathbf{E}^{\prime})$  denoting the state density, and:

$$T^{b}_{\ell',j}(\varepsilon) = T^{b}_{\ell'}(\varepsilon)$$
, independent of j'. (15.b)

The latter assumption is also often introduced into Hauser-Feshbach calculations through an averaging procedure over j'. The first assumption is less realistic, the level density being described by:

$$\rho_{b}(I',\Pi',E') = \sum_{n} f(n,I') P(\Pi') \omega(n,E'), \qquad (16)$$

where  $\omega(n,E')$  is the particle-hole state density,  $P(\Pi')$  is the parity distribution (assumed to be 1/2 here) and f(n,I') is the spin distribution of exciton levels, given by:

$$f(n,I') = \frac{(2I'+1)}{2\sigma^3(n,E')\sqrt{2\pi'}} \exp\left[-\frac{(I'+1/2)^2}{2\sigma^2(n,E')}\right].$$
 (17)

The spin cut-off parameter, which from the numerical calculations to be presented will turn out to be a crucial parameter, is proportional with n for small n [9]. It is important to point out that in this region the spin cut-off parameter is essentially independent of the energy [9,12]. With increasing exciton number, there will occur a saturation of the value of  $\sigma^2(n,E')$ , cf. [12]. Here, we assume a maximum value equal to the one taken for standard Hauser-Feshbach calculations, i.e.,  $\sigma^2_{eq}(E')$ . Accordingly, we may use for  $\sigma^2(n,E')$  the minimum of:

$$\sigma_{\text{preeq}}^2(n) = \langle m^2 \rangle_n = 0.24 \ A^{2/3}n,$$
 (18.a)

$$\sigma_{eq}^{2}(E') = \langle m^{2} \rangle_{gt}, \qquad (18.b)$$

where g is the single-particle level-density parameter and t is the thermodynamic temperature. This very simple expression satisfies Eq. (16) in good approximation. For more detailed calculations the formulae from the recent study by Fu [12] could be used. Equation (18.b) leads to somewhat higher values than usual, but is consistent with Eq. (18.a) (the current value is probably too small, cf. Ref. [20]).

It follows from Eqs. (16) and (17) that the assumption (15.a) is valid only for very large values of the spin cut-off parameter. Application of the assumptions (15), then, to the angular-momentum conserving model formulae (6) or (12) yields the standard exciton model according to Eq. (2), with  $\tau(n) = \sum \tau^{J\Pi}(n)$ . This elegant relationship between the two models is gratifying, <sup>JII</sup> because it coincides with the one expected beforehand on the basis of fundamental statistical considerations.

65

Thus, the Hauser-Feshbach model as well as the standard exciton model can be viewed as limiting cases of the spin-dependent master-equation model proposed in Sec. 2. A diagram clarifying the relationships between the various models is presented in Fig. 1. We conclude that the proposed model may genuinely be called a unified pre-equilibrium/Hauser-Feshbach model.

#### 4. COMPUTATIONAL PROCEDURES: THE MEAN-LIFETIME ANSATZ

As has already been remarked in Sec. 2, the unified model, as represented by Eqs. (4) to (9), is not yet a really practical one. For each J and I a set of master equations must be solved for  $\tau^{JI}(n)$ , while within each set a collection of transition and emission rates has to be computed, each one on its turn requiring the evaluation of involved angular-momentum coupling functions. As compared to Hauser-Feshbach calculations, we further need to carry out additional summations over exciton states, cf. Eq. (12). This situation is similar to that with respect to the multi-step compound model [4, 21, 22]. Introduction of the never-come-back approximation into Eq. (12) indeed leads to an expression that bears much resemblance to the FKK multi-step compound model; compare also Refs. [6] and [15].

Consequently, one may look for approximative expressions for the mean lifetimes  $\tau^{J\Pi}(n)$  that avoid the computational difficulties indicated above. As a physically plausible and numerically very convenient approximation we suggest the following mean-lifetime Ansatz:

$$\tau^{J\Pi}(n) \stackrel{\sim}{=} \frac{\sigma_{a}^{J\Pi}}{\sigma_{a}} \quad \frac{W_{t}(n)}{W_{t}^{J\Pi}(n)} \tau(n), \qquad (19)$$

where  $W_t(n)\tau(n)$  is computed from the standard exciton model, Eq. (3). Expression (19) may be made plausible as follows. The exciton state  $n = n_0$ , which is mainly responsible for the pre-equilibrium emission, is strongly occupied only when the time t is close to zero. Assuming that the transition and emission rates do not depend strongly on J. Eq. (9) for the initial condition will also approximately hold for  $n = n_0$  at t > 0. Integrating over t we get:

$$\tau^{J\Pi}(n_0) \approx \frac{\sigma_a^{J\Pi}}{\sigma_a} \tau(n_0) , \qquad (20)$$

66

which is close to Eq. (19), due to the rather weak variation of  $W_t^{JR}(n)$ with the spin. Next, we look at the high-n values,  $n \approx \bar{n}$ , which produce the equilibrium part of the emission. In this case Eq. (14) holds, and we add that the ratio  $\rho(n,J,\Pi,E)/\rho(J,\Pi,E)$  is independent of the spin for  $n \approx \bar{n}$ , since for these values of n the spin cut-off factor does no longer depend on the exciton state (see the discussion related to Eq. (18)). This brings us to the conclusion that, for exciton states close to the equilibrium value  $\bar{n}$ , Eq. (19) will be valid. Combination of this observation with Eq.(20), with the probability-conservation property (10) and its spinless equivalent  $\sum W_t(n)\tau(n) = 1$ , yields the approximation (19). It may be further demonstrated that Eq. (19) does not destroy the attractive limiting properties of the unified model as discussed in Sec. 3.

We have checked the correctness of the above Ansatz by directly calculating the J-dependence of the transition and emission rates and, on this basis, of the mean lifetimes. Results are presented in Fig. 2. Figure 2.a demonstrates that the transition and emission rates are indeed only weakly dependent on J. Not shown are the An=-2 rates. At low n their J-dependence is stronger than that of the An=+2 rates, but in this case their influence on the mean lifetimes is negligible, as a result of their being several orders of magnitude smaller. At high n there is essentially no J-dependence both for the An=+2 rates. Figure 2.b compares the calculated results of Eq. (19) (dashed lines) with the full solution of the spindependent master equation (5). It is concluded that the Ansatz (19) represents an excellent approximation to the exact solution for the mean exciton-state lifetimes.

The expression (19) considerably reduces the computational effort related to the unified model as represented by Eq. (12). If we insert Eq. (19) together with the probability-conservation property (10) into Eq. (12), we obtain an expression for the emission cross-sections according to the unified model, that is also the most suitable one for numerical calculations:

$$\frac{d\sigma}{d\varepsilon} (a,b) = \pi x^2 \sum_{J\Pi} \frac{(2J+1)}{(2s+1)(2I+1)} \sum_{\ell j} T^a_{\ell j} (E) \times$$

$$\sum_{n}^{\Sigma} W_{t}(n)\tau(n) \frac{\sum_{\substack{I'\ell' j', \Pi' \\ I''\ell' j'' \Pi''; b'}} T_{\ell'j}^{b}(\epsilon)\rho_{b}(n-b, I', \Pi', E') Q_{b}(n)}{\sum_{\substack{I''\ell'' j'' \Pi''; b'}} f_{d\epsilon'} T_{\ell''j''}^{b'}(\epsilon')\rho_{b}(n-b', I'', \Pi'', E'')Q_{b}(n)}.$$
 (21)

add that the ratio  $\rho(n,J,\Pi,E)/\rho(J,\Pi,E)$  is independent of the spin for  $n \approx \bar{n}$ , since for these values of n the spin cut-off factor does no longer depend on the exciton state (see the discussion related to Eq. (18)). This brings us to the conclusion that, for exciton states close to the equilibrium value  $\bar{n}$ , Eq. (19) will be valid. Combination of this observation with Eq.(20), with the probability-conservation property (10) and its spinless equivalent  $\sum W_t(n)\tau(n) = 1$ , yields the approximation (19). It may be further demonstrated that Eq. (19) does not destroy the attractive limiting properties of the unified model as discussed in Sec. 3.

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fied model, that is also the most suitable one for numerical calculations:

$$\frac{d\sigma}{d\epsilon} (a,b) = \pi \kappa^{2} \sum_{J\pi} \frac{(2J+1)}{(2s+1)(2I+1)} \sum_{\ell j} T_{\ell j}^{a} (E) \times \sum_{n} W_{t}(n)\tau(n) \frac{\sum_{l'\ell',j'\pi'} T_{\ell',j'}^{b}(\epsilon)\rho_{b}(n-b,I',\pi',E')Q_{b}(n)}{\sum_{l'\ell',j'\pi'',b'} \int d\epsilon' T_{\ell',j'}^{b'}(\epsilon')\rho_{b}(n-b',I'',\pi'',E'')Q_{b}(n)}.$$
 (21)

As compared to a standard Hauser-Feshbach calculation, the additional summation over the exciton states cannot be avoided. Nevertheless, it appears possible to strongly speed up some of the spin summations in Eqs. (12) and (21) (as well as in the usual Hauser-Feshbach formula) by means of highly accurate analytical approximations. These are derived by exploiting the factorization properties of the level-density formula (16). Details are found in Ref. [23]. The combined result of the optimizations with respect to the computational procedures, as indicated in this section, is that the computational effort related to the unified model becomes comparable to and in many cases less than that of a normal Hauser-Feshbach calculation.

The above equation (21) has been coded in a programme called UNIMOD. To ensure compatibility between the precompound and Hauser-Feshbach calculations (a feature usually not present in model codes), the Williams particle-hole state density [24] has been renormalized to the backshifted Fermi-gas formula of Dilg et al. [25], as follows [26]:

$$\rho(n, I, \pi, E) = f(n, I) \frac{1}{2} r(U) \omega(n, U), \qquad (22)$$

where  $\omega(n,U)$  denotes the usual Williams formula

$$\omega(n,U) = \frac{g(gU-A(p,h))^{n-1}}{p!h!(n-1)!},$$
(23)

where r(U) is a renormalization factor:

$$\mathbf{r}(\mathbf{U}) = \sqrt{\frac{\pi}{3}} \frac{\mathbf{U}}{\mathbf{a}^{1/4} (\mathbf{U} + \mathbf{t})^{5/4}} .$$
 (24)

After summation over all possible values of n Eq. (22) becomes asymptotically equal to the level-density formula of Dilg et al. [25]. Further details about this renormalization procedure are found in Ref. [26]. We remark that Eq. (16) is obeyed. The symbols used in Eqs. (22) to (24) have their usual meaning, cf. [24,25]: U = E-A (A is the energy shift); a and g are level-density parameters  $(a=\pi^2 g/6)$ ; t is the thermodynamic temperature and A is a Pauli correction.

In the present version of the code the emission probabilities  $W_t(n)\tau(n)$  have to be given as input. These are computed with the GRAPE code [27], that is completely consistent with UNIMOD. The model in GRAPE is based upon Eqs. (1) to (3), whereby instead of the level densities (22) the state densities  $r(U)\omega(n,U)$  are used throughout the code. It has been checked numerically that insertion of Eq. (15) into UNIMOD leads to virtually the same results as those of GRAPE. This also guarantees a sound methodological basis on which the numerical differences between semiclassical and quantum-mechanical models for precompound decay can be evaluated.

## 5. DISCUSSION OF NUMERICAL RESULTS

A number of sample calculations with the unified model presented above has been carried out for neutron-induced reactions on <sup>33</sup>Nb (I=9/2) and <sup>1 e 2</sup>Ru (I=0). One of the angular-momentum effects which cannot be reproduced by the standard pre-equilibrium models might be due to variations in the ground-state spin, cf. also Ref. [11]. For this reason also some calculations were performed with the fictious target-spin values I'=1/2 for <sup>33</sup>Nb and I'=4 for <sup>1 e 2</sup>Ru, keeping all other model parameters the same.

Calculated results for the neutron inelastic scattering spectra according to the unified model (UM) and the semi-classical exciton model (EM) are shown in Figs. 3 and 4. It is seen that the difference between these two models is related to the value of the ground-state spin of the target nucleus. For high target spins the emission spectrum according to the unified model turns out to be very close to that of the exciton model. At low target spin the UM spectrum is slightly softer than the EM one, but the difference is quite small. These observations pertain to the high68

energy end of the spectrum, i.e., the region that is dominated by preequilibrium emission. Calculations show, however, that this situation is reversed for the equilibrium emission region, where the spectrum becomes harder with decreasing target spin. This is brought out more clearly in Fig. 5, where we have plotted the UM results for the initial exciton state (i.e., pure precompound decay) against those according to the Hauser-Feshbach (HF, i.e, pure equilibrium emission) model. We conclude that in considering angular-momentum effects a distinction needs to be made between the precompound and compound decay mechanisms.

The key to physically understand these results is the behaviour of the spin cut-off parameter. In HF calculations  $\sigma^2$  is an increasing function of energy which implies that there are more final states with high spins at low emission energy than at high emission energy. Accordingly, a high target spin leads to increased low-energy and decreased high-energy emission in HF calculations. On the other hand, in UM calculations the value of  $\sigma^2$  in the precompound region is both small and independent of energy, compare the discussion related to Eq. (18). This means that in the case of a high ground-state spin relatively high outgoing orbital angular momenta ( $\ell^2$ ) are needed to excite the low-n states, independent of their energy.

Since transitions with high l' are easier with high outgoing energies, the excitation of low-lying states is favoured. This explains the increased high-energy emission.

It has been confirmed through a numerical analysis that these effects are indeed due to the behaviour of the spin cut-off parameter. In particular, if  $\sigma_{eq}^{i}$  (no n-dependence) is inserted in the UM the target-spin dependence is reversed (like in HF). It is noted that this incorrect assumption has been employed in several, for pre-equilibrium effects corrected, HF codes, cf. [2].

We have further investigated the relative contributions of the incident partial waves with different orbital angular momenta (l) to the equilibrium and pre-equilibrium emission cross-sections. It has been claimed (e.g., [1], [28]) that in pre-equilibrium decay surface reactions contribute significantly as compared to the evaporative stage. This assumption has motivated the development, notably by Blann [28], of so-called geometry-dependent pre-equilibrium models. The unified model presented in this paper is able to give an independent check on the validity of this assertion. Figure 6 presents calculated results for  $10^2 \operatorname{Ru}(n,n'x)$  at incident energies of 14.5 and 30.0 MeV. First, it is shown that with higher incident energy and, accordingly, higher pre-equilibrium emission fractions, the relative contributions of the high orbital angular momenta  $\ell$  increase. Second, it is observed that, for given incident energy, the high- $\ell$  contributions are somewhat enhanced for the pre-equilibrium processes as compared to the equilibrium decay mechanism. At 14.5 MeV the difference between the contributions of the large  $\ell$  waves ( $\ell$ >5) to the two reaction mechanisms is near 4 per cent, whereas it amounts about 10 per cent at 30.0 MeV.

Thus, there is some evidence, especially at higher incident energies, that the pre-equilibrium emissions occur at slightly higher angular-momentum states of the composite nucleus relative to the equilibrium ones. Reformulated in quasi-classical terms this means that surface reactions are somewhat more favoured in the precompound stages. Interestingly, numerical simulations demonstrate that these differences between the compound and precompound mechanisms are, again, essentially due to the behaviour of the spin cut-off parameter as a function of the exciton number and the residual excitation energy. Since the spin cut-off parameter appears to be such a crucial variable, it seems worthwhile to replace the present simple estimates of  $\sigma^2(n,E)$  by more realistic ones.

# 6. CONCLUSIONS

The conservation of angular momentum has been included in a straightforward manner in a master-equation model, that gives a unified description of precompound and compound decay. Efforts have been made to computationally optimize this generalized model, so that it is easy and fast to use for applications, without the need to admit an unfavourable trade-off with respect to the various consistency requirements that can be formulated. The resulting unified model may be considered as a practicable version of the quantum-mechanical AWM theory [3] and contains the standard exciton model as well as the Hauser-Feshbach and Weisskopf-Ewing models as limiting cases. The relationships between the various statistical models have been clarified, see the diagram in Fig. 1.

Sample calculations have been performed for neutron-induced reactions on <sup>33</sup>Nb and <sup>102</sup>Ru in order to evaluate the importance of angular-momentum effects in pre-equilibrium decay. The results show that the spin cut-off parameter of the final states plays a crucial role. As a consequence of the energy independence of this parameter at low exciton numbers it follows that the unified model predicts softer emission spectra for low target spins than the semi-classical precompound models, although the differences are small. Another consequence is that for pre-equilibrium emission the average incoming orbital momentum is somewhat higher than for equilibrium emission.

Further refinements of the unified model are possible, for instance by introducing more realistic expressions for the spin cut-off parameter and the particle-hole level densities, e.g., those proposed by Fu [12,29]. Other possible and quite straightforward improvements are: an extension of the model to excitation of discrete levels, the introduction of Y-ray competition and the inclusion of multi-particle emission. Finally, we mention that it may also be of interest to generalize the model to predict angular distributions. Immediate generalization, using the random-phase approximation, gives the symmetric (multi-step compound) component of the angular distribution, consistent with the predictions of the HF model at equilibrium. To calculate the odd-order Legendre coefficients more involved assumptions are needed, that are beyond the scope of this paper (see e.g. Ref. [2]).

The central conclusion of this paper may be formulated as follows. It goes without saying that quantum-mechanical models for precompound decay [3,4] represent an important conceptual and theoretical improvement over the older, phenomenological ones. The present work has, however, provided evidence that the numerical differences between these models are small, so that in this sense the semi-classical models can be considered reliable. Therefore we expect that these fast and easy-to-use models will continue to play a useful role in applications.

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Fig. 1. Schematic of the relationships between the unified model (UM) proposed in this paper, the Hauser-Feshbach model (HF), the Weisskopf-Ewing model (WE) and the usual exciton model (EM). The arrows denote a mathematical reduction by means of simplifying assumptions, the equation number of which is indicated between parentheses.



<u>Fig. 2.</u> J-dependence of transition and emission rates and mean lifetimes, for the composite nucleus <sup>1+3</sup>Ru at  $E_{exc.}$  =20.6 MeV.

- <u>a.</u> Results for the transition and emission rates. For clarity, a linear scale has been used and  $\lambda_{+}(n=3)$  has been normalized to unity for J=4.5.
- b. Comparison of the mean lifetimes, as exactly calculated from the J-dependent master equation (solid lines), with the approximation according to Eq. (19) (dashed lines).


Fig. 3. Comparison between the unified model (UM) and the exciton model (EM) for the reaction "Nb(n,n'x) at 14.6 MeV. The full curve represents the EM spectrum, the dotted line represents the UM with the target spin  $I^{*}/_{2}$ , and the dashed one corresponds to the UM with a fictitious target spin  $I^{*}_{2}$ .



<u>Fig. 4.</u> Comparison between the UM and the EM for the reaction <sup>1+2</sup>Ru(n,n'x) at 14.5 MeV. The full curve represents the EM spectrum, the dashed line corresponds to the UM with the target spin I=0, and the dotted line (in this case coinciding with the solid one) shows a UM calculation with a fictitious target spin I'=4.



Fig. 5. Comparison between the behaviour of the unified model (UM) and the HF theory for different target spins. The reaction is  $*^{1}Nb(n,n'x)$  at E=14.6 MeV. For the UM only the contribution from the initial exciton state n=3 is given, which means that these curves describe the pure pre-equilibrium emission.



<u>Fig. 6.</u> Ratio of the contributions of the incident partial waves with  $lSL_{\rm M}$  to the all- $\ell$  contributions in the equilibrium and the pre-equilibrium processes as a function of  $L_{\rm M}$ . The reaction is <sup>1+2</sup>Ru(n,n'x) at 14.5 MeV and 30.0 MeV, respectively. The ratio is defined as

$$R(L_{M}) = \frac{L_{M}}{\ell = 0} \frac{d\sigma^{\ell}(E,\varepsilon)}{d\varepsilon} \frac{d\sigma(E,\varepsilon)}{d\varepsilon} .$$

Neutron capture in the frame of the exciton model and total gamma-ray spectra calculations

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Abstract

We realized the necessity of introducing the preequilibrium contribution to the neutron capture process in order to satisfy the need for gamma-ray spectra following neutron induced reactions in the structural material of the fusion technology.

In this paper we describe and discuss the theoretical approach adopted. As an example, gamma-ray spectra calculations are shown for Nb, Co and Al.

Introduction

Gamma-ray spectra following neutron induced reactions are needed for the structural material in fusion technology.

At the typical energies of fusion neutrons the important reaction mechanisms include in particular preequilibrium one in addition to collective capture and compound nucleus processes.

In what it follows we shall deal with the description of the exciton model adopted for the calculation of the preequilibrium contribution to the total capture. The contribution from the different reaction mechanisms will be shortly discussed.

As an example the energy spectrum of total gamma-ray emission following 14.5 MeV neutrons in Al will be illustrated.

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The model

According to refs.1,2,3,4,5,6 the adopted generalized master equation reads

$$\frac{d}{dt} P(E,J,\pi,n,\Omega,t) = \sum_{m=n-2}^{n+2} \lambda_{m \to n}^{J,\pi}(E) \int G(\Omega,\Omega')P(E,J,\pi,m,\Omega',t)d\Omega' + \dots$$
(1)
$$- P(E,J,\pi,n,\Omega,t) \left[ \sum_{a} \int W_{a}^{J,\pi}(E,c_{a},n)dc_{a} + \sum_{a} \lambda_{a}(E) \right]_{m=n-2} \dots \rightarrow m$$

Here  $P(E,J, \pi, n, \Omega, t)$  is the occupation probability at time t of the state characterized by n excitons, spin J, parity  $\pi$ , total excitation energy E and by a leading nucleon in the direction  $\Omega$ .

 $G(\Omega, \Omega') = (d \sigma^F/d\Omega) / \sigma^F$  being  $\sigma^F$  the free nucleon-nucleon scattering cross-section.

 $\lambda = J,\pi$  (E) is the transition probability from the exciton configuration m to n when the composite system is characterized by the set of quantum numbers (E,J, $\pi$ );  $W_{a}J^{\pi}(E,E,n)$  is the decay probability of the state (E,J, $\pi$ ,n) by emission of "a".

Solution of the set of master equations gives the total occupation probability

$$\tau^{J, \tau}(E, n, \Omega) = \int P(E, J, \star, n, \Omega) dt$$
 (2)

The double differential cross section for the binary reaction (a,b) is then given by

$$\frac{d^2\sigma(\mathbf{a},\mathbf{b})}{dc_b d \mathbf{a}_b} = \sum_{\mathbf{a},\mathbf{J},\mathbf{1}_a,\mathbf{j}_a} \sigma^{\mathbf{c}}_{\mathbf{a},\mathbf{J},\mathbf{1}_a,\mathbf{j}_a} (c_a) \cdot \sum_{\mathbf{n},\mathbf{b}} W^{\mathbf{J},\mathbf{T}}(\mathbf{E},c_b,\mathbf{n}) \tau^{\mathbf{J},\mathbf{T}}(\mathbf{E},\mathbf{a},\mathbf{n})$$
(3)

Where  $\sigma_{\pi,J,l_{B},j_{B}}^{c}$  (c a) is the usual optical model compound nucleus cross section in channel  $(\pi,J,l_{B},j_{B},c_{B})$ .

The decay term  $W_D^{J},\,{}^{T}\!(E,\,\epsilon_D\,\,,n)$  is different for particles or gamma-rays.

For particles

$$W_{b}^{J,\pi}(E,c_{b},n) \propto \left[ J_{b},j_{b},l_{b} t_{l_{b},j_{b}}(c_{b}), \frac{\rho(U-c_{b}, J_{b},\pi, n-n_{b})}{\rho(U,J,\pi,n)} \right]$$
(4)

 $t_{1,j}(\epsilon)$  being optical model transmission coefficients and U the total effective excitation energy of the composite system.

For gamma-rays, in the usual Hauser-feshbach theory, in analogy to particle transmission coefficients from optical model, gamma-ray trasmission coefficients are also introduced by way of the detailed balance principle

$$t_{\gamma}(\varepsilon)\alpha\varepsilon^{2}\sigma_{\gamma}(\varepsilon_{\gamma},U)$$
 (5)

The inverse El photo-absorption cross section  $\sigma_\gamma(\epsilon_\gamma,U)$  for simplicity is approximated by a lorentzian curve  $\sigma_L(\epsilon_\gamma)$ , under the assumption

$$o_{\gamma}^{E1}(\epsilon_{\gamma},U) \approx o_{\gamma}^{E1}(\epsilon_{\gamma},0) = o_{L}(\epsilon_{\gamma})$$
(6)

namely that the photo-absorption cross section from an excited state can be assumed to be very similar to that from the ground state.

In the use of the exciton model further complications arise becouse the inverse process of the photon absorption takes place from various exciton configurations (U,n) of the composite system.

Akkermans et al. /7/ suggests a factorization

$$\sigma_{\gamma}^{El}(\epsilon_{\gamma}, n \rightarrow k) = \sigma_{\underline{L}}(\epsilon_{\gamma}) b(n \rightarrow k, \epsilon_{\gamma})$$
 (7)

under the condition that eq.7 reduces to (6) in the limit case of equilibrium and of gamma-ray scattering respectively. This can be achieved uniquely if

$$\sum_{k} b(n \rightarrow k, \epsilon_{\gamma}) = 1$$
 (8)

According to the condition (8) the "b"'s are the branching ratios which subdivide the total photo-absorption cross section into its various components. Becouse the gamma-decay of the composite system takes place either via a p-h annihilation  $\Delta n=-2$ . or via an internal transition  $\Delta n=0$  with partial deexcitation of one particle, one has

$$\sigma_{\gamma}^{E1}(\epsilon,n) = \sigma_{L}(\epsilon) \left[ b(n \rightarrow n-2, \epsilon) + b(n \rightarrow n, \epsilon) \right]$$
(9)

According to Betak et al. /8/ b( $n \rightarrow n-2,\epsilon$ )=1 and b( $n + n,\epsilon$ )=gn/ $\rho(2,c)$  being g=( $\pi^2/b$ ).a and "a" the level density parameter.

In order to satisfy the condition (8) the "b"'s by Betak et al. must be normalized to give

$$b (n \rightarrow n-2, c) = \rho(2, c) / [\rho(2, c) + g(n-2)] \text{ and}$$

$$b (n \rightarrow n, c) = gn / [\rho(2, c) + gn]$$
(10)

Accordingly the gamma-decay probability through El transitions become

$$W_{\gamma}^{J, *}(E, c_{\gamma}, n) \alpha \frac{J_{\gamma}^{-1}}{|J-1|} J' (1-\delta_{J=0, J'=0}) \frac{c_{\gamma}^{2} \alpha_{L}(c)}{\rho(n, U, J, *)} .$$
(11)
$$n$$

$$K=n-2 b(n + k, c) \rho(k, U-c_{\gamma}, J', -*)$$

Becouse not much is known about the parity distribution of the exciton states, in the present calculations the additional assumption has been made of an equal distribution of exciton states between the two parities.

In practice this leads to parity independent W by way of a general cancellation of the factor 1/2 so introduced.

#### Results and discussion

In the compound nucleus picture, compound nucleus capture may take place after all the energy of the incoming projectile has been statistically shared among all nucleons in the composite system, i.e. when statistical equilibrium is reached. The equilibrium configuration represents the limit case of the intranuclear cascade when the internal transition rate n=2 and n=-2 become equiprobable.

According to Lane /9/ the direct capture model is based on the assumption that the incident nucleon during its movement inside the mean nuclear potenzial field of the target nucleus (1p-0h state) is captured into an unoccupied bound state, emitting a gamma-ray.

In terms of exciton model one expects the direct nucleus capture corresponds to the n=1 contribution to nucleon capture.

According to ref. /10/, /11/, /12/, in the direct semidirect capture model the collective modes of the target may be excited. The incoming nucleon may be scattered into some empty particle state with excitation of a 2p-lh configuration before a gamma ray is emitted.

In fig. 1 the gamma-ray spectrum following the radiative capture of 14.1 neutrons by 93Nb is shown. The results of the calculations according to the exciton model described in the present paper are compared with the measurements /14/ and /15/.

The various components corresponding to the gamma decay of different exciton configurations n=1,...,n=9 are given separately. As it can be seen, the high energy tail of gammaray spectrum is dominated by the n=3 preequilibrium component.

In fig. 1 arrows indicate the gamma-energies corresponding to the maxima of each preequilibrium component plotted. It is interesting to note how these energies decrease at encreasing exciton numbers. This being consistent with our knowledge that the maximum of equilibrium gamma-ray emission spectrum lies at very low energies. The n=1 and n=3 stand in the ratio 1/10 as predicted by /13/ and /16/ even if the energy of the respective maxima are reverted with respect to the exciton model predictions. On the whole around 14 MeV the contribution from all the components other than n=3 is 1/3 of the total capture process and it is dominated by the n=5 component. This indicates that compound nucleus, direct and semidirect capture are not completely adequate to describe the neutron capture gamma-ray spectrum in the whole energy range.

In fig. 2 and 3 with the examples of 93Nb and 59Co respectively at 14.1 MeV neutron energy the direct semidirect calculations by /14/ and /15/ are compared with the sum of the n=1 and n=3 contributions according to the present exciton model calculations. Measurements are also shown for comparison.

The discrepancies which can be observed at both tails of the gamma-ray spectrum are an exciton level density effect. In the hard tail of the spectrum corresponding to gamma-rays from transitions to the discrete level, the direct-semidirect calculations take into account discrete levels separately, whereas our adopted exciton level density treats the discrete levels very roughly. On the other hand at the lower energy tail corresponding to gamma-transitions to continuum levels, our level density formula (based on statistical assumptions) holds better, while the Longo and Saporetti treatment fails becouse it doesn't include transitions to continuum levels.

In fig. 4 and 5 the total gamma-ray spectrum following 14.5 MeV neutron induced reactions on 27Al is shown. Measurements are also given for comparison. As it can be seen a reasonably good agreement could be obtained in the whole energy range by use of equilibrium and preequilibrium contributions only.

#### Conclusions

In view of the fact that no free parameters are involved, the unified exciton model offers a valid tool for a reliable and consistent description of nucleon capture processes, otherwise described in terms of several different reaction mechanism models. This seems to be an interesting step forward in the theoretical description of the capture mechanism.

From the technological application view point this model is an important tool for shielding and radiation damage calculations in fusion technology.

The direct semidirect models are much more involved and do not include contributions neither from n=3 exciton states, nor from transitions to continuum exciton states.

Introduction of the total angular momentum conservation is a necessary improvement in particular for the description of the particle capture process.

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Fig. 1 Plot of the different n-exciton capture contributions in 93Nb for 14.1 MeV neutrons.



Fig. 2 Comparison of measurements with our preequilibrium calculations and with direct semidirect calculations by /14/.



Fig. 5 The dashed line gives the contribution to the capture spectrum from the pure compound nucleus capture; the full line gives the total spectrum which includes equilibrium and preequilibrium capture contributions.



Fig. 4 The dashed line gives the gamma-ray spectrum from Hauser-Feshbach calculations including only gamma-ray following the neutron inelastic scattering; the full line gives the total gamma-ray spectrum including the gamma-ray following from all open reaction processes.

## SESSION

DESCRIPTION OF DIRECT PROCESSES

ROLE OF DIRECT AND PRE-EQUILIBRIUM PROCESSES IN THE DESCRIPTION OF THRESHOLD REACTION EXCITATION FUNCTIONS

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## Abstract

This paper gives consideration of the method of threshold reaction calculations which takes into account phenomenologically the integral contribution of direct processes in inelastic scattering of particles.

## INTRODUCTION

81

The statistical approach which describes decay of equilibrium compound nucleus is widely used at the present for the calculations of the threshold reaction excitation functions. However the analy sis of observed energy spectra and angular distributions of emitted particles shows that already at the sufficient low energy of inci dent particles the hard component of emission spectra is formed as a results of nonstatistical mechanism of reactions. The integral contribution of the nonstatistical component in the cross sections of different reactions grows quickly enough with the increasing of incident particle energy.

The nonstatistical component of nuclear reactions is often treated as sum of multistep direct and multistep compound transitions /1/. It is seen from the angular distributions of secondary partic les that the direct mechanism plays leading role in the formation of nonstatistical component of the cross sections of different reacti ons /2/.

Exact calculations of multistep direct transitions appear however to be very complicated. That is why more simple exciton model of pre-equilibrium particle emission is broadly used now for description of various experimental data /3,4/. The recent formulation of the exciton model uses many ideas of the intranuclear scattering cascade /4/. That enables to consider the exciton model as phenomenological description of mul tistep. incoherent direct transitions.

The main parameters of pre-equilibrium model are the singleparticle state density g, specifying the number of intermediate n - quasiparticle configurations of nucleus, and the square of matrix element  $/M/^2$ , which characterizes probabilities of intranuclear transition. Usually /3/ the dependence of matrix element on nucleus excitation energy U is approximated by expression.

$$/M/^2 = K A^{-3} U^{-1}$$
 (1)

As for as the quasiclassical estimation of g = 0.075 A Mev<sup>-1</sup>is adopted more often for single - particle state density the coefficient K appears to be one parameter of pre - equilibrium model which deter - mines the nonstatistical component of nuclear reactions.

It was early remarked /2/ that for inelastic scattering of neutrons or protons the pre - equilibrium model does't enable to describe the observed energy spectra the hard part of which is formed as a results of intensive coeherent direct transitions. It was also shown /5/, that it is impossible to achieve the consistent simulta neous description of the particle spectra and excitation functions of  $(n, \mathcal{L})$ , (n,p) and (n,2n) - reactions at any choice of parameter K.

To remove discrepancy in the choice of coefficient K it is ne - cessary to add to the pre - equilibrium model calculations the cont - ribution of direct coeherent transitions, which excite collective - states of the target by inelastic scattering. Microscopic calcula - tions of such transition intensities using theory of direct reac - tions give the sufficiently good description of observed hard "plateau - like" component of energy spectra /2/. It was noted in /6/, that comparatively weak dependence of hard part of spectra on incident particle energy  $E_o$  allows to obtain simple empirical estimation of integral contribution of direct coeherent transitions:

$$\mathcal{G}_{dir}(E_o) = \left(\frac{d\delta}{dE'}\right)_{og_s} \left(E_o - E_{low}\right) \tag{2}$$

where  $(dG/c(E')_{ols}$  - the observed differential inelastic scattering cross section in the "plateau" region and  $E_{low}$  - the effective boundary energy of direct transitions.

The analysis of the neutron inelastic spectrum fives the values  $(dG'/dE')_{abs} \simeq 20$  <sup>mb</sup>/MeV and  $E_{bw} \simeq 5$  MeV.

### THE CALCULATIONS OF EXCITATION FUNCTIONS

Adding the description of direct transitions with the formula (2) to the calculations of pre - equilibrium model, we can obtain the threshold reaction cross sections which is in good agreement with experimental data available. As example Fig. 1 and 2 show the excitation functions of  $^{56}$ Fe(n,2n) and  $^{56}$ Fe(n,p) reactions and secondary particle spectra from these reactions correspondently. The phenomenological representation for the contribution of direct processes allows to describe the excitation functions of (n,2n) -, (n,p) - reactions with consistent set of the level density parame  $\sim$  ters g and the coefficient  $K = 700 \text{ MeV}^3$ . Similar description was obtained by authors also for the same reactions on other neighbou - ring nuclei.

Our analysis in spite of simplifyed features display qualitatively the main results of time consuming theoretical calculati – ons /2/. This is a reason that the phenomenological account of di – rect collective transitions is more logical as compared with the description of the same data in the frame of pure pre – equilibrium model using adjustment of coefficient K. This adjustment does not enables to avoid disagreement in the description of the neutron spectra and (r, 2n) – reaction cross sections together with the same data for (n,p) – reaction.

It is necessary to remark that the choice of level density parameters plays important role for consistent description of cross sections of different threshold reactions. The using of the back - shifted Fermi-gas formula with parameters, obtained from experimental data on neutron resonance density, does not give as a rule good agreement with the observed excitation functions of (n,p) and (n,d) - reactions. The example of such calculations is shown for the  $^{56}$ Fe (n,p) - reaction on Fig.1 b ( dotted line). The great discrepance between the calculated and the experimental data in low energy region is directly connected with the value of level density parameter of the residual nucleus. Of course the similar discrepancies can be removed always by the renormalization of level density parameters

(Fig. 1b, solid line), but in this case the inconsistense in fitting of different experimental data does not eliminate. This contradiction can be resolved only by the using more physical approach for level density taking into account the shell, superfluid and collective effects. The example of such calculations is shown in Fig. 1b (dashed - dotted line) where for the description of level density it was used the model described in /5/.

#### CONCLUSION

We have considered the method of calculation of threshold reaction cross section which phenomenologically takes into account the contribution of direct process in entrance channel. The method proposed enables to obtain in a simple way a consistent description of the excitation function and particle emission spectrum of different reactions. Early the similar description was obtained only as a result of using essentially different values of the main parameter K of pre - equilibrium model for inelastic scattering and exchange reaction channels.

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Fig. 1. The excitation functions of (n,2n) - and (n,p) - re - actions for <sup>56</sup>Fe. The experimental data are taken from /7/, theoretical curves were obtained by account of pre - equilibrium decay and direct mechanism. The solid curve - calculation using the back - shift Fermi-gas model wich adjustment of parameters on excitation functions, The dash curve - calculation using the back-shift Fermi-gas model without parameter adjustment. The dash - dotted curve - calculation using superfluid model.



Fig. 2. The secondary particle spectrum of the reactions  $^{56}$ Fe (n,2n) (a) and  $^{56}$ Fe (n,p) (b) for incident neutron energy 14,6 MeV. The theoretical curves are obtained taking into account of the direct and pre-equilibrium processes. The experimental data are taken from /9/. On Methods for the Calculation of Neutron Induced Reactions

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I. Analysis of neutron induced reactions on Cr isotopes

In the first part of this work a complete and consistent analysis of the more important interactions of neutrons with Cr isotopes in the energy range 2-20 MeV is presented.

As it is well known, in the energy range considered the reaction mechanism changes in character. At lower excitation energies, most reactions leading to the particle emission are well described by the compound-nucleus evaporation model (e.g. Hauser-Feschbach or Weisskopf-Ewing theory), at higher excitation energies, however, the contribution from the precompound mechanism becomes significant and cannot be neglected. The exciton model of preequilibrium decay has been widely used to describe that fraction of cross sections.

In this work the integral cross sections and the emission spectra are described using a combination of both the compound--nucleus and preequilibrium models. Emphasis is put on a simultaneous analysis of many reaction channels involved in the interactions of neutrons with Cr isotopes, using a consistent set of parameters.

## I.1 Optical model calculations

The optical model calculation constitutes an important part of the nuclear data analysis. Usually it employs either a phenomenological or microscopically derived optical potential. In this work, the optical model calculations were made using the spherical optical model code SCAT2 of O. Bersillon (1981). The global optical potential parameters of Perey (1963) for protons, and those of McFadden and Satchler (1966) for alphas were used. The neutron optical potential parameters for Cr and V were taken from the evaluations by Vozyakov (1983) and Tanaka (1982), respectively.

## I.2 Statistical model calculations

85

All calculations were made using the Weisskopf-Ewing evaporation model in combination with the modified precompound exciton model.

Since the Weisskopf-Ewing theory is well known, only the relevant features of our precompound exciton model will be briefly discussed here.

The emission rate of the particle  $\beta$  from an n-exciton state is given by the usual expression

$$W_{\beta}(m, E, \varepsilon_{\beta}) = \frac{2 s_{\beta} + \Lambda}{\pi^{2} \hbar^{3}} \omega_{\beta} \varepsilon_{\beta} \delta^{-\mu\nu}(\varepsilon_{\beta}) Q_{\beta}(\rho) \times \frac{\omega(\rho - \rho_{\beta}, h, U, E_{\mu})}{\omega(\rho, h, E, E_{\mu})}$$
(1)

Here, the proton-neutron distinguishability factor  $Q_{A}(p)$  makes it possible to use the one-fermion density of exciton states.

We used the n-exciton state density  $\omega(p,h,E,E_{\rm H})$  corrected for the Pauli principle and the finite depth of hole excitation. This is given by

$$\omega(p, h, E, E_{H}) = \frac{g^{m}}{p! h! (m-1)!} \sum_{l=0}^{h} {\binom{h}{l}} {(-1)}^{l} \times (2)$$

$$\times \left[ E - R_{p,h} - lE_{H} \right]^{m-1} \ominus \left( E - R_{p,h} - lE_{H} \right)$$

where A p,h is the correction factor due to the Pauli principle (Meneses 1983)

$$A_{p,h} = \frac{1}{g} \left[ ph - p(p+1)/4 - L(L+1)/4 \right], \quad (3)$$

and  $E_{\rm H}$  is the finite depth of hole excitation. In fact, the inclusion of the correction for the finite depth of hole excitation is the only major difference between the commonly used exciton model and that used in this work. It may be noted, that euch a type of correction is in accord with the dominating role of the nuclear surface in nuclear interactions. In terms of energy this means that the depth of hole excitation is expected to be comparable with the strength of the effective residual interaction which amounts to a few MeV. This may be compared with the total depth of the Fermi sea i.e. several tens of MeV.

Indeed, the recent evaluation of the equilibration of finite fermion systems by Wolschin (1981) showed that during the relaxation process, the occupation probabilities of only a small part of the nucleons below the Fermi energy (holes) were changed substantially. The remaining part of nucleus continued to be inviolable. The width of the energy region influenced by the equilibration was approximately equal to the thermodynamic tempsrature of the resulting compound nucleus.

Thus, the following relation based on the reasoning given above was adopted for the evaluation of the effective finite depth of hole excitation

$$E_{H} \approx T_{eq} \approx \sqrt{E/a}$$
 (4)

a being the level density parameter of the compound nucleus.

The next important quantity in the closed-form exciton model is the transition rate forming the n+2 - exciton state.

This is given by the "golden rule" as

86

$$\lambda^{*}(m, E) = \frac{2\pi}{\pi} |M|^{2} \omega_{\ell}^{*}(m, E, E_{\mu})$$
 (5)

where we use the density of accessible final states  $\omega_{f}(n, E, E_{H})$ , corrected for the finite depth of hole excitation as given by Betak and Dobes (1976).

For the normalization of the absolute magnitude of the transition rate it is necessary to know the averaged squared matrix element  $|M|^2$ . In this work  $|M|^2$  is expected to behave approximately as (Gmuca 1982).

$$|M|^{2} = K q^{-3} E_{H}^{-1}$$
 (6)

The single particle density g is related to the level density parameter a by

$$g = \frac{c}{\pi c} \alpha \qquad (4)$$

The dimensionless free parameter K was determined to be 0.30 for neutron induced reactions (Gmuca 1982).

In Weisskopf-Ewing model calculations the level density formula of the traditional Fermi-gas form

$$\rho(U) = \frac{V_{\overline{x}}}{12} \frac{\exp\{2\left[\alpha\left(U-S\right)\right]^{4/2}\}}{\alpha^{4/4} \left(U-S\right)^{5/4}}$$
(8)

was used at higher excitation energies, joining smoothly to the constant temperature formula for excitation energies below 5 MeV.

## I.3 Results and discussions

The model described above was used to calculate both. the angle integrated secondary particle emission spectra and excitation functions for the more important neutron threshold reactions on Cr isotopes in the energy range up to 20 MeV. At low energies the reactions (n,p) and  $(n, \alpha)$  dominate, while at higher energies (n,2n), (n,pn),  $(n,n^*p)$  and  $(n,n^*\alpha)$  become also important. The remaining possible reactions, (n,3n), (n,2p) and those embracing the complex particle other than  $\alpha$ , do not contribute appreciably below 20 MeV and were excluded from consideration.

Results of calculation were compared with the available experimental data (see Figs. 1-5). In general, the model is ' able to reproduce properly both, the angle integrated emission spectra and integral cross sections with a consistently taken set of parameters though some discrepancies remain. Due to its simplicity, the model is especially suited for evaluation purposes. For a better understanding of underlying physics, however, more microscopic models are needed.

# II. Microscopic description of direct contribution to neutron inelastic scattering

The second part of this work is devoted to the calculation of double-differential cross sections of neutron inelastic scattering. We shall concentrate mainly on the calculation of the direct continuum contribution to these spectra.

During the past decades, the direct reaction methods (DR) have been used extensively and successfully in analyzing a large smount of experimental data for nuclear reactione. These applications, however, have been limited mainly to processes in which the reeidual nuclei were left in their respective discrete states.

Contrary, the purpose of the present work is to apply the DR methods to the calculation of continuum cross sections. We shall focus our attention on the description of the inelastic neutron scattering around 14 MeV on even-even targets.

## II.1 Direct reaction methods

The simplest version of the DR methods is the distorted wave Born approximation (DWBA). In that approach, the angular distribution of inelastic scattering on a particular discrete state is given as (Glendening 1983)

$$\left(\frac{d}{d\Omega}\right)_{onl} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k_{\ell}}{k_{\star}} \left(\beta_{\ell}R_{o}\right)^2 \sum_{m} |B^{\ell m}|_{l}^2 \qquad (9)$$

where

87

$$B^{\ell m} = \frac{i}{(2\ell+1)^{4/2}} \int d\vec{x} \chi^{(-)\ell}(\vec{k}_{l},\vec{x}) \frac{dU}{dn} \chi^{(m)}(\vec{x}) \chi^{(\ell)}(\vec{k}_{2},\vec{x}), \quad (10)$$

and we use explicitly the collective form-factor.

In the continuum region, there will be contained a lerge number of states, even when a relatively narrow energy interval is taken, and to calculate cross sections to excite these states individually is impracticable. Rather an averaging procedure over a large number of these states has to be taken. Thus, the continuum cross section per unit energy should be interpreted as the incoherent sum of the energy averaged cross sections for states contributing to the given energy bin.

One may write

$$\left(\frac{d^2 6}{d \varepsilon d \Omega}\right)_{i} = \sum_{e} \langle \left(\frac{d \sigma}{d \Omega}\right)_{o \to I} \rangle_{i} \rho_{i}^{e} \qquad (11)$$

where an index i stands for the i-th energy bin over which an averaging is performed and terms on the right-hand side of eq. 11 are given by eq. 9. The quantity  $\rho_{\star}^{4}$  represents the number of states with a multipolarity 1 contributing to the i-th energy bin.

The energy dependence of the right-hand side of eq. 9 is contained mainly in the dynamic deformation parameters  $\beta_{j}$ which fluctuate strongly with the excitation energy, while the reduced amplitudes  $B^{lm}$  vary smoothly and slowly (due to the smooth and slow variation of the optical potential U). Thus, the problem of an energy averaging of eq. 9 is in fact, reduced to an averaging of the  $\beta_{\ell}$ 's. In the standard collective model of nucleus (Bohr and Mottelson 1974) the  $\beta_{\ell}$ 's are related to the reduced matrix elements and thus, the problem is further shifted to the field of the nuclear structure theory.

#### II.2 Nuclear structure calculations

In this work we have used the quasiparticle-phonon nuclear model (QPNM) to predict energies, wave functions and matrix elements of excited states. Since this model has been described in detail elsewhers (Soloviev 1978, Vdovin and Soloviev 1983) only the essential features will be given here.

The starting point of the QPNM is the Hartree-Fock-Bogolyubov (HFB) theory. The model Hamiltonian of the QPNM used in this work consist of the mean nuclear field (of the Saxon-Woods form) and the effective interaction in the form of the monopole pairing interaction plus the separable multipole-multipole isoscalar and isovector forces.

One may write this Hamiltonian in the second quantization as

$$H = H_o^{(n)} + H_o^{(p)} + H_{pnik}^{(n)} + H_{pnik}^{(p)} + \sum_{\lambda} H(\lambda) \qquad (12)$$

where

$$H_{o}^{(t)} + H_{PAIR}^{(t)} = \sum_{jm} E_{j} Q_{jm}^{+} Q_{jm}^{-} - \frac{G^{(t)}}{4} \times (A3)$$

$$\times \sum_{jj'} \sum_{mm'} (-A)^{j-m} (-A)^{j'-m'} Q_{jm}^{+} Q_{j-m}^{+} Q_{j'-m'}^{-} Q_{j'm'}^{-} j$$

$$38H(\lambda) = -\frac{1}{2} \sum_{du} \left\{ (x_{0}^{(\lambda)} + x_{1}^{(\lambda)}) \left[ M_{\lambda_{du}}^{*}(m) M_{\lambda_{du}}(m) + M_{\lambda_{du}}^{*}(p) M_{\lambda_{du}}(p) \right] + (x_{0}^{(\lambda)} - x_{1}^{(\lambda)}) \times (44) \right\}$$

$$\times \left[ M_{\lambda_{du}}^{*}(m) M_{\lambda_{du}}(p) + M_{\lambda_{du}}^{*}(p) M_{\lambda_{du}}(m) \right] \right\} i$$

Transforming the model Hamiltonian (12)-(15) by the canonical Bogolyubov transformation, one passes from nucleon operators  $a_{jm}, a_{jm}$  to quasiparticle creation and annihilation operators  $\alpha_{jm}, \alpha_{jm}$ . The pairs of operators  $\alpha'_{jm}, \alpha'_{jm}$ , and  $\alpha'_{jm}, \alpha'_{jm}$  are then expressed through phonon operators  $Q_{\lambda\mu}, Q_{\lambda'\mu'}$ , and thus the quasiparticle operators remain only in the form  $\alpha'_{jm}, \alpha'_{jm}, \alpha'_{jm}$ . In such a way we have finally obtained the Hamiltonian which contains the free quasiparticles, free phonors and the quasiparticle-phonon interaction. Then, the random phase approximation (RPA) method has been applied to this Hamiltonian.

The RPA equations have been solved to determine the energies and wave functions of one-phonon states. It has been already demonstrated (see references cited above) that such an approach is very useful for describing excited states. The one--phonon states provide a unique description of collective, waaky collective and two-quasiparticle states.

Having determined the energies and structure of one-phonon states one may calculate the transition matrix elements. We are interested in both, the proton and neutron reduced matrix elements  $B(X\lambda)$  (X=P,N) induced by external multipole fields. For this purpose we have calculated the RPA multipole response functions for multipolarities  $\lambda$  from 1 to 6. Typical examples of the response functions for the neutron and proton systems of  $^{56}$  Fe of the multipolarities  $\lambda$  =2 (for the 2  $^+$  states) and  $\lambda$  =4 (for the 4  $^+$  states) are given in Fig. 6 and Fig. 7, respectively.

Please, nute a strong energy variation of the response functions.

Since in DWBA calculations we use a collective form factor, for simplicity, we have to express the RPA reduced matrix element for a particular state  $B(X \lambda)$  (where X is N for the neutron and P for the proton systems) in terms of the dynamic deformation parameter

$$\beta^{2}(x\lambda) = B(x\lambda) \left\{ \frac{3}{4\pi} N_{x} R_{o}^{\lambda} \right\}^{-2} \qquad (\Lambda 6)$$

where N<sub>X</sub> is the number of particles of the type X. Finally, for the effective dynamical deformation of inelastically scattered neutrons we may write

$$\beta_{m,m'}(\lambda) = \left| \frac{V_{mp} N_p \beta(P\lambda) + I V_{mm} N_m \beta(N\lambda)}{V_{mp} N_p + V_{mm} N_m} \right|, \quad (14)$$

where  $N_p$ ,  $N_n$  are numbers of protons and neutrons building the level under consideration and  $V_{np}$ ,  $V_{nn}$  are the strength (relative) of n-p and n-n forces, respectively. The parameter I represents the isoecalar (+1) or isovector (-1) excitation of the given level.

## II.3 Results and discusions

The model has been used to calculate the double-differrential cross sections of inelastic scattering of 14 MeV neutrons on  ${}^{52}$ Cr,  ${}^{56}$ Fe and  ${}^{58}$ Ni nuclei. Since this model gives the direct contribution only, the compound nucleus portion of the cross section has been added.

The results of calculations have been compared to the experimental data of Takahashi et al. (1983). The agreement is encouraging. The typical results may be seen in Figs. 8-12, where the neutron inelastic spectra from the reaction  $^{56}$ Fe+n are shown at several angles. Similar results were obtained also for  $^{52}$ Cr and  $^{58}$ Ni nuclei.

## III. Conclusions

In the first part of this work the simple model for the calculation of neutron threshold reactions is presented. The model is based on a combination of the compound-nucleus Weieskopf-Ewing evaporation model and the modified exciton model of the preequilibrium emission. In such an approach the angle integrated particle spectra as well as the excitation functions of many competing reactions may be simultaneously described using a consistent set of parameters. Due to its simplicity the model is well suited for evaluation purposes.

The second part of this work is devoted to the microscopic description of the direct contribution to neutron inelastic scattering. The model consists of one-step DWBA approach and the quasiparticle-phonon nuclear model for nuclear structure calculations. In fact, the model is very close to that of Tamura, Udagawa and Lenske (1982) except the underlying model of nuclear structure. Our one-phonon states contain collective, weakly collective as well as two-quasiparticle states and thus describe a good portion of the spectrum of excited states. At this stage it eeems the model is well suited for the description of 14 MeV neutron inelastic scattering, where one-step DWBA approach is sufficient. At higher energies, however, two--step contributions may be required to correctly describe the experimental data.

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Fig. 1: Calculated and experimental proton emission spectra from 15 MeV neutron bombardment of <sup>50</sup>Cr. The solid curve is the total proton emission spectrum while the long-dashed end short dashed curves represent contributions coming from (n,px) and (n,n'p) reactions. The dot-dashed curve is a preequilibrium part of the first proton emission spectrum.



Fig. 2: Calculated and experimental alpha emission spectra from 15 MeV neutron bombardment of <sup>52</sup>Cr. No preequilibrium alpha emission is needed to describe experimental data.



Fig. 3: Calculated and experimental cross sections for the  ${}^{52}Cr(n,p){}^{52}V$  reaction from near threshold to 20 MeV.



Fig. 4: Same as Fig. 3 for the 53Cr(n,p) reaction



Fig. 5: Calculated and experimental cross sections for the <sup>50</sup>Cr(n,2n)<sup>49</sup>Cr reaction to 20 MeV. The dashed curve represents results of the ENDF/B-V evaluation.



Fig. 6: Quadrupole RPA response functions of neutron (N) and proton (P) fields of  ${}^{56}\textsc{Fe}$ .



,Fig. 7: Same as Fig. 6 for the multipolarity  $\lambda = 4$ .



Fig. 8: Double-differential cross-sections for 14 MeV scattered neutrons in <sup>56</sup>Fe to the laboratory angle 37°. The dashed histogram represents the direct contribution, the thick solid histogram is the total theoretical prediction (direct + compound) and the thin histogram is the evaluation from ENDF/B-IV. The cireles are exparimental data of Takahashi et al.



Fig. 9: The same as Fig. 8 for the scattering angle 65°.



Fig. 10: The same as Fig. 8 for the scattering angle 100°.







Fig. 12: The same as Fig. 8 for the scattering angle 139<sup>0</sup>.

## GAMMA-RAY SPECTRA AND ANGULAR DISTRIBUTIONS OF PHOTONS FOLLOWING THE CAPTURE OF FAST NEUTRONS

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#### Summary

It can be useful in fusion reactor research to obtain information on the production of high energy photons. For this purpose an outline of the direct-semidirect (DSD) model is given and the model is applied to calculate the cross sections for the production of 10-50 MeV photons following radiative capture of 4-50 MeV neutrons by  ${}^{40}\text{Ca}, {}^{48}\text{Ti}, \text{nat Ni}$ and  ${}^{120}\text{Sn}$ . It is shown that the model can allow useful predictions about the relative yield of high-energy gamma-rays emitted in different directions with respect to incident neutrons and that the angular distributions depend greatly on the parameters of giant multipole resonances and on the level structure of final nuclei.

#### 1. Introduction

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Fusion reactors require a large range of nuclear data for structural materials at energies above 5 MeV. Most of these data are not experimentally known so that nuclear model codes should be used to supply the necessary information.

Neutron-induced photoproduction cross sections and angular distributions of emitted high-energy photons can be of interest in shielding, dosimetry and radiation damage problems connected with fusion reactors and facilities that utilize neutrons up to about 50 MeV, e.g. d+T, d+Li, or p+Li neutron sources. The (n,gamma) reaction, though constituting only a small fraction of the non-elastic cross section for high energy neutrons, becomes one of the dominant mechanisms for producing photons with energies higher than about ten MeV. This hardest part of the gamma-ray spectrum may be important not only to protect fusion reactor components, but to satisfy biological safety requirements. Since the necessary experimental information is rather scarce, one must use model calculations to fill gaps and supply the energy-angle data required. Different mechanisms (statistical<sup>1)</sup>, valence<sup>2)</sup>, preequilibrium<sup>3)</sup>, direct and semidirect<sup>4-8)</sup> have been proposed in attempts to account for the experimental data of the nucleon capture reaction in the energy-region of interest.

Among the different models proposed attention is here focused on the direct-semidirect model which, up to now, seems the more adequate to reliably calculate cross sections and angular distributions for radiative capture by heavy and medium-mass target nuclei of nucleons with energies greater than about 5 MeV. The mechanism of nucleon capture is essentially the same for neutrons or protons. However, taking into account the purpose of the present Meeting the examples examined here refer only to neutrons.

#### 2. The direct-semidirect model

Following the direct capture model the incident neutron, during its movement in the mean nuclear potential field of the target nucleus, emits a gamma-ray undergoing a direct transition to an unoccupied particle bound state.

In the semidirect model the capture proceeds through intermediate states. In this picture the target nucleus may have shape oscillations and an incident nucleon experiences a slightly deformed potential. The interaction of the nucleon with the nucleus through such a potential can excite collective modes of the target. In the capture process the nucleon is scattered into an empty particle bound state and the nucleus is excited to a giant resonance state. The latter then decays emitting a gamma-ray. According to the direct or semidirect model the capture of neutrons leading to bound final states by the emission of one photon is favoured. Therefore a dominance of high-energy photons in the spectra is expected.

In the present formulation the direct-semidirect differential cross section for capture to a given final state is written as

$$\frac{d\sigma}{d\Omega} = \left| \sum_{\mathbf{L},\mu} \mathbf{A}_{\mathbf{L},\mu}(\mathbf{E}) \cdot \overline{\mathbf{X}}_{\mathbf{L},\mu}(\boldsymbol{\theta}, \boldsymbol{\phi}) \right|^2 , \qquad (1)$$

where  $A_{L\mu}$  is the radiative capture amplitude for an electric multipole transition of order L from an initial state (l'j') to a final bound state (lj)

$$A_{L\mu} = (4\pi \frac{Me^2}{\pi^2 k'} \frac{L+1}{L[(2L+1)!!]^2} k_{\gamma}^{2L+1})^{\frac{1}{2}} \sum_{j'} (jL, \frac{1}{2}-\mu, \mu | j' \frac{1}{2}) Z(2'j'2j; \frac{1}{2}L) \sum_{T=0,1}^{M} M_{TLj'}$$

with k' and  $k_{\Upsilon}$  the nucleon and photon wave numbers,  $M_{TLj},$  , the direct-semidirect radial matrix elements, while X are the vector spherical harmonics

$$\overline{\mathbf{X}}_{L\mu}(\vartheta, \phi) = -i \left[ L(L+1) \right]^{-\frac{1}{2}} \left( \overline{\mathbf{r}} \times \overline{\mathbf{7}} \right) \mathbf{Y}_{L\mu}(\vartheta, \phi) \quad . \tag{3}$$

M in formula (1) is the radial part of the matrix element TLj'

$$M = \langle \Psi_{fin} | \Xi_{L\mu}^{(N)} | \Psi_{in} \rangle + \frac{\langle \Psi_{fin} | \Xi_{TL\mu}^{(N)} | \Psi_{inc} \rangle \langle \Psi_{inc} | H'_{TL\mu} | \Psi_{in} \rangle}{\varepsilon_{2'j'} - \hbar \omega_{TL} - \varepsilon_{2j} + \frac{i}{2} \varepsilon_{TL}},$$
(4)

whose first and second terms correspond to direct and semidirect capture respectively. Here  $\boldsymbol{\epsilon}_{\ell'j'}$  and  $\boldsymbol{\epsilon}_{\ell j}$  are the initial and final nucleon energies and  $\boldsymbol{\pi}_{\omega_{TL}}$  the excitation energy of the giant (TL) state in the target nucleus (A,N,Z).

The initial, intermediate and final states are given respectively by

$$\begin{aligned}
& \Psi_{in} = \frac{1}{2'j'} e^{i\sigma L'} \left[ 4\pi (22'-1) \right]^{\frac{1}{2}} (2'0\frac{1}{2}) \phi_{j'n} (\Omega, \sigma) \Psi_{2'j'} (\tau) \phi_{\sigma\sigma} \\
& \Psi_{inc} = \phi_{jn} (\Omega, \sigma) \Psi_{2j} (\tau) \phi_{T_{2}-\Psi} , \quad (5) \\
& \Psi_{fin} = \phi_{jn} (\Omega, \sigma) \Psi_{2j} (\tau) \phi_{\sigma\sigma} ,
\end{aligned}$$

with  $\sigma_{\ell'}$ , the Coulomb phase shift ( $\sigma_{\ell'}$  =0 for incident neutrons),  $\phi$  the target functions and  $\Phi$  the spin-angular wave functions

$$\Phi_{\mathbf{M}} = \sum_{\lambda} (\mathfrak{L}, \mathfrak{M} - \lambda, \mathfrak{j}, \lambda) \mid \mathcal{M}) \Upsilon_{\mathfrak{L}, \mathfrak{M} - \lambda} \chi_{\mathfrak{j}, \lambda}$$
(6)

The direct multipole transition operator in (4) is given by

$$\mathcal{I}_{Lu}^{(N)} = e \sum_{i=1}^{N+1} q_i r_i^L Y_{Lu}(\hat{n}_i)$$
(7)

with  $q_i = \frac{1}{2}(1+\tau_{3i})=1,0$  for protons and neutrons respectively. To estimate the direct transition matrix element an effective charge  $\tilde{e}$ , is usually introduced:

$$\mathbf{e}_{L} = \mathbf{e} \sum_{i=1}^{A+1} q_{i} \overline{\mathbf{r}}_{i}^{L} = \mathbf{e} \left[ q(\overline{\mathbf{r}}_{p} - \overline{\mathbf{r}}_{s})^{L} + Z(\overline{\mathbf{r}}_{p} \overline{\mathbf{r}}_{s})^{L} \right]$$

with r, r and r = (r + Ar)/(A+1) being the location vectors in an arbitrary system of coordinates for the incident particle, the target CM and the system (particle + target) CM respectively. With the notation  $r = r_p - r_t (r - r_t = r/(A+1))$  this formula can be rewritten as

$$\tilde{e}_{L} = eM^{L}(q + \frac{Z}{(-A)^{L}}) r^{L}$$
, (8)

where M is the reduced mass. It is immediately clear from formula (8) that for L>1 the direct matrix element can be neglected in <u>neutron</u> capture. It is this elimination of the non-E1 direct amplitudes that highly increases the sensitivity of  $(n,\gamma)$  experiments to collective radiation.

The particle-vibration coupling interaction for excitation of giant multipole states in (4) can be written as

$$H^{*}_{\Pi_{u}} = \frac{7}{2} \nabla_{T} h_{\overline{T}} (\Xi, r) Y^{*}_{L_{u}} (\Omega) \alpha_{\overline{T}_{u}}$$
(9)

with  $\vartheta_1 = 1$ ;  $\vartheta_1 = \tau_3$ ;  $\alpha_{TL\mu} = \sum_i \vartheta_{TI} r_i r_{L\mu}(\Omega_i)$  the collective coordinates of the target. The radial form factor  $h_{TL}(E,r)$  is here expressed in the general form

$$h_{TL}(r, E) = \frac{1}{\rho_{o}} \left[ v_{T}^{V}(E) \xi(r) + v_{T}^{S}(E) \eta(r) + i w_{T}^{V}(E) \xi(r) + i w_{T}^{S} \eta(r) \right], \quad (10)$$

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with

$$\begin{cases} \xi(r) = \frac{4\pi}{\lambda} \frac{r^{2} \sigma_{+}(r)}{cr^{2}L_{>}} \\ \eta(r) = -\frac{4\pi}{\lambda} \frac{r^{L-1} dc_{+}(r)/dr}{(2L+1) < r^{2}(L-1)_{>}} \end{cases}$$
(11)

where  $v_T^{V,S}$ ,  $v_T^{V,S}$  are the "volume" or "surface" depths of the optical potential used,  $\rho(r)/\rho$  are Woods-Saxon form factors f(r) with the same geometrical parameters as in the optical potential, while the radial form factors  $\xi(r)$  and  $\eta(r)$  satisfy the normalization condition

$$\int \xi(\mathbf{r}) \mathbf{r}^{L+2} d\mathbf{r} = \int \gamma(\mathbf{r}) \mathbf{r}^{L+2} d\mathbf{r} = 1$$
 (12)

In order to evaluate the matrix elements of  $\mathcal{H}_{TL\mu}^{(t)}$  direct use of the experimental values for the fractions of the EWSR exhausted can be made, taking into account the relation:

$$S_{TL}(EWSR) \equiv \sum_{K} (E_{K} - E_{0}) \sum_{U}^{2} \langle x, Lu | Q_{TLU} | 0, CO \rangle |^{2} = \frac{A\pi^{2}}{8\pi M} L(2L+1)^{2} \langle r^{2}(L-1) \rangle \cdot \begin{cases} z^{2}/A^{2} & (T=0) \\ NZ/A^{2} & (T=1) \end{cases}$$
(13)

By introducing the operators mentioned into (4) the radial part of the direct-semidirect matrix element  $M_{TLi}$ , is found to be

$$M_{TLj} = \tilde{e}_{L} D_{Lj} + \frac{G_{TL} C_{TLj}}{E_{\gamma} - \pi \omega_{TL} + \frac{1}{2} C_{TL}}$$
(14)

with  $E_{\gamma} = \mathcal{E}_{\ell',j} - \mathcal{E}_{\ell,j}$ , the energy of the photon emitted,  $\tilde{\tilde{e}} = \tilde{e}/er^{L}$ , and

$$G_{TL} = \frac{3}{\pi u_{TL}} - \frac{\hbar^2}{M} L < r^{2(L-1)} > . \qquad \begin{cases} Z^2/\lambda^2 & (T=0) \\ NZ/\lambda^2 & (T=1) \end{cases}$$
(15)

where  $\beta_{TL}$  is the fraction of the EWSR exhausted and  $D_{L,j}$ ,  $C_{TL,j}$ , are the direct and semidirect (collective) integrals respectively:

$$\begin{cases} D_{Lj}, = \int u_{\ell j}(r) r^{L} \psi_{\ell' j}, r^{2} dr \\ C_{TLj}, = \int u_{\ell j}(r) h_{TL}(\Xi, r) \psi_{\ell' j}, r^{2} dr \end{cases}$$
(16)

Thus, after calculating the bound-state  $u_{j}(r)$  and continuumstate  $\psi_{j',j}$ , wave functions, the radiative capture amplitude (2) and the differential  $(n,\gamma)$  cross section (1) can be obtained.

To analyse the angular distributions of photons following neutron radiative capture the differential cross section is expanded in the standard form

$$\frac{d6}{d\Omega} \begin{pmatrix} E_n, \theta_1 \end{pmatrix} = \frac{\sigma \begin{pmatrix} E_n \end{pmatrix}}{4\pi} \begin{bmatrix} 1 + \sum_{m=1}^{2L} a_m(E_n) P_m(\cos \theta_1) \end{bmatrix} (17)$$

with  $\sigma_0$  the cross section integrated over the  $4\pi$  solid angle and the  $a_m$  - coefficients expressed through combinations of the amplitudes  $A_{r,n}$ .

The angular distributions of emitted photons are therefore obtained as

$$W(E_{n}, \theta_{\gamma}) = 1 + \sum_{m=1}^{2L} a_{m}(E_{n}) P_{m}(\cos \theta_{\gamma})$$
 (18)

To our knowledge no description of DSD codes for calculation of angular distributions of emitted photons is presently available. In the next section attention is focused on some results of angular distribution calculations.

#### 3. Production of high-energy photons

96

It has been pointed out in previous papers <sup>9)</sup> that the available experimental data associated with gamma-ray production chiefly concern the thermal- and low-MeV neutron energy region. Such experimental data are usually limited to photons below  $\sim 10$  MeV, which is a very large fraction of the total gamma-ray production cross section from nonelastic and radiative capture reactions for fast neutrons. Knowledge of this main part of the gamma-ray production is important for nuclear heating studies as well as for material damage estimates. For higher energy photons, it is the transmission of the gamma-ray flux through shielding that may be of interest, but information on production of high-energy photons is rather scarce.

The main part of gamma-ray production from reactions induced by neutrons is essentially due to nonelastic reactions that produce photons whose intensity rapidly decreases with energy. For producing photons with energy above  $\sim 10$  MeV, radiative capture is one of the dominant mechanisms. In this energy region the use of DSD calculations is required due to the lack of experimental data.

Following the model, the incident neutrons are captured to states in the final nucleus that have a single-particle structure. This implies that to a given neutron energy there should be a corresponding group of monochromatic emitted gamma rays.

As an example the calculated <sup>9)</sup> gamma-ray spectra for radiative capture of 9.2 and 13.2 MeV neutrons by <sup>208</sup>Pb is shown in fig. 1. By introducing corrections for the detector gamma-ray efficiency and spectrometer response function the calculated spectra can be compared with experimental points , as fig. 2 shows. As can be seen, the essential features of the spectral shapes are reproduced. In this case, as in others, a discrepancy between measured and calculated spectra generally remains for high excitation energies up to the neutron separation energy  $B_N$ .

This disagreement disappears taking into account the compound nucleus contribution as shown in fig. 3 reproduced from ref.  $^{11)}$ .

The gamma-ray spectra considered in figs. 1-3 refer to photons produced over the  $4\pi$  solid angle. Let us now illustrate the results (part of which were presented at the Kiev<sup>13)</sup> and Santa Fe<sup>14)</sup> conferences) for angular distributions of high energy gamma-rays due to radiative



Fig. 1. Calculated gamma-ray spectra for radiative capture of monochromatic neutrons by <sup>208</sup>Pb.







Fig. 3. Comparison between the experimental<sup>12)</sup> and the calculated<sup>11)</sup> spectrum of high-energy photons emitted in the <sup>89</sup>Y(n,y) reaction. (----DSD;-----compound; ---- total).

capture of fast neutrons by  $^{40}$  Ca,  $^{48}$  Ti, Ni and  $^{120}$ Sn (natural nickel is considered as an admixture of  $^{58}$ Ni and  $^{60}$ Ni, neglecting the 6% of other isotopes).

Calculations are performed by using the extended formulation  $^{6-7)}$  of the DSD model, which includes higher multipole contributions. The differential  $(n,\gamma)$  cross sections for E1+E2+E3 capture are calculated versus the incident neutron energy E and the angle  $\theta_{\gamma}$  between incident neutrons and emitted photons by using formula (17).

The explicit expressions for the  $a_m$ -coefficients show that interference between opposite-parity transitions gives rise to symmetry breaking in the photon angular distributions.

The  $(n,\gamma)$  cross sections are obtained, as in ref.<sup>6</sup>, without recourse to free parameters, that is: 1) EL contributions up to L=3 are taken into account with energies, widths and strengths of giant states taken directly from experimental data, 2) the same depths and geometrical 15 are used both for the optical potential and the energydependent complex coupling interaction having a mixed surface- and volume-form, 3) the same potential geometry is adopted both for bound and scattering states, 4) the depth of the bound-state potential is adjusted to give the final-particle binding energies, obtained as the centre of gravity of the nuclear levels listed in "Nuclear Data Sheets".

The reliability of the  $(n, \gamma)$  cross sections thus obtained has been checked: 1) by a comparison between experimental points for photons emitted at a fixed angle  $(\theta_{\gamma}=90^{\circ})$  and the corresponding curves calculated for neutron capture in Ca and Ni (see figs. 4 and 5);





Fig. 4. The  ${}^{40}Ca(n,\gamma_0)$  calculated cross section compared with data  ${}^{17)}$ .





2) by a comparison between calculated curves and the experimental points for angular distributions of photons following radiative capture in  $^{40}$ Ca of neutrons at the fixed energies indicated in fig. 6.

From the  $(n,\gamma)$  cross sections, the spectra of emitted  $\gamma$ -rays are obtained for  $E_n = 4-50$  MeV with  $\Delta E_n = 0.2$  MeV and for  $\theta_{\gamma} = 0^{\circ} - 180^{\circ}$ with  $\Delta \theta_{\gamma} = 10^{\circ}$ . From these spectra the photoproduction cross sections  $d^2\sigma(E_{\gamma}, \theta_{\gamma})/dE_{\gamma}$  dA and the angular distributions  $\Psi(E_{\gamma}, \theta_{\gamma})$  are obtained as average values for photons produced in a one-MeV energy interval.

Of course, the case of strictly monochromatic neutrons is not the most important in reactor technology. Attention should also be devoted to those neutrons having a continuous spectrum of energies; for example, resulting from scattering and other nuclear reactions after passing through the first wall, the blanket, and other structures of a reactor.

Fig. 6. Comparison between calculated <sup>16)</sup> angular distributions and those measured in refs.<sup>17)</sup> for the  $^{40}Ca(n,\gamma_0)$  reaction.

Therefore, for application purposes, knowledge of  $G' = \phi(E_n) \ \delta(E_{\gamma})$ , the photoproduction cross section  $\sigma(E_{\gamma})$  weighted to the relative incident neutron fluxes  $\phi(E_n)$  is of greater interest. As an example these values are calculated for incident energy distributions corresponding to neutron spectra from d+T and d+Li reactions.

In fig. 7 the calculated differential cross sections for gamma-rays produced by neutron radiative capture on  $^{40}$  Ca (fig. 7,a) and  $^{120}$  Sn (fig. 7,b) are plotted versus the photon energy for three fixed angles  $\theta_{\rm Y}$  =90°, 30° and 150° corresponding to curves 1, 2 and 3, respectively.



Fig. 7. Photoproduction differential cross sections for  $^{40}$  Ca (a) and  $^{120}$ Sn (b):  $1-\theta_{\gamma}=90^{\circ}$ ;  $2-\theta_{\gamma}=30^{\circ}$ ;  $3-\theta_{\gamma}=150^{\circ}$ .

The curves reproduce the distinctive feature of the giant dipole resonance, while no resonance-like shape can be connected to the position of E2- and E3-giant resonances. The presence of E2- and E3-radiation, however, highly influences the angular distributions of emitted photons. The E2- and E3-giant resonances are weak in  $^{40}$ Ca, so the angular distribution of photons is almost symmetric in the whole energy range considered (fig. 7,a). Conversely, the interference between opposite-parity transitions for the  $^{120}$ Sn(n, $\gamma$ ) reaction gives rise to cross section values which, for  $\theta_{\gamma} = 30^{\circ}$ , are greater in the high energy range by about a factor 2 with respect to those for  $\theta_{\gamma} = 150^{\circ}$  (fig. 7,b).

This situation is illustrated more distinctly in figs. 8,a ( $^{40}$  Ca ) and 8,b ( $^{120}$ Sn). On the left part of the figure photoproduction differential cross sections are plotted versus the cosine of  $\theta_{\gamma}$  for three fixed energies equal, for  $^{40}$ Ca, to 15, 25 and 50 MeV (curves 1, 2 and 3, respectively) and, for  $^{120}$ Sn, to 15, 22 and 35 MeV (curves 1, 2 and 3, respectively). On the right of fig. 8 the angular distributions are shown for the same photon energies. The latter clearly indicates a forward peaking, growing with energy for photons produced in the Sn(n, $\gamma$ ) reaction.

A similar strong forward peaking of high-energy photons is obtained for gamma-rays produced by neutron radiative capture in  $^{48}$  Ti and nat<sub>Ni</sub> as shown in fig. 9.

This asymmetry is particularly pronounced for capture to high-spin final states, which in the nuclei considered have a great statistical factor. For energies greater than about 20 MeV the asymmetry of the angular distributions would be further enhanced taking into account the isovector quadrupole giant resonance. This resonance is here ignored, its existence still being controversial<sup>18</sup>.

The three-dimensional representation of figs. 10 and 11 allows one to take a general look at the angular-energy dependence of the photoproduction cross section and angular distributions for the nuclei considered.

The  $\gamma$ -yields, integrated over the  $4\pi$  solid angle and weighted to three different incident neutron energy distributions ranging from 4- to 50 MeV, are plotted in fig. 12 for the  $^{120}$  Sn(n, $\gamma$ ) reaction. The incident fluxes shown in the inset to fig. 12 are: 1- a uniform energy distribution, 2- a distribution corresponding to part of the neutron energy spectrum from a d+T source, 3- a



Fig. 8.

Differential cross sections (left) and angular distributions (right) for gamma-rays from calcium (a) and tin (b). a):  $1-E_{\gamma}=15$  MeV;  $2-E_{\gamma}=25$  MeV;  $3-E_{\gamma}=50$  MeV. b):  $1-E_{\gamma}=15$  MeV;  $2-E_{\gamma}=22$  MeV;  $3-E_{\gamma}=50$  MeV. b):  $1-E_{\gamma}=15$  MeV;

distribution corresponding to part of the neutron spectrum resulting at 8° from 35-MeV deuterons incident upon lithium. As can be seen from fig. 12, curve 1, obtained for a uniform neutron-energy distribution and corresponding to those of part b of figs. 7-8, shows a resonance-like shape due to the presence of the giant dipole resonance. Curve 2, corresponding to neutrons from the d+T source, exhibits strong enhancement in the yield of 16- to 22 MeV photons with two distinct peaks both due to the neutron distribution and the level structure of the target nucleus. Curve 3, corresponding to the d+Li source, shows enhancement of the gamma-ray yield in the whole energy region from 10- to 30-MeV with a rapid decrease at higher energies.

The upper and lower sections of fig. 13 show the angular-energy dependence, of the  $\gamma$ -yields corresponding to the neutron energy distributions shown respectively in the insets 2 and 3 of fig. 12.

A similar plot is given in fig. 14 for the  $\gamma$ -yields from radiative capture of neutrons by natural nickel. In the left and right sections of fig. 14, the incident neutron fluxes correspond to the 4-20 MeV part of a neutron energy spectrum from d+T and d+Li reactions respectively. The left surface, corresponding to neutrons from the d+T source, shows strong enhancement in the yield of photons with  $E_{\gamma}>18$  MeV, the peak being displaced from ~17 MeV (fig. 9) to about 20 MeV. The right surface, corresponding to the d+Li source, exhibits a moderate enhancement of the  $\gamma$ -ray yield at the peak, and a decrease at higher and lower energies.

To our knowledge no experimental data on the cross sections for the production of 10- to 50-MeV photons are available, so direct comparison of the present calculations with experiment is not possible. However, the reliability of the present estimates can be inferred from the agreement of calculations with  $(n, \gamma)$  experimental data for capture of 6- to 15-MeV neutrons (see figs. 4-6).



Fig. 9. Upper: photoproduction cross sections for Ni,  $\theta_{\gamma} = 30^{\circ}(-)$ ,  $\theta_{\gamma} = 90^{\circ}(--)$ ,  $\theta_{\gamma} = 150^{\circ}(-.-)$ . Lower: angular distributions for  $^{48}$ Ti,  $E_{\gamma} = 12 \text{ MeV}(--)$ ,  $E_{\gamma} = 18 \text{ MeV}(--)$ ,  $E_{\gamma} = 35 \text{ MeV}(--)$ .











Differential cross section (left) and angular distribution (right) for  $\gamma$ -rays from the  $^{48}$ Ti(n, $\gamma$ ) and the  $^{nat}Ni(n,\gamma)$  reactions.





120Sn(n, $\gamma$ ) reaction. The  $\gamma$ -yields, integrated over the  $4\pi$  solid angle and weighted to the incident neutron energy distributions shown in the inset: 1 - uniform energy distribution; 2 - d+T neutron source; 3 - d+Li neutron source.





The angular-energy dependence of the  $\gamma$ -yields for the radiative capture by  $^{40}$  Ca and  $^{120}$  Sn of neutrons from a) a d+T source, b) a d+Li source.



Fig. 14.

Gamma-yields for the radiative capture by natural Ni of neutrons from a d+T source (left) and a d+Li source (right).

#### 4. Conclusions

These results show, that the strength and position of giant multipole resonances and the level structure of the final nuclei highly influence the angular distributions of high-energy  $\gamma$ -rays emitted by the constituents of the structural materials. The reliability of estimated angular distributions is closely related to the experimentallyknown values for the GMR parameters taken as input values in the calculations. The cross section magnitude depends mainly on the level structure and giant-dipole state parameters adopted. To improve the reliability of calculations more experimental data are needed on the GMR parameters, especially IVQR, and on  $(n, \gamma)$  cross sections in the high-energy range. It follows that DSD calculations based on the knowledge of the positions and strengths of giant multipole resonances, can allow useful predictions about the relative yield of high-energy  $\gamma$ -rays emitted in different directions with respect to incident neutrons. These calculations can be of interest in problems connected with the protection of fusion reactor components and with biological safety requirements.

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## SESSION

## PARAMETRIZATION OF OPTICAL MODEL, LEVEL DENSITY FUNCTIONS, GAMMA-RAY STRENGTH FUNCTIONS
Calculation of  $\gamma$ -ray Cascades in Code ALICE<sup>\*</sup>

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We describe the methods used to calculate  $\gamma$ -ray cascades in the code ALICE/LIVERMORE 300. Results are compared with experimental spectra for  ${}^{93}$ Nb (n,x $\gamma$ ),  ${}^{27}$ Al (n,x $\gamma$ ) and  ${}^{197}$ Au (n,x $\gamma$ ) at  $c_n = 9.5$ , 14 and 18.5 MeV (average bin energies), and for  ${}^{181}$ Ta (n,x $\gamma$ ) at 14 MeV: The  ${}^{93}$ Nb and  ${}^{181}$ Ta  $\gamma$ -ray spectra are also compared with results of the ENEA code PENELOPE.

## I. INTRODUCTION

The code ALICE is a nuclear reactions code which was designed for versatility and ease of use in the bombarding energy range of a few MeV to several hundred MeV.<sup>1</sup> The requirement of detailed input parameters was sacrificed to achieve these goals. The minimum input required to run ALICE is the target and projectile charge and mass numbers, projectile energy, and a title card.

Many options exist for types of reactions to be considered, e.g., heavy ion fusion-fission with angular momentum dependent fission barriers, light ion fusion-fission, precompound decay reactions and evaporation reactions. The ALICE code provides yields and spectra for all reactions populated by all combinations of n, p, d and  $\alpha$  decay, and can provide all input parameters internally (with the exception of the minimum input parameters listed above). The running time of the code is very short, being typically 0.5 sec on a CDC-7600 computer and 20 sec on a MICRO VAX.

The ALICE code has been successfully used to reproduce data of (HI, xnypzaf) reactions, (n,xnypzaf) reactions, photonuclear reactions for  $\epsilon_{\chi} \leq 140$  MeV, and stopped pion capture reactions. In this paper, we describe the addition of a routine to calculate  $\gamma$ -ray spectra from de-excitation of the excited nuclei formed during the precompound/compound reaction cascade. Excellent codes exist to accomplish this task with sophisticated physics and with detailed nuclear structure input. Our goal is to see how well we can do within the framework of the ALICE code, requiring no additional input information than required to run earlier code versions. A listing of the  $\gamma$ -ray subroutine and changes to the ALICE code required for the  $\gamma$ -ray calculation are in the appendix.

## II. ADOPTED TREATMENT OF Y-RAY CASCADES

## A. Equilibrium y-rays

The primary assumption made in the present treatment is that the preponderance of equilibrium  $\gamma$ -rays come from excited but particle stable nuclei. We therefore assume that where n or p may be emitted (i.e., the excitation energy exceeds the neutron binding energy or the p or a binding plus an increment for an effective coulomb barrier) there is no  $\gamma$ -ray competition. If this is so, we may sum populations of all residual nuclei as a function only of excitation, since we follow no discrete levels, nor do we keep account of spin and parity population.

This situation is summarized in Fig. 1, where we indicate at the bottom of the figure the summing up of all particle emission stable residual cross-sections as a function of residual excitation. The upper part of the figure pictorially represents the sequence with which the ALICE code considers all de-excitation paths by n, p, and a decay, giving the residual nucleus populations which we sum for the  $\gamma$ -ray cascade calculation. The summed populations  $\sigma(u)$  at each excitation energy u are next used to generate the  $\gamma$ -ray cascade.

<sup>107 \*</sup> This paper was published as preprint UCRL-95374 (1986).

108

We replaced the Fermi gas level density of ALICE

$$\rho(u) = u^{-5/4} \epsilon^2 \sqrt{\alpha(u-\Delta)}$$
 (Eq. 1)

by a constant temperature, form

$$\rho(u) \propto \frac{1}{T} e^{U/T}$$
 Eq. 2)

for residual excitations below the average neutron binding energy of the first two neutrons emitted. The constant temperature density was normalized to the Fermi gas form at the matching excitation  $U_{\chi}$ . The temperature was defined in the usual way as:

$$T = \sqrt{U_{x}/a}$$
 (Eq. 3)

where a = A/9 and  $U_x$  is the average neutron binding energy referred to above. These constant temperature level densities affected both particle emission and  $\gamma$ -ray spectra.

The  $\gamma$ -ray spectra are calculated using a Lorentzian form for the photon absorption cross-section, <sup>2</sup>

$$\sigma_{L}(c) = \sum_{R=1}^{2} \sigma_{R} = \frac{c^{2} \Gamma_{R}^{2}}{(c^{2} - E_{R}^{2}) + c^{2} \Gamma_{R}^{2}}$$
(Eq. 4)

where  $c_0 = 43.4 \ A^{-0.215}$ ,  $E1 = E_0 (1 - \beta/3)^2$ ,  $\sigma_1 = 0.0145 \ A/E1$ ,  $\Gamma_1 = 0.232 \ E_1$ ,  $E_2 = E_0 (1 - 0.16\beta)$ ,  $\sigma_2 = 0.0235 \ A/E2$ , and  $\Gamma_2 = 0.275 \ E_2$ . While B could be made an input parameter, we have simply set  $\beta = 0$  internally.

We assume only El radiation, so that the relative  $\gamma$ -ray cross-section from de-excitation of a population at excitation energy U with cross-section  $\sigma(U)$  is given by

$$\sigma_{\gamma}(c_{\gamma}) = c_{\gamma}^{2} \sigma_{l}(c) \rho(u) \sigma(u),$$
 (Eq. 5)

and this expression is normalized to the total emission to give absolute cross-sections.

Results of  $\gamma$ -ray spectra calculated with this formulation were found to be too soft. Prompted by this shortcoming, we made one additional assumption, that the levels accessible for each  $\gamma$ -ray transition were half the total. This may be justified by the argument that generally half the levels are even parity and half are odd parity, and El  $\gamma$ -ray transitions can populate only levels of a single parity for a given initial parity. Results of calculations with this modification are shown in Figs. 2-11. The agreement with experimental results is generally satisfactory, and we have adopted this approach for the code.

## B. Precompound y-rays

Some  $\gamma$ -rays of energy 15-22 MeV have been seen in 14 MeV neutron bombardment of several targets.<sup>5,6</sup> We have taken a purely empirical approach to reproduce these results for applications where high energy  $\gamma$ -rays, though in low abundance, may be important (e.g., in shielding calculations).

Our first step was in plotting the log of the experimental cross-sections versus log of residual excitation. This indicated a proportionality of the precompound  $\gamma$ -ray spectra to U and U<sup>3</sup>, similar to 3 and 5 exciton state densities. By considering the dimensionality, we parametrized the  $\sigma_{\nu}(c)$  as:

$$\sigma_{\gamma}(c) = \frac{\sigma_{R} c_{\gamma}^{2}}{AE^{2}} [k_{1} U + k_{2} \frac{U^{3}}{E^{2}}]$$
(Eq. 6)

where a fit to the <sup>59</sup>Co (n,x $\gamma$ ) data gave k<sub>1</sub>=0.0011 and k<sub>2</sub>=0.02B. In Eq. 6,  $\sigma_R$  is the projectile + target reaction cross-section, A is the target mass number, U the residual nucleus excitation energy and E the compound nucleus excitation energy. This algorithm is applied only to the compound nucleus. A total calculated <sup>93</sup>Nb(n,x $\gamma$ ) spectrum is shown in Fig. 12, including the high energy precompound  $\gamma$ -rays, compared with experimental results. We should emphasize that the procedure used for these high energy precompound y-rays is ad-hoc and arbitrary. It is not physics. The method may be useful for reactions induced by neutrons of around 14 MeV. Extrapolation to other regimes is unwarranted and dangerous, until such time as the algorithm may be tested versus experimental results for various projectile energies and target mass numbers.

## III. CONCLUSIONS

The Lorentzian line shape has been used for El radiation for equilibrium  $\gamma$ -ray emission in the code ALICE. No spins or parities are followed or retained in the calculation, and no additional input parameters are required with respect to the earlier code version. The results are in quite reasonable agreement with experimental spectra for the wide range of target masses considered.

## IV. ACKNOWLEDGEMENTS

109

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Figure 1 Diagrammatic representation of the ALICE de-excitation calculation, beginning with a composite nucleus of mass number A and charge Z. Precompound n and p are emitted, followed by equilibrium n,p,d and  $\alpha$ . The daughter products in turn decay by evaporation of n,p,d and  $\alpha$ . Each nuclide has a population  $\sigma_U$  versus excitation energy U. Following the conclusion of all n,p,d, $\alpha$  emission processes, all particle stable populations are added to give a single population distribution  $\sigma(U)$ , as shown at the bottom of Fig. 1. This summed buffer is used to calculate the  $\gamma$ -ray cascade.

U



Figure 2 Experimental  $^{27}A1$  (n,xy) data with 14.2 MeV neutrons compared with results of the ALICE calculation with T=  $\sqrt{E/a}$  below B<sub>n</sub>. Data are from Ref. 4.



Figure 3 As in Fig. 2 for 93Nb (n,xy) with neutrons of average energy 9.5 MeV. Data are from Ref. 4. The dashed histogram represents y-ray spectra calculated with the ENEA code PENELOPE.



Figure 4 As in Fig. 3 with 14.2 MeV average neutron energy. Data are from Refs. 3 and 4.



Figure 5 As in Fig. 3 for neutrons of average energy 18.5 MeV.



Figure 6 As in Fig. 3 for the 181Ta (n,xy) reaction with 14.2 MeV incident neutron energy. Data are from Refs. 3 and 4.



Figure 7 As in Fig. 2.





112



Figure 12 Comparison of experimental  $^{93}$ Nb (n,x $\gamma$ ) data for 14.2 MeV neutrons and ALICE calculation including the precompound algorithm. Data are from Refs. 3-6.

## CONSISTENT DESCRIPTION OF SHELL, SUPERCONDUCTIVE AND COLLECTIVE EFFECTS IN THE LEVEL DENSITY OF STRUCTURAL MATERIALS

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#### ABSTRACT

The paper presents the results of a level density analysis based on the superfluid nuclear model. Using the random phase method, the temperature dependence of the coefficients of vibrational enhancement of level density was studied. On the basis of the results obtained, a phenomenological approach was developed to describe the level density of spherical nuclei in the mass number range A=50-65 in which the shell effects of the single-particle spectrum, the pair correlations of the superconducting type and the increase in level density due to collective vibrational modes are taken into account.

#### 1. INTRODUCTION

The statistical approach has been used successfully for evaluating particle spectra and cross-sections in nuclear reactions at low and medium energies since in many cases the contribution of the compound process is dominant [1,2]. The state density of excited nuclei plays an important role in all practical applications of the statistical theory of nuclear reactions. Because of its simplicity, the Fermi-gas model is the one most widely used for describing the density of nuclear levels. The principal parameters of this model are the parameter "a", which is associated with the density of single-particle states near the Fermi energy, and the phenomenological parameter  $\delta$ , which allows the difference in the level density of even and odd nuclei to be taken into account [3,4]. However, analysis of the statistical properties of nuclei based on microscopic methods developed in studies of ground and low-lying states of nuclei has shown that the Germi-gas model does not take into account many important effects due to the shell structure of the singleparticle spectrum, pair correlations of nucleions of the superconducting type and coherent collective nuclear excitations [5-8].

The use of microscopic methods developed to describe ground and low-lying nuclear states has enabled systematic calculations of nuclear level density to be performed which include the shell structure of the single-particle spectrum and the superconducting-type pair correlations of nucleons [5]. This approach has provided a better understanding of the limitations of the Fermi-gas model and an explanation of a number of deviations from its predictions, in particular the features of the energy dependence of the level density of near-magic nuclei and the weakening of the influence of shell structure with increasing of excitation energy. However, with correct selection of average field and superconducting-type correlation interaction parameters, it has proved impossible with the independent quasi-particle model to describe for most nuclei and absolute value of level density at an excitation energy equal to neutron binding energy. These discrepancies are a direct indication of the existence in excited nuclei of fairly strong collective effects which are due to residual interaction of a coherent nature and lead to an increase in the excited state density of nuclei. Many examples of the experimental occurrence of such effects in various nuclear reaction cross sections have also now been stored [7].

The problem of consecutive separation of different types of coherent collective motion of nucleons has not yet been fully resolved. It appears that the influence of rotational effects on excited state density can be described for a wide range of excitation energies in an adiabatic approximation. The use of this approach has substantially improved the theoretical description of the neutron resonance density of deformed nuclei [9,10] and enabled a number of earlier inconsistencies in the interpretation of the energy dependence of nuclear fission cross sections to be eliminated [11]. Analysis of the contribution of vibrational motion is complicated by the fact that the adiabatic approximation cannot normally be used to evaluate it. These effects can be investigated using the combinatorial microscopic approach generalized to the region of highly excited nuclei by Solov'ev et al. [6]. A similar study based on thermodynamic methods of describing coherent excitations of heated nuclei was conducted in Ref. [7]. Unfortunately, sufficiently vigorous methods of calculating nucler level density are extremely laborious, what severely limits their practical application.

Research is urgently required to find a description of level density which takes into account of the main ideas of theory on the structure and properties of highly excited nuclei and at the same time is sufficiently simple and convenient for practical application. Ref. [9] is an example of such an approach: the authors have succeeded in constructing a phenomenological description of level density for heavy nuclei with A>150 which is in good agreement with the results of theoretical calculations in a Woods-Saxon potential scheme and with experimental data on neutron resonance density. Certain problems prevent the extension of such an approach to the lighter nuclei region. First of all, the rotational increase in level density is absent for spherical nuclei, and the contribution of vibrational motion can vary strongly from one nucleus to another. For transitional nuclei, both the adiabatic evaluation of rotational motion, and the liquid-drop evaluation of the stiffness coefficients which govern the average contribution of vibrational modes in deformed nuclei [9] may prove to be too rough. To overcome these difficulties it is very important therefore to have reliable experimental data on level density behaviour over a wide range of excitation energies. Unfortunately, direct experimental data on level density exist only for limited energy ranges, namely near the ground state and at neutron binding energy [3,4]. Indirect information on level density can be derived from an analysis of nuclear reaction cross sections and the spectra of the particles emitted therein.

The aim of this paper is to study the role of the vibrational increase in level density in a description of the existing set of experimental data.

2. ANALYSIS OF NEUTRON RESONANCE DENSITY IN A NON-INTERACTING QUASI-PARTICLE MODEL

Before examining the influence of collective effects, we shall discuss the differences between experimental data and the results of calculations of level density in a non-interacting quasi-particle (NQP) model. In the statistical approach the nuclear level density at a given excitation energy and angular momentum is calculated using the relation in Ref. [5]:

$$\mathcal{P}_{NQP}(U,J) = \frac{2J+1}{8JT^2G^3D_{e}t^{1/2}} \exp\left\{S - \frac{(J+1/2)^2}{2G^2}\right\}, \quad (1)$$

where the entropy S and the spin cut-off parameter  $\sigma^2$  are determined by:

$$S = \sum_{v} (2j_{v}+1) \{ t^{-1} E_{v} n_{v} + ln(1-n_{v}) \},$$

$$G^{2} = \sum_{v} j_{v} (j_{v}+1) (2j_{v}+1) n_{v} (1-n_{v}) / 3.$$
(2)

Here  $n_v = [1 - exp (E_v/t)]^{-1}$  is the average occupation numbers of quasi-particle states with energy  $E_v = [(\varepsilon_v - \lambda_{\tau})^2 + \Delta_v]^{1/2}$ ,  $j_v$  and  $\varepsilon_v$  are the angular momentum and the energy of the corresponding single-particle level. The chemical potentials  $\lambda_{\tau}$  and the temperature of the excited (heated) nucleus t are determined by the equations of state:

$$E = \sum_{v} (2j_{v}+1) \left\{ \varepsilon_{v} \left[1 - \frac{\varepsilon_{v} - \lambda_{\tau}}{E_{v}} (1 - 2n_{v})\right] - \frac{\Delta_{v}}{2E_{v}} (1 - 2n_{v}) \right\}$$

$$\frac{Z}{N} = \sum_{\nu}^{(\gamma)} (2j_{\nu}+1) \left[ 1 - \frac{\varepsilon_{\nu} - \lambda_{\gamma}}{\varepsilon_{\nu}} (1 - 2n_{\nu}) \right],$$
(3)

and the excitation energy U is related to the total energy of the nucleus E by the relation U = E(t)-E(t = 0). At full length the expressions for

the determinant of second-order derivatives Det as well as a more detailed treatment of the relations for thermodynamic functions (2) and (3) can be found in Ref. [12].

When calculating the level density, the correlation parameters  $\Delta_{v}$ , were used which depend both on the temperature of the nucleus and the quasi-particle state energy. Both these dependences are derived from the model considered in Ref. [12],

$$\Delta_{v}(t) = \Delta (\varepsilon_{v} - \lambda \tau) \varphi_{\tau}(t),$$

$$\Delta (\varepsilon_{v} - \lambda_{\tau}) = (\varepsilon_{v} - \lambda_{\tau}) sh^{-1} (\frac{\varepsilon_{v} - \lambda_{\tau}}{t_{\tau} cr}),$$
(4)

where the function  $\phi_{\tau}(t)$  characterizing the temperature of the correlation parameters is defined by the equation:

$$\Psi_{\tau}(t) = th\left[\frac{t_{\tau}cr}{t}\Psi_{\tau}(t)\right] \qquad (5)$$

The critical temperature  $t_{cr}$  of the phase transition from the superconducting to the normal state is related to the correlation function at the Fermi surface  $\Delta_r(0)$  by the relation:

$$t_{TCF} = \Delta_{\tau} (0) / 2.$$
 (6)

The difference between this model and the traditional superfluid one [15], in which matrix elements of the pair interaction are replaced by a constant, is manifested mainly in a slightly different connection between the critical temperature and the correlation function  $\Delta_{\tau 0}$  of the ground state of the system

115 
$$t_{\tau cr} = 0,567 \Delta_{\tau o}$$
. (7)

If for a given single-particle spectrum the correlation interaction parameters are selected so that the critical temperatures in the two models coincide, then the differences in the temperature and energy dependence of the level density and in other thermodynamic characteristics of the system will be negligibly small. This conditions satisfied by the parameter connection

$$\Delta_{\tau} (0) = 1,134 \bullet \Delta_{\tau 0},$$
 (8)

which we have used in all subsequent calculations. Figure 1 shows the energy dependence of the entropy, the spin cut-off parameter and the temperature of the  $^{56}$ Fe nucleus calculated using relations from both models. It is clear that the differences in the thermodynamic functions in the two approaches are very small. However, from the standpoint of calculations, the model used is simpler and more convenient for the purposes of analysing experimental data.

We calculated the neutron resonance density in the non-interacting particle model using a spectrum of single-particle levels of the Woods-Saxon potential and the correlation parameters obtained in Ref. [13] from an analysis of a set of experimental data on proton and neutron pair energies of spherical nuclei with 40 < Z < 60 and 50 < N < 90. A similar analysis was conducted for nuclei with 50 < A < 70 in which the parameters were assumed to the same as for the heavier nucleus range [13, 14]. The results of our calculations are given in Fig. 2a. The mean neutron resonance spacing is related to the level density by the correlation D<sub>theor</sub>. =  $\rho_{\rm theor}^{-1}$ , where

$$\rho_{\text{theor.}} \begin{cases} 1/2 \left\{ \rho(B_{n}, I_{o}^{+1/2}) = \rho(B_{n}, I_{o}^{-1/2}) \right\} \text{ for } I_{o} \neq 0, \\ \\ \\ 1/2 \rho(B_{n}, 1/2) \text{ for } I_{o} = 0. \end{cases}$$
(9)

116

Here I is the target nucleus spin and B is the neutron binding energy. The data given in Ref. [15] were used as the experimental values D . It should be pointed out that for many of the nuclei studied, and particularly the near-magic nuclei, the experimental errors for the mean resonance spacing are very significant. The different systematics of D for these nuclei diverge by several times. These divergences are illustrated in Fig. 2c which shows the ratios of the experimental data D\_\_\_\_\_ from Ref. [16] to those in Ref. [15], which we use as reference data. For purposes of comparison with our calculations, Fig. 2b shows the results of similar calculations of D /D carried theor. exp. out in Ref. [10] for the spectrum of single-particle levels of the Woods-Saxon potential, but using somewhat different potential parameters and another procedure for selecting the correlation functions. From an analysis of the results presented in Fig. 2, it can be concluded that it is not possible whith the independent quasi-particle model to obtain a self-consistent description of neutron resonance density for a wide class of nuclei. However, the independent quasi-particle model correctly reflects the shell structure and the influence of pair correlations on the level density energy dependence. It is natural to link the discrepancies that exist in the description of the experimental data on neutron resonance density to the existence of coherent effects of a collective nature which are not taken into account in the independent quasi-particle model. These effects will be considered in Section 4 below.

We should point out, however, that sufficiently rigorous microscopic methods for calculating level density are extremely laborious, and this severely restricts their practical application. Research is urgently required, therefore, to find a description of level density which takes into account the main ideas of theory and is at the same time simple enough and convenient to be used in practice.

## 3. PHENOMENOLOGICAL APPROACH TO LEVEL DENSITY BASED ON THE SUPERFLUID NUCLEUS MODEL

In the continuous spectrum approximation in Ref. [9] a phenomenological method (model) was worked out for calculating level

density which includes both shell effects and correlation of the superconducting type. Let us examine the main relations of this method, which are similar to the Fermi-gas model.

One of the chief parameters in this model is the correlation function  $\Delta_{o}$ ; according to (7), the critical temperature  $t_{cr.}$  of the phase transition from the superfluid to the normal state is directly related to this parameter. At temperatures above critical (t >  $t_{cr.}$ ), the equations of state differ from the Fermi gas equations of state only by the shift of excitation energy on condensation energy  $E_{cond.}$ :

$$U = at^{2} + E_{cond},$$
  

$$S = 2at = 2 [a(U - E_{cond})]^{1/2},$$
  

$$O^{2} = \frac{6}{2T^{2}} \alpha \overline{m}^{2} t, \quad Det = \frac{144}{2T} \alpha^{3} t^{5}.$$
(10)

Below the phase transition point (t < t ) we use the method developed in Ref. [12] to describe the same thermodynamical functions:

$$U = U_{cr} (1 - \varphi^{2}), \quad S = S_{cr} \frac{t_{cr}}{t} (1 - \varphi^{2}),$$

$$G^{2} = G_{cr}^{2} (1 - \varphi^{2}), \quad Det = Det_{cr} (1 - \varphi^{2}) (1 + \varphi^{2})^{3}.$$
(11)

In relations (11) the index "cr." denotes the corresponding values at the critical point for  $t = t_{cr}$ , namely:

$$V_{cr} = a_{ort} t_{cr}^{2} + E_{cond}$$
,  $S_{cr} = 2a_{cr} t_{cr}$ , (12)

$$G_{y}^{2} = \frac{6}{3\pi^{2}} \alpha_{y} m^{2} t_{y}$$
,  $Det_{y} = \frac{144}{3\pi} \alpha_{y}^{3} t_{y}^{5}$ .

Here and above it is assumed that  $m^2 = 0.24 A^{2/3}$ . The function  $\phi^2 = (I - \frac{U}{U_{cr.}})$  is related to the temperature by the equation:

$$\varphi = th\left(\frac{t_{\rm or}}{t}\varphi\right) \tag{13}$$

Solving this equation allows us to obtain the temperature corresponding to a particular excitation energy or, conversely, to find  $\varphi$  for a given t < t<sub>cr.</sub>, and then - with the help of Eq. (11) - to determine the remaining values. The condensation energy, which characterizes the reduction in ground state energy due to the correlation interaction, is determined by:

$$E_{cond} = \frac{3\alpha_{cr}\Delta_{o}^{2}}{2\pi^{2}}$$
(14)

In order to include shell effects in the consideration, it is necessary in relations (10-14) to use the value of the level density parameter, a, which has a certain dependence on the excitation energy. For this purpose we employ the relations:

$$a(U,Z,N) = \tilde{a} (A) \{1 + \delta \xi_{0} (Z,N) f(U)/(U-E_{cond})\},$$
  
$$\tilde{a}(A) = \alpha A + \beta A^{2/3},$$
(15)  
$$f(U) = 1 - \exp\{-\gamma (U-E_{cond})\},$$

which was successfully used earlier for the systematics of the level density parameters in the Fermi-gas model. In relations (15), "a" is the asymptotic value of the parameter "a" at high excitation energies,  $\delta \xi_0$  is the shell correction at nuclear binding energies (nuclear masses) and f(U) is the "universal" dimensionless function which determines the energy dependence of the parameter "a". The influence of

shell effects on in the superfluid phase (11) is reflected by the thermodynamical functions the value of the level-density parameter at the critical point  $a_{cr}$ , which should be determined from the equation

$$\alpha_{\text{Gr}} = \widehat{\alpha} \left\{ 1 + \delta \widehat{2} \circ \left[ 1 - \exp\left( - \gamma \alpha_{\text{Gr}} t_{\text{Gr}}^2 \right) \right] / \alpha_{\text{Gr}} t_{\text{Gr}}^2 \right\} . \quad (16)$$

The differences in the statistical characteristics of even and odd nuclei are determined by the ground state energy shift [9]. They can be obtained using the following values for the excitation energy in relations (10,11)

(0, for even-even nuclei;  

$$U^* = U + (\Delta_0, \text{ for odd nuclei}; (17))$$
  
( $2\Delta_0, \text{ for odd-odd nuclei}$ 

For the subsequent discussion it is important to note the following main features of the description used for the level density:

- 1. The correlation function for the ground states of nuclei was taken to be  $\Delta_0 = 12/\sqrt{A}$  MeV. This choice of  $\Delta_0$  agrees on average with the nuclear mass systematics in Ref. [17] and also with the results of the analysis of neutron resonance density of heavy nuclei [9].
- 2. The parameter  $\gamma = 0.064 \text{ MeV}^{-1}$  was kept the same as in the description of neutron resonance density of heavy nuclei in Ref. [9].
- 3. The asymptotic value of the level density parameter a = 0, III. A MeV<sup>-1</sup> was determined by comparing the phenomenological approach in question with the results of microscopic calculations of level density for a spectrum of single-particle levels of the Saxon-Woods potential [5].
- In calculating the level density parameters (see (15)) for shell correction, the values given in Ref. [17] were used.

118

The above relations (10-16) of the superfluid model are, of course, more complex than the simple expressions of the Fermi-gas model. However, such complication is unavoidable if we wish to achieve a consistent description of the level density over a wide range of excitation energies. The number of parameters defining an excited nucleus in the model considered remains the same as in the Fermi-gas model. The use of this model for the analysis and the systematics of experimental data thus seems highly promising.

## 4. ANALYSIS OF THE VIBRATIONAL ENHANCEMENT COEFFICIENTS IN A RANDOM PHASE APPROXIMATION

A feature of vibrational excitations in heated nuclei is the damping of collective low-energy modes due to the disintegration of coherent excitation into close-lying incoherent states of quasi-particle pairs. Using the temperature Green functions, it was shown in Ref. [7] that it is possible in a random phase approximation to write the variations of nuclear excitation energy and entropy induced by coherent effects in the form

$$SS_{\lambda} = \pm \sum_{i} (2\lambda + 1) \left[ \frac{\omega_{i}}{2t} \operatorname{cth} \frac{\omega_{i}}{2t} - \operatorname{In} \left( 2\operatorname{sh} \frac{\omega_{i}}{2t} \right) \right],$$

$$SU_{\lambda} = \pm \sum_{i} (2\lambda + 1) \frac{\omega_{i}}{2} \left( \operatorname{cth} \frac{\omega_{i}}{2t} - 1 \right),$$
(18)

where  $\lambda$  is the multipolarity of the vibrational excitations studied. The frequence spectrum  $\omega_i$  is determined by the secular equations [19]:

$$1 = \frac{x_{i}}{x_{i+1}} \sum_{jj'} \left| f_{jj'}^{(i)} \right|^{2} \left\{ u_{jj'}^{2} \frac{(E_{j} + E_{j'})(1 - n_{j} - n_{j'})}{(E_{j} + E_{j'})^{2} - \omega_{i}^{2}} - \omega_{i}^{2} \frac{(E_{j} - E_{j'})(n_{j} - n_{j'})}{(E_{j} - E_{j'})^{2} - \omega_{i}^{2}} \right\},$$

where

$$\mathbf{U}_{jj}$$
, =  $\mathbf{U}_{j}\mathbf{V}_{j}$ , +  $\mathbf{V}_{j}\mathbf{U}_{j}$ ,;  $\mathbf{V}_{jj}$ , =  $\mathbf{U}_{j}\mathbf{U}_{j}$ , -  $\mathbf{V}_{j}\mathbf{V}_{j}$ ,;  $\mathbf{U}_{j}$  and  $\mathbf{V}_{j}$ 

are the variational coefficients of the superfluid nuclear model,  $f_{jj}^{(\lambda)}$ , are the reduced matrix elements of the effective multipolar forces and  $\kappa_{\lambda}$  is the corresponding strength constant. In Eq. (18) the plus sign corresponds to the roots of the secular equation and the minus sign to the poles.

With an accuracy of up to insignificant changes in the pre-exponential factor, the level density taking into account collective effects can be presented in the form

$$\rho(U,J) = \rho_{NQP} (U,J) \kappa_{vibr} (U), \qquad (20)$$

where the coefficient of vibrational increase of level density is defined by the relation

$$K_{\text{vibr}} = \prod_{i} \left[ \frac{1 - \exp(-\omega_i^2/t)}{1 - \exp(-\omega_i^2/t)} \right]^{2\lambda + 1}$$
(21)

Here  $\omega_i$  and  $\omega_i^o$  are the roots and poles of Eq. (19) respectively. When the difference between  $\omega_i$  and  $\omega_i^o$  is small, the corresponding factor in Exp. (21) tends to unity, and hence a major contribution to the level density increase will be made only by coherent excitations for which the roots of the secular equation are shifted sufficiently strongly relative to the poles. The appearance in Exp. (21) of the statistical sums of the poles reflects the non-adiabatic nature of the effects under consideration.

The spectrum of solutions  $\omega_i$  of secular equation (19) depends strongly on the nuclear temperature, and this dependence is displayed directly in the behaviour of  $\kappa_{vibr}$ . Figure 3 shows, for a number of

nuclei, the temperature dependences of the coefficients of the level density increase due to quadrupol  $\kappa_2$  and octupol  $\kappa_2$  coherent modes [20]. The solid curves represent calculations which include temperature variations in the root and pole spectrum of secular equation (19), while the dotted curves correspond to calculations for the spectrum of roots and poles obtained at zero temperature. The effective force form factors in both variants were based on the self-consistent approach [21], but the strength constants were selected by the fitting to the position of the first vibrational levels in the cold nuclei. Let us pay attention to the characteristic maximum in the temperature dependence of  $\kappa_{a+}$  at t  $\simeq 0.7$  MeV in Fe and Sn nuclei. This non-monotonic dependence of the  $\kappa_2$  + coefficient is associated with the reduction - in the 0.5-0.7 MeV temperature range - of the correlation function  $\Delta(t)$  and of the corresponding rearrangement of the coherent excitation spectrum. Hence the disruption in a heated nucleus of pairing-type correlation effects leads to a considerable weakening of coherent effects in the quadrupolar nuclear excitation spectrum, and similar behaviour of  $\kappa_2$  can be expected in all nuclei with well-developed pairing. In contrast, pair correlations have only a very slight effect on the octupol excitation spectrum, and their disruption does not affect the temperature dependence  $\kappa_3^{-}(t)$ . This property of octupolar excitations already shows up in cold nuclei as a relatively weak energy dependence of the first 3 level of spherical nuclei on the nucleon composition.

In calculation of  $\kappa_{\rm vibr.}$  the selection of the effective interaction constants is of crucial importance. The influence of the strength constants on  $\kappa_{\rm vibr.}$  is similar to the analagous effect of the constants on the position of low-lying phonon nuclear excitations [22]. Thus, although calculations using a theoretical value of constants correctly depict the main qualitative characteristics of the behaviour of  $\kappa_{\rm vibr.}$  coefficients, it is better for a quantitative presentation of level density to correct the constant values on the basis of available data on the energy of the lowest collective levels. In so doing, it is advisable to retain the temperature dependence of constants [21] since this dependence may be essential for  $\kappa_{\rm vibr.}$  calculations in far-from-magic nuclei. The results of thermodynamic calculations of  $\kappa_{vibr.}$  can be compared with analogous values obtained from combinatorial calculations of multiphonon nuclear excitations in Ref. [6]. Table 1 shows the  $\kappa_{vibr.}$  values obtained for a number of nuclei by us and in Ref. [6] at an excitation energy equal to neutron binding energy. Ideologically, the two approaches are close and are based on the same Hamiltonian. However, since the relations used in the level density calculations differ substantially, this is reflected to some extent in the  $\kappa_{vibr.}$ values obtained. On the whole the values of the level density increase coefficients obtained in the two approaches are sufficiently close, at least for the nuclei considered in Ref. [6].

In comparing theoretical calculations of level density with experimental data, it is necessary to bear in mind that the description of collective effects in the random phase approximation underestimates the role of excitation damping. In cold nuclei low-lying collective states have a negligibly small damping width, while in heated nuclei the collective low-lying mode must be considered as a resonance with a significant width  $\sim$  2-3 MeV. This width results from the interaction of the collective mode with close-lying excitations of quasi-particle pairs, in other words its damping mechanism is similar to that of plasma oscillations [21]. Broadening of collective modes should occur also as a result of excited quasi-particle collisions. Strict treatment of collisions is a fairly complicated problem for which no satisfactory microscopic solution has yet been found in nuclear theory. However, a rough estimation of the effects that occur can be received if the relation defining the damping of zero-sound in Fermi-liquid theory [23] is used for the parametrization of the damping of vibrational excitation of heated nuclei:

$$\gamma(\omega,t) = \text{const } \omega^2 \left[ 1 + \left(\frac{2\pi t}{\omega}\right)^2 \right] \qquad (22)$$

Allowing for damping in secular equation (19) in the first approximation is equivalent to replacing the roots and poles of Eq. (18) by complex values, the imaginary parts of which are determined by the corresponding 120 width values (22). For the coefficients of vibrational increase in level density in this approximation, we obtained instead of Exp. (21) the relation [24]

$$K_{vi6r} = \prod_{i} \left[ \frac{(1 + e^{-\tilde{\omega}_{i}/t})^{2} - 4e^{-\tilde{\omega}_{i}/t} \cos^{2}(\tilde{y}/2t)}{(1 + e^{-\omega_{i}/t})^{2} - 4e^{-\omega/t} \cos^{2}(y/2t)} \right]_{(23)}^{\lambda + 1/2}$$

As an example, Fig. 4 shows the results of calculations of  $\kappa_2^+$  in the <sup>58</sup>Fe nucleus using different constants in Exp. (22). Phenomenologically, this constant can be evaluated from experimental data on the width of the giant quadrupol resonance  $\gamma = 2.5 - 3$  MeV. It is clear that allowing for vibrational mode damping yields a significant reduction in the coefficients of vibrational increase in level density only at excitation energies U = 10 - 15 MeV. At lower excitation energies the role of such damping is small compared with the temperature-induced weakening of coherent effects.

## 5. DESCRIPTION OF NEUTRON RESONANCE DENSITY IN A MICROSCOPIC APPROACH

It was demonstrated in Ref. [20] that neutron résonance densities calculated using the independent quasi-particle model depend strongly on the correlation parameters employed. For this reason the calculation of the neutron resonance density taking into account the coherent effects we performed first of all for near-magic nuclei such as Ni, Zr, Sn and Pb which have filled proton or neutron shells. This makes it possible to lessen the dependence of the calculations on the parameters of the superfluid model.

For these nuclei, the level density vibrational enhancement coefficients were calculated at an excitation energy equal to the neutron binding energy. For even-even nuclei, the effective interaction constants were selected from the fitting of experimental values of first vibrational level energy. The coefficients  $\kappa_{vibr.} = \kappa_{2+} \times \kappa_3$ obtained are shown in Fig. 5b [20]. When calculating these coefficients for odd nuclei, the strength constants were determined by extrapolating from adjacent even-even nuclei.

Figure 5a gives the ratios  $D_{theor}$ ,  $D_{exp}$ , obtained taking into account the collective enhancement in level density. It can be seen that including collective effects in the description eliminates the systematic excess of the  $D_{theor}$ , value over the experimental one which existed earlier for near-magic nuclei.

Let us look at certain details of the theoretical description. First, the value  $D_{theor}$ ,  $D_{exp}$  for the <sup>62</sup>Ni nucleus stands out. It was already found in the non-interacting particle model that  $D_{NQP}/D_{exp}$ , ~1, and that is why the inclusion of the collective increase gives D /D < 0.1. It should be pointed out here, though, that for this nucleus there are large discrepancies in the experimental data themselves  $D_{exp}$  [14]  $\approx 0.5 \times D_{exp}$ [15]. Accordingly, the lack of sufficiently accurate and consistent data on the experimental neutron resonance density values affects the magnitude of the discrepancy in D ... Further, while agreement between theory and experiment may generally be considered satisfactory, the situation is much worse for isotopes of tin and antimony with A > 120. Characteristic for such nuclei is the low contribution of collective modes of  $(r_{vibr.} = 2-3, Fig. 5a)$ . There are also large discrepancies between the D values calculated in the independent guasi-particle model and experimental data (Fig. 2a). It is possible that, to achieve a more consistent description of collective increase in level density, it will be essential to take anharmonic effects into account.

It can be seen from Fig. 5a that the inclusion of collective effects does not eliminate the irregular fluctuations of the ratio  $D_{theor}$ ,  $D_{exp}$ , which appeared earlier in Fig. 2a for nickel, zirconium, tin and lead isotopes. To eliminate these fluctuations, it seems necessary to conduct a more careful analysis of the average field parameters and pairing interaction constants and to perform fuller testing of the effective interaction constants with respect to both the position of the vibrational level and the corresponding transition probability.

6. PHENOMENOLOGICAL DESCRIPTION OF THE COEFFICIENTS OF VIBRATIONAL INCREASE IN LEVEL DENSITY

It follows from an analysis of Eq. (21) that a major contribution to  $\kappa_{\rm vibr.}$  is made only by those vibrational states whose energy  $\omega_{\rm l}$  is strongly shifted in relation to the energy of the two-quasi-particle state  $\omega_{\rm l}^0$ . Besides only excitations with an energy below the heated nucleus temperature (i.e.  $\omega < t$ ) make a notable contribution to  $\kappa_{\rm vibr.}$ . As nuclear excitation energy grows, so the coherent effects of a vibrational nature diminish [19,21], and under these conditions  $\omega_{\rm l}$  approaches  $\omega_{\rm l}^0$ . The corresponding cofactor in Eq. (21) thus tends to unity. It is therefore essential to take proper account of temperature variations of  $\omega_{\rm l}$  in order to obtain the correct value of the coefficient  $\kappa_{\rm vibr.}^{-1}$  at very high nuclear excitations [21].

It was shown in Ref. [19] that the following approach can be used to study coherent effects in heated nuclei: within certain energy ranges, the spectrum of vibrational states  $\omega$  should be treated as a single collective mode which has disintegrated into two-quasi-particle states. Following the energetically weighted sum rule, it is possible to determine the average energy of the collective mode

$$\overline{\omega}_{\lambda} = \sum \omega_{i} \beta_{\lambda}(\omega_{i}) / \sum \beta_{\lambda}^{2}(\omega_{i}), \qquad (24)$$

$$\omega_{1} < \omega_{i} < \omega_{2} \qquad \omega_{4} < \omega_{i} < \omega_{2}$$

where  $\omega_1$  and  $\omega_2$  are the boundaries of the energy region included in this mode and  $\beta_{\lambda}^2(\omega_1)$  are the deformation parameters. It is possible in the same way to determine the average two-quasi-particle excitation energy  $\overline{\omega}_1^{\circ}$ , which corresponds to the set of non-collective modes with energies  $\omega_1^{\circ}$ . In Refs. [19,25] a study was made of the temperature dependences of such modes and it was shown that  $\tilde{\omega}_{\lambda} \rightarrow \tilde{\omega}_{\lambda}^{0}$  at large excitation energies (t > 1 MeV). For nuclei with A = 50 - 70, it was also demonstrated that the overall contributions of vibrational states to level density, which were calculated using all the solutions of  $\omega_{1}$  from secular equation (19) and the average energies  $\tilde{\omega}_{\lambda}$ , are close to each other. In constructing a phenomenological description the temperature dependence  $\omega_{\lambda}$ (t) was approximated by the following relations:

$$\overline{\omega}_{\lambda} = \left[ \overline{\omega}_{\lambda}^{\circ} - \overline{\zeta}(t) \left( \overline{\omega}_{\lambda}^{\circ} - \omega_{\lambda}^{exp} \right) \right]^{1/2}$$
(25)

$$Z(t) = \exp\left(-ct^{2}/\omega_{\lambda}^{exp}\right), \qquad (26)$$

where  $\omega_{2+}^{\circ} = 20/A^{1/3}$  MeV,  $\omega_{3-}^{\circ} \simeq 41/A^{1/3}$  MeV and  $\omega_{\lambda}^{\exp}$  are the experimental values of the energy of the first collective levels  $2^+$  and  $3^-$ .

We used relations (22-26) to describe the energy dependence of the level density, with the constants of Exp. (22) and (26) obtained from an analysis of experimental data on level density of <sup>56</sup>Fe isotope. Figure 6 shows the temperature dependences of  $\kappa_{vibr.} = (\kappa_2^+) * (\kappa_3^-)$ for <sup>56</sup>Fe and <sup>60</sup>Ni nuclei. These dependences are close both to the results of the corresponding microscopic calculations [20] and to the behaviour of  $\kappa_{vibr.}$  (t) obtained in Refs. [26,27] for the <sup>56</sup>Fe nucleus on the basis of various empirical approaches.

The phenomenological description of the average energies (25) and the damping of corresponding excitations (22) was used then for the calculations of the coefficients (23) in many nuclei.

7. ANALYSIS OF LEVEL DENSITY OF ATOMIC NUCLEI OF STRUCTURAL MATERIALS

Within the framework of the phenomenological approach presented in this paper, experimental data on the level density of the following nuclei were analysed:  $51,53,54,55_{CT}$ ,  $55,56_{Mn}$ ,  $55,56,57,58,59_{Fe}$ ,  $58,59,60_{Co}$ ,  $58,59,60,61,62,65_{Ni}$ ,  $64,66_{Cu}$ . The reason for choosing these nuclei was that enough experimental data on level density exist for most of them both in the low excitation energy range [28] and at neutron binding energy [4,15,29]. For  $^{56}$ Fe,  $^{55}$ Mn and  $^{60}$ Ni nuclei experimental values of  $\rho(\upsilon)$  are also available in the high excitation energy range 17-23 MeV [30]. Figures 7-10 show the results obtained. In these Figures  $\rho(\upsilon)$  are presented in the form of histograms close to the ground state. The histograms were constructed in accordance with Ref. [28]. Experimental data on neutron resonance density as well as the theoretical description of such densities are shown in the inserts. For purposes of comparison, the results of  $\rho(\upsilon)$  calculations in the Fermi-gas model are also presented [4].

It is clear from Figures 7-10 that, in general, a satisfactory description was achieved for level density over a wide range of excitation energies. However, attention should be drawn to the principal differences in the selection of the parameters used in the different versions of the Fermi-gas model [3,4,15] and in the superfluid nuclear model presented by us. In the back shift Fermi-gas model, for example, the parameters for each nucleus considered were selected from existing experimental data on  $\rho(v)$ . In this case the level density parameters a and  $\delta$  lose their physical significance and become purely adjustment values. In the level density model proposed by us the parameters are determined from a detailed analysis of experimental and theoretical data on collective excitations in nuclei and also from an analysis of shell and superfluid effects. It is thus possible to conclude that our description of level density is based on physically meaning parameters. This is demonstrated clearly in those nuclei for which direct experimental information is not available. Examples of such situations are the description of the level density of 55,57 Fe (see Fig. 8) and

<sup>55</sup> Mn (Fig. 10) nuclei for which the experimental values of  $\rho(v)$  are not described satisfactorily by the Fermi-gas model [4].

Thus a sufficiently good description of the energy dependence of the level density of a number of spherical nuclei was obtained in the A=50-66 mass number range using the approach explained above. The choice of physically meaning parameters presented in thus paper gives us reason to hope that ourmodel yields correct level density values for those nuclei for which the experimental values of  $\rho(v)$  are not known at present. To study level density energy dependence further, it would be interesting to analyse experimental data on evaporation spectra in inelastic scattering reactions or in charged particle exchange reactions and to study excitation functions of threshold reactions.

### 8. CONCLUSION

A method has been examined for calculating the density of excited states of spherical nuclei in the A=50-65 mass number range in which account is taken phenomenologically of shell effects and their reduction as excitation energy grows, pair correlations of the superconducting type and the level density enhancement due to collective vibrational models. This method yields a good description of existing experimental data on level density in the iron region close to the ground state and at neutron binding energy. Its advantage compared with systematics based on the Fermi-gas model relations are that it takes into account important physical effects and makes it possible to select parameters to calculate level density when direct experimental data are not available. Information on particle spectra and the excitation functions of threshold reactions may be an effective means of improving our knowledge of nuclear level density in a wide range of energies. However, to achieve this it will be necessary to carry out a detailed analysis of the whole set of experimental data on both excitation functions and particle spectra in all competing channels, in which being used the correct current ideas regarding nuclear reaction mechanisms.

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Fig. 1: Dependence of entropy, spin cut-off parameter and temperature on the excitation energy of the <sup>56</sup>Fe nucleus in the superfluid model with traditional dependence  $\Delta_{\tau}(t)$ (solid lines) and with  $\Delta_{\upsilon} = \Delta$  ( $c_{\upsilon}$ )  $f_{\tau}$  (t) (dotted lines).



- Fig. 2a,b: Ratio of theoretical and observed average neutron resonance spacing obtained in this paper (lower part of figure) and in Ref. [10] (middle part of figure). Even-even nuclei are denoted by open circles (0), even-odd by closed circles (0) and odd-odd by crosses (+).
- Fig. 2c: Ratio of different systematics for D to the data  $D_{exp}$ , in Ref. [15].  $\triangle$  represents D from Ref. [16] and  $\square$ represents D from Ref. [4].



Fig. 3: Temperature dependence of the level density enhancement coefficient due to quadrupol (upper part of figure) and octupol (lower part of figure) coherent modes. The solid lines show  $\kappa_{vlbr}$  values calculated taking into account the effect of temperature on the phonon spectrum, and the dotted lines - without this effect.



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Fig. 4: Influence of excitation damping on the level density vibrational enhancement coefficient due to quadrupol coherent modes of the  $^{58}$ Fe nucleus. The dotted curve shows  $\kappa_{vibr}$ , without allowance for damping, and the solid and dot-dashed curves show  $\kappa_{vibr}$ , with allowance for damping for two values of the constant in relation (22).



Fig. 5: Nuclear level density enhancement coefficient at excitation energies equal to neutron binding energy (upper part of figure) and ratio of theoretical and observed average neutron resonance spacing (lower part).



Fig. 6a: Temperature dependence of average low frequency modes for quadrupolar (dotted line) and octupolar (solid line) excitations in <sup>56</sup>Pe and <sup>60</sup>Ni nuclei.



Fig. 6b: Temperature dependence of the level density vibrational enhancement coefficient obtained using the phenomenological approach for nuclei of <sup>56</sup>Fe and <sup>60</sup>Ni nuclei.









Experimental data on, and results of calculations of, the level density of \$1,53,54,55Cr nuclei. The solid curves were obtained taking into account shell and collective effects, and the dashed lines were obtained for the back shift Fermi-gas model [4].



As above, for SS.57.58.59Fe nuclei.

Fig. 9:

As above, for S6Fe, 60Co, 64,66Cu nuclei.



Fig. 10: As above, for <sup>56</sup>Fe, <sup>55</sup>Mn, <sup>60</sup>Ni nuclei.



G.D.H. PRE-EQUILIBRIUM EMISSION MODEL AND STATISTICAL MODEL PARAMETERS FOR STRUCTURAL MATERIAL FAST NEUTRON DATA CALCULATIONS

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## Abstract

Inclusion of the angular momentum conservation in the Geometry Dependent Hybrid (GDH) pre-equilibrium emission subroutine of the Hauser-Feshbach code STAPRE is discussed. The consistency of the statistical model nuclear level density and the equivalent particle-hole state density has been acyieved following a unitary use of an energy dependent level density parameter.

The neutron and charge particles optical model potentials selected from literature are commented. The El gamma-ray strength functions, used in the gamma-ray transmission coefficient evaluation, have been taken from an empirically modified energy-dependent Breit-Wigner (EDBW) model.

The proper account of the nuclear level density over a large energy range has been obtained through the use of the empirical back-shifted Fermi gas (BSFG) model, at medium excitation energies, and of a realistic analytical formula with microscopic suggested parameters at the high excitation energies. The necessary transition excitation range between the two different density approaches, in the mass range 40 < A < 65, has been discussed.

127

128 Introduction

The main goal of the Research Contract 3802/R1/RB is the achievement of pre-equilibrium emission and statistical model calculations of fast neutron activation cross sections and secondary particle energy distributions for the stable Fe, Cr, and Ni isotopes, in the incident energy range from threshold to 20 MeV. To improve the result accuracy a great care has been taken for:(i) as suitable as possible nuclear models, however with well enough established or able to be derived parameter systematics including all the nuclei of interest, (ii) use of consistent sets of input parameters, determined or validated by means of various independent types of experimental data, and (iii) unitary account of a whole body of related data (isotope chains and neighbouring elements). The present progress report concerns the first two points above.

## Nuclear models

The Hauser-Feshbach-Moldauer statistical model and the Geometry Dependent Hybrid (GDH) pre-equilibrium emission model have been involved in these calculations, using a local version of the computer code STAPRE. In the present work [1] inclusion of the angular momentum conservation in the GDH model is reported. The consistency of the statistical model nuclear level density and the equivalent particle-hole state density has been also achieved following a unitary use of an energy dependent level density parameter. GDH and Hauser-Feshbach calculations for proton

emission spectra from 15 MeV neutron induced reactions on <sup>46,48</sup>Ti isotopes have given a first validation of the present approach.

Statistical model parameters

a. Neutron optical model potential

The spherical optical model potential (OPM) parameters for the neutron transmission coefficient calculation in the energy range from few tens of keV to 20 MeV have been selected according to the SPRT method [2]. The experimental values of the:

- (i) s- and p-wave neutron strength functions,  $S_0$  and  $S_1$ [3, 4];
- (ii) potential scattering radii [3];
- (iii) total neutron cross sections of elemental chromium. from 1.0 to 4.5 MeV [5], of the isotope <sup>52</sup>Cr, compiled between 1.0 and 9.0 MeV [6], of the isotope <sup>58</sup>Ni, from 1.0 to 4.5 MeV [7], of elemental nickel, compiled between 0.1 and 30 MeV [8] and of the even nickel isotopes, compiled between 0.5 and 9.0 MeV [9]

have been compared with the calculated values using the OMP parameter sets of:

- (i) Pasechnick et al. [10] (global OMP parameter set);
- (ii) TUNL 82 [11], including particular parameter sets for <sup>54,56</sup>Fe and <sup>63,65</sup>Cu isotopes, derived through the analysis of the elastic and inelastic scattering of neutrons from 8.0 to 14 MeV, as well as a global parameter set finally deduced;
- (iii) Guenther et al. [5], obtained through a simultaneous fit of the elastic and inelastic scattering angular

<sup>\*)</sup> The references 1, 29 and 30 herein are counterparts of this Progress Report.

distributions for elemental chromium from 1.5 to 4.0 MeV incident energies and reproducing the total neutron cross sections;

- (iv) Arthur and Young [12], resulted from a simultaneous fit of the S<sub>o</sub> and S<sub>1</sub> strength functions and potential scattering radii, total neutron cross sections from 2.0 to 40 MeV and elastic scattering angular distributions from 6.0 to 14 MeV, for  $^{54,56}$ Fe target nuclei;
- (v) Kawai [13], which has been reproducing the total neutron cross sections of elemental nickel taking account of the systematic trends among neighbouring nuclei, from Ti to Cu isotopes, and has been also successfully used to describe the total and elastic and inelastic cross sections of the even nickel isotopes from 0.5 to 9.0 MeV [9], as well as in the JENDL-2 evaluation [14];
- (vi) TUNL 85 [8], deduced for the <sup>58,60</sup>Ni isotopes and neutron energies up to 80 MeV through an extension of the SPRT method.

The calculations have been performed with the spherical optical model (SOM) computer code SCAT2 [15]. The same OMP have been used to describe the interactions of neutrons with both the target nuclei (Fe, Cr, Ni isotopes) and the proton channel nuclei (Mn, V, Co isotopes) able to be involved in the (n, pn) reaction calculations. The comparison of the experimental and calculated strength functions and potential scattering radii is shown in Fig. 1. Finally, the following OMP have been selected to be used in Hauser-Feshbach calculations for:

- (i) the Cr isotopes: Guenther et al. [5] OMP for  $E_n \leq 4$  MeV and Pasechnik et al. [10] OMP for higher energies, where the latter one is giving total neutron cross sections close to the experimental data and intermediary between the predictions of the refs. [5] and [7] OMPs;
- (ii) the Fe isotopes: the OMP of Arthur and Young [12], confirmed by the particular OMPs of TUNL 82 [11] at the energies  $E_n \stackrel{>}{\sim} 5$  MeV (it is worthy of note the intermediate total neutron cross sections given by these OMP between the global parameter set [10, 11] predictions, at the higher energies);
- (iii) the Ni isotopes: the OMP of Kaway [13] for  $E_n \leq 10$  MeV and TUNL 85 parameter set at higher energies, where the lower total neutron cross sections given by the former underestimates the experimental data.

## b. Charged particle optical model potentials

Special attention has been devoted to the low energy behaviour of the proton OMP parameters and to the consistency of the low and high energies optical model predictions. The main point in the low energy region is the strong A - dependence of the imaginary surface potential depth  $W_D$  [16], while at higher proton energies questions arise from the differences between the predictions of the well known global OMP parameter sets of Perey [17] and Becchetti - Greenlees [18](as well as of those derived

- 130 on their base). The total reaction cross sections given by the following OMPs have been compared in the present work:
  - (i) the BARC potentials [16], for sub-Coulomb proton energies, with an empirical variation of the imaginary surface potential depth with the atomic number deduced from fits of the (p,n) reaction excitation functions of nuclei from  $^{45}$ Sc to  $^{80}$ Se and incident energies from ~2 to 5 MeV, as well as that covering the large proton energy range between 4 and 180 MeV, for medium weight nuclei;
  - (ii) the Arthur and Young [12] parameter set, acquires in the study of fast neutron interactions with the 54,56 Fe isotopes and derived from the OMP of Perey [17] to better fit the experimental cross sections of the low energy (p,n) reactions and the (p,n) and (p,2n) reactions on 56 Fe for incident energies up to 40 MeV (while this goal has been realized through the addition of an energy dependence to the imaginary potential depth, Haetrick et al. [19] extended this OMP's use to the study of the fast neutron interactions with the 63,65 Cu isotopes taking explicitly into account the real Coulomb correction term and isovector strength);
  - (iii) the recent OMP of Romanovskii [20]for the <sup>51</sup>V nucleus and energies ≤ 10 MeV, found to reproduce satisfactorily the experimental differential elastic scattering cross sections, polarization and total cross sections;
  - (iv) the OMP of Matsuzuki and Arai [21], derived from proton strength functions ( $E_p \approx 3$  MeV) in the mass region

30 < A < 70. The resulted energy dependence of the total reaction cross sections has been found however inadequate.

The following remarks have been made:

- (i) A proper account of the transition from the specific sub-Coulomb behaviour to the high energy trends of the global sets [17,18] is given by the particular BARC parameters up to  $E_p \approx 5$  MeV, followed by the global BARC OMP [16] (see Figures 2 and 3 for the <sup>51</sup>V and <sup>55</sup>Mn respectively).
- (ii) The total reaction cross sections given by the OMPs of BARC and Romanovskii for  ${}^{51}$ V are in the same agreement with the experimental data [20] (Fig. 2). Therefore, in spite of the Romanovskii's criticism [20] with reference to the BARC potential, the latter seems to be preferably, taking into account its global attribute and the purpose of the present work.
- (iii) The total reaction cross sections calculated for the <sup>56</sup>Mn nucleus (Fig. 3) with the OMPs of BARC [16] and Arthur and Young [12] are differing nearly by the same amount as those obtained with the OMPs of Becchetti -Greenlees [18] and Perey [17] (from which the first ones are derived) are. Consequently for n + Fe interactions the proton OMP of Arthur and Young will be used with priority.

The alpha particle emission has been generally described by means of the OMP of McFadden and Satchler [22], proved to be more adequate in the mass region A  $\approx$  50 [23]. The alpha particle OMP derived by Arthur and Young [12], adjusted to better fit the low energy ( $\alpha$ , n) data and also used by the ORNL group in the n + <sup>63,65</sup>Cu interaction study [19], is generating total reaction cross sections in close agreement with those given by the parameters of Mc Fadden and Satchler. Therefore the OMP of Arthur and Young [12] has been used in the calculations of neutron interactions with the Fe isotopes and those of McFadden and Satchler [22] for Cr (global set) and Ni (particular set number 2) isotopes.

## c. Gamma - ray transmission coefficients

The gamma-ray transmission coefficients have been related to the gamma-ray strength functions which are showing a relatively small variation for the isotopes of the same element [24]. The strength function  $f_{F1}(E_{y})$  for the electric dipole radiation - the dominant transition - has been taken according to the giant dipole resonance (GDR) model [24], while the strength functions for the M1. E2 and M2 transitions also taken into account are normalized to the first one, at the neutron binding energy, using the Weisskopf single-particle model [26]. Although the Lorentzian curve parameters usually involved to describe the GDRs do not greatly influence the Hauser-Feshbach calculations [27], the energy-dependent Breit-Wigner (EDBW) model [28] has been used concerning this goal. As the EDBW model is better reproducing the energy dependence of the experimental strength functions, compared to the Lorentz resonance shapes, but not also the absolute values, a further analysis of this model and its parameter systematics has been performed in the present frame [29]. Empirical correction factors for medium mass nuclei are finally taken

as representing the result of the exchange term contributions to the dipole sum rule and of the extent to which the sum rule is exhausted.

## d. Nuclear level densities [30]

Nuclear level densities of interest over a large excitation energy range, as required in statistical model calculations, are also investigated in the present frame [30]. A proper account of the nuclear level density has been obtained through the use of the empirical back-shifted Fermi gas (BSFG), at medium excitation energies, and of a realistic analytical formula with microscopic suggested parameters at the high energies. The BSFG model parameters have been determined by a least-squares fit of recent experimental total numbers of the low-energy discrete levels and s-wave neutron resonance spacings. The necessary transition excitation range between the two different density approaches, in the mass range 40 < A < 65, has been discussed.

## Work in progress

Based upon the above nuclear model parameters set up, GDH pre-equilibrium emission and Hauser-Feshbach calculations are performed for the (n,p),  $(n,\alpha)$  and (n,2n) reactions on Ti, Fe, Cr and Ni isotopes which are well experimentally described over a large energy range. The main calculational aspects which are investigated in these conditions are the pre-equilibrium approach and the nuclear level density at energies above the neutron binding energy. The former has to be validated through the analysis of the particle emission spectra, while the latter is expected to be established by the excitation function analysis.

131

132 Furthermore the (n,p),  $(n,\alpha)$ , (n,2n), (n,3n),  $(n,n^{\circ}p)$  and  $(n,n^{\circ}\alpha)$ reaction cross sections will be calculated for all stable isotopes on Fe, Cr and Ni from threshold to 20 MeV.

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Comparison of the experimental and calculated strength functions and potential scattering radii for the V (•), Cr (o), Mn (\*), Fe (•), Co (•) and Ni (□) isotopes. The experimental data are from Refs. [3, 4]. Fig. 1.

Total reaction cross sections for the system  $p + {}^{51}V$ . The experimental data are from: • -Ref. [20], • - Ref. [20] (other data corrected).

Fig. 2.

Total reaction cross sections for the system  $p + \frac{56}{Mn}$ .



133

# SESSION

## METHODS OF CROSS-SECTION EVALUATIONS

Neutron Scattering on Nuclei Near A=60 and A=90\*

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#### <u>Abstract</u>

Over a wide range of incident energies, the total cross section and angular distributions for elastic scattering of neutrons from nuclei in these mass regions are analyzed using the spherical-optical-statistical model. The effect of a real-surface-peaked potential, predicted by dispersion relations, is considered. It is found that when the data on a given nucleus between say, 4.5 and 10 MeV, are analyzed simultaneously one obtains a smooth energy variation of the optical model parameters. Moreover, this parameterization may be used to predict, quite accurately, at least the total cross sections up to 20 MeV. The parameters characterizing the model are quite different in the two mass regions. However, a comparison of the optical model results for  $^{89}_{\rm Y}$  and  $^{93}_{\rm Nb}$  indicates that near A=90 the real well parameters are nearly the same for the two nuclei and that the volume integrals of the imaginary potentials are similar.

In this paper we report on the theoretical analysis of neutron scattering data on targets in the A=60 and A=90 mass regions. Experimentally, we have acquired high quality data over a wide energy range (~ 2-10 MeV) on both the elastic angular distributions and the total cross sections for several nuclei in these regions. This data has been interpreted in terms of the spherical- optical-statistical model by use of the ANL code ABAREX. <sup>(1)</sup> The "ground rules" for modeling the data have been:

- 1. We require that the optical model parameters have a smooth energy variation and that the parameterization give the gross properties  $(\sigma_{total})$  outside the energy region of the fit.
- 2. The optical model parameters are determined by minimizing the function

$$\chi^{2} = \sum_{i=1}^{N} \left\{ \frac{\sigma_{expt}^{(i)} - \sigma_{theory}^{(i)}}{\delta \sigma_{expt}^{(i)}} \right\}^{2}$$
(1)

where N is the number of data points and

$$\sigma_{\text{expt}} = ((SN)^2 + S^2 + C^2 + \Delta \theta^2)^{1/2}$$
 (2)

In Eq. (2) SN is the systematic' normalization uncertainty which is independent of angle and is ~ 3%. S is the statistical error which Is ~ 1% except at the cross section minima, C is the uncertainty due to data correction procedures (e.g., multiple scattering corrections) which is ~ 1% except at the minima of the distributions and  $\Delta\theta$  is the angular uncertainty (in absolute value  $\Delta\theta \simeq 0.5^{\circ}$ ) which is obviously most important where  $\sigma(\theta)$  is changing rapidly.

We have actually used two different optical models to parameterize the data:

Model I - Conventional Model

V, the real potential, is assumed to have the Woods-Saxon form with diffuseness, a, radius, r,  $(R_v = r_v A^{1/3})$ , and depth, V<sub>0</sub>.

W, the imaginary potential, is taken to be a derivative Woods-Saxon well characterized by  $a_{\omega},r_{\omega}$  and  $W_{\omega}.$ 

 $v_{spin orbit}$  is the Thomas spin-orbit interaction which is assumed to be real and have well parameters  $a_{so}$ ,  $r_{so}$  and  $v_{so}$ .

The compound elastic scattering was calculated using the Moldauer modification<sup>(2)</sup> of the Hauser-Feshbach theory.<sup>(3)</sup> For odd A nuclei (which we shall discuss in this report) discrete levels up to approximately 3 MeV excitation energy were explicitly included. Above 3 MeV the statistical formalism of Gilbert and Cameron<sup>(4)</sup> was used.

Model II - Surface Real Potential Added

There is a dispersion relationship which connects the real and imaginary parts of the optical model potential  $^{(5)}$ 

$$V(r,E) = V_{WS}(r,E) + \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{W(r,E')}{E - E'} dE'$$
(3)

<sup>\*</sup>Work supported by U. S. Department of Energy, Nuclear Energy Programs, under Contract W-31-109-Eng-38.

where P implies the principal value integral. Thus, if W(r,E') is surface peaked this implies that the real part of the optical model potential should also have a derivative Woods-Saxon part. In Model II we include this component.

It should be stressed that the final optical model parameters, particularly in the A=60 region, often depend on the starting guess that one makes in the fitting procedure. Therefore, the parameters we quote may not be unique.

#### A=90 Region

For the purposes of this meeting the most important data to analyze would be the Zr results. However, we have not quite finished the experiments and analysis on this nucleus. On the other hand, we have extensive data and the analysis completed on the neighboring nucleus  $^{89}$ Y. In Fig. (1) we compare the angular distributions for 8 MeV neutrons scattering from  $^{89}$ Y and a natural Zr target. It is clear that the angular distributions are quite similar and, therefore, one would not expect the optical model parameters to change much in going from  $^{89}$ Y to Zr. Therefore, in order to illustrate our methods and the quality of the results we obtain in the A=90 region, we present an analysis of the  $^{89}$ Y data.  $^{(6)}$ 

Thirteen energies were involved in the fitting: 2.75 (simultaneous fitting of all results in the 1.5-4.0 MeV range), 4.5, 5.0, 5.5, 5.9, 6.5, 7.14, 7.5, 8.03, 8.4, 9.06, 9.5 and 10.0 MeV. At first we attempted a nine parameter fit to the data using the conventional approach. Model I, discussed above. The parameters were  $V_0$ ,  $a_v$  and  $r_v$  for the real potential and the analogous quantities for the surface imaginary and the spin-orbit interactions. Although an excellent fit to the data could be obtained, the parameters tended to spatter and one could detect no systematic energy dependence of them. We, therefore, studied the sensitivity of the fits to the various parameters and found that  $r_v$ ,  $V_{s0}$ ,  $a_s$  and  $r_s$  could be taken to be independent of energy and to have the values

$$r_v = 1.24 \text{ fm}$$
  
 $V_{so} = 5.75 \text{ MeV}$  (4)  
 $r_{so} = 1.025 \text{ fm}$   
 $a_{so} = 0.4 \text{ fm}$ 

However, a fit to the data required that the geometry of the imaginary potential vary with E, the incident laboratory energy of the neutron. An adequate representation of this energy dependence is

$$r_{W} = 1.5336 - 0.0255E \text{ fm}$$
  
a\_w = 0.1661 + 0.0284E fm (5)

With these constraints, we then minimized  $\chi^2$  of Eq. (1) as a function of  $a_v$ ,  $v_o$  and  $W_o$ . The angular distributions obtained by these fittings are shown in Fig. (2-a). The values of  $a_v$  and the volume integrals of the real and imaginary potential.

$$J_{V} = \frac{4\pi}{A} \int V(r)r^{2}dr' \simeq \frac{4\pi}{3} r_{v}^{3} V_{o} \left[ 1 + \left(\frac{\pi a_{v}}{R_{v}}\right)^{2} \right]$$
(6)

$$J_{W} = \frac{4\pi}{A} \int W(r) r^{2} dr \simeq \frac{16\pi R_{W}^{2} a_{W}}{A} W_{O} \left[ 1 + \frac{1}{3} \left( \frac{\pi a_{W}}{R_{W}} \right)^{2} \right] .$$
 (7)

are shown in Fig. (3) for each value of E considered. The energy dependence of these quantities was then determined by making a least squares fit to the empirically determined parameters. In this way, one finds that  $a_v$  and  $J_w$  are energy independent, whereas  $J_v$  decreases linearly with E.

$$a_{v} = 0.7033 \pm 0.0049 \text{ fm}$$

$$J_{w} = 66.47 \pm 1.29 \text{ MeV-fm}^{3}$$

$$J_{v} = 455.64 \pm 5.96 - (3.89 \pm 0.83) \text{E MeV-fm}^{3}.$$
(8)

The errors shown in Fig. (3) and quoted in Eqs. (8), are calculated on the assumption that the uncertainty at energy E is proportional to the value of  $\chi^2/N$ , where N is the number of observables at energy E. The proportionality constant was chosen separately for  $a_v$ ,  $J_v$  and  $J_w$  so that  $\chi^2$  per degree of freedom was unity for each of these quantities.

In Fig. (2-b) we show the predictions obtained when the optical model potential for  $^{89}$ Y is given by Eqs. (4), (5) and (8). From comparison of Figs. (2-a) and (2-b) we see that this characterization of the potential reproduces experiment almost as well as does the explicit three parameter fit at each energy.

As a test of the predictive powers of this potential, we have looked at gross properties outside the 1.5-10.0 MeV region. In Fig. (4) we compare the total cross section with the predicted values. Up to 20 MeV the total theoretical cross section is always within 1.35% of experiment.<sup>(7)</sup> Turning to low energies, theory gives a value of S<sub>o</sub>, the s-wave strength function, of  $0.1 \times 10^{-4}$  whereas the experimental value<sup>(8)</sup> is

13

 $(0.27\pm0.05) \times 10^{-4}$ . Although the theoretical prediction is outside the experimental error, one must remember that S<sub>0</sub> is small and that the theoretical estimate is extremely sensitive to  $r_w$  (in fact if  $r_w$  is changed by ~ 5%, theory and experiment are in agreement for S<sub>0</sub>).

Thus we conclude that a good fit to the  $^{89}$ Y data can be obtained with the smooth energy variation of the parameters given by Eqs. (4), (5) and (8). Moreover, this potential gives a good fit to the gross data from 0-20 MeV as well as a detailed fit to experiment in the 1.5-10 MeV range.

We now turn to fitting the yttrium data using Model II, which has a surface peaked real potential added to the usual Woods-Saxon well. According to Eq. (3), in order to estimate the strength of this added potential, one must know W(r,E') for all energies E', while our experiments only give information from 1.5 to 10 MeV. A further complication is the energy-dependent geometry of W. To simplify matters we have estimated the strength of the surface real potential using the volume integral of the imaginary potential in the following way:

- (i) In the range  $0 \le E \le 13.77$  MeV we assume  $J_{W}(E')$  is given by Eq. (8).
- (ii) For  $13.77 \le E' \le 57.22$  MeV we calculate, from the potential of Walter and Guss<sup>(9)</sup>

$$J_{W}(E') = 87.54 - 1.53E' MeV - fm^{3}$$
. (9)

At 13.77 MeV, Eqs. (8) and (9) give the same values of  $J_W$  so the function is continuous. Also, the Walter-Guss potential implies  $J_W$  vanishes at 57.22 MeV.

(iii) On the basis of the dilute Fermi-gas model it can be shown  $\binom{10}{10}$  that near the Fermi energy (approximately -9.1 MeV for  $\binom{89}{Y}$ ) W(E') is proportional to  $(E'-E_F)^2$ . Thus for  $-18.2 \le E' \le 0$  MeV we assume.

$$J_{m}(E') = 0.8029(E'+9.1)^{2} \text{ MeV-fm}^{3}.$$
 (10)

With these assumptions  $J_{\omega}(E')$  has a continuous value over the range -18.2

.

 $\leq$  E'  $\leq$  57.22 MeV. When Eqs. (8), (9) and (10) are inserted into the dispersion relationship, the volume integral of the surface peaked real potential is given by

$$J_{R}(E) = \frac{P}{\pi} \int_{-18.2}^{57.22} \frac{J_{w}(E') dE'}{E-E'}$$
(11)

Thus Eq. (3) becomes

$$V(r,E) = V_{WS}(r,E) + 4\lambda(E)W_{0}a_{W}\frac{d}{dr}\left\{\frac{1}{1+\exp[(r-r_{W}A^{1/3})/a_{W}]}\right\}$$
(12)

where  $V_{WS}(r,E)$  has been taken to be the usual Woods-Saxon potential and

$$\lambda(E) = J_{R}(E)/J_{\omega}(E)$$
(13)

With this added potential and the constraints of Eqs. (4) and (5),  $V_0$ ,  $a_v$  and  $W_0$  were varied so as to give a best fit to the data. Since  $W_0$  was allowed to vary, the fitting should have been done in an iterative manner, i.e. after a fit the values of  $J_R(E)$  should be recalculated, a new value of  $\lambda(E)$  computed, and then the fit repeated. However, this effect is small and the self-consistency criterion was not imposed.

The fits to the experimental data obtained in this way are almost as good as those arising when the conventional model is used. The values of  $a_v$  and the volume integral of  $V_{WS}(r,E)$ , denoted by  $J_{WS}$ , are shown in Fig. (5). In contrast to the constant value of  $a_v$ , Eq. (8), obtained with Model I,  $a_v$  now shows a quadratic dependence on energy. On the other hand,  $J_{WS}$  is independent of energy so that the entire energy dependence of the real potential comes from the principal value integral of Eq. (3). In Fig. (6) the volume integral of the imaginary and total real potential, V(r,E) of Eq. (12), are shown.  $J_w$  now shows a slight increase with E instead of the constant value it had in the conventional fit. The volume integral of the real potential, Eq. (12), has a complicated energy dependence arising from the dispersion integral. Eq. (11). However, within the energy range 1.5-10 MeV,  $J_v$  can be represented as a linear function of E. The energy dependences of the various parameters arising when Model II is used to fit the vtrium data are summarized in Table I.

To test the predictive powers of this model outside the 1.5-10 MeV energy range, we have used the value of J given in Table I to calculate new values for  $J_p(E)$  and  $\lambda(E)$  to be used in Eq. (12). When these results are combined with the parameterization given in Table I one predicts an s-wave strength function of  $0.257 \times 10^{-4}$  in excellent agreement with the experimental value of  $(0.27 \pm 0.05) \times 10^{-4}$ . As to the total cross section, the model overestimates experiment by 0.26% at 11 MeV and at 20 Mey underestimates it by 3.73%. Thus we obtain nearly as good a prediction for the total cross section using this model as is obtained with the conventional potential, despite the large differences in the parameterizations.

#### A=60 Region

In this region we have excellent experimental data, (11) ranging in energy from 0.36 to 10 MeV, for the nucleus  $^{59}$ Co. Therefore, in this section we present the results obtained when a fit is made to this data base using a spherical-optical-statistical model in which the real potential has a surface peaked component (Model II discussed earlier). Because fluctuations are evident in the neutron total and differential-elastic-scattering cross sections of cobalt to at least 4 MeV, we have been mainly concerned with fitting elastic scattering angular distributions at energies  $\geq 4.5$  MeV.

At higher energies the cross section at the back angle minimum  $(\sim 130\circ)$  is extremely sensitive to the spin-orbit interaction. The parameters of this potential were determined from a detailed survey of the 9-10 MeV data and were finally taken to have the values  $V_{c}$ =5.5 MeV,

 $r_{so} = 1.005$  fm and  $a_{so} = 0.65$  fm.

In determining the geometry of the real and imaginary potentials, we required that not only the elastic scattering angular distributions be reproduced but also that the predicted s-wave strength function and low-energy total cross sections be close to their experimental values. With these constraints it was found that the radii of both the real and imaginary wells could be taken to be independent of energy but that both diffusenesses had to vary linearly with E. The values chosen for these quantities are given in Table I. Having fixed seven of the nine opticalmodel parameters, a least-squares fit to the angular distributions was made minimizing  $\chi^2$  of Eq. (1) as a function of V and W. The added surface potential in Eq. (12) depends on the value of  $J_\omega$  through the dispersion integral, Eq. (3). In the case of Cobalt the added surface potential was calculated self consistently. That is, after a fit to the data was made a new value of  $J_{p}(E)$  was calculated and a new depth for the

$$J_{\omega} = 124.12 \pm 3.73 - (3.73 \pm 0.50)E$$
.

(14)

In computing  $J_{R}^{(E)}$  it was assumed that Eq. (14) represented  $J_{\omega}$  between 0 and 33.28 MeV, the energy at which J becomes zero. It was further assumed that J was continuous and symmetric about the Fermi energy,  $E_{\rm F}$  = -13 MeV, and that between 0 and -26 MeV J is proportional to  $(E-E_r)^2$ .

The fits to the measured angular distributions, shown in Fig. 7, are clearly comparable to those shown in Fig. (2-a) for  $^{89}$ Y. In Fig. (8-a) the volume integral of V<sub>WS</sub>, Eq. (12), is seen to be independent of the bombarding energy. Thus, as in the  $\Lambda$ =90 region, the entire energy dependence of the real potential comes from the dispersion integral. The total real potential, Eq. (12), has a complicated energy dependence, but within the 4.5-10 MeV range this dependence is more than adequately approximated by the linear dependence shown in Fig. (8-b) and given in Table I. Finally, from Fig. (8-c) one sees that the volume integral of the imaginary potential decreases with increasing energy with a best fit to the data being given by Eq. (14). Since the imaginary optical-model interaction is introduced to "mop up" those open channels which are not explicitly included in the analysis, one would expect the imaginary potential would either remain constant or increase with increasing energy since the number of open channels increases at higher energy. (12) Thus, although we obtain an excellent fit to the data, our imaginary potential seems to be unphysical. We have examined the possibility that this may be due to the neglect of volume absorption but find no evidence for this when we fit the data. However, we have shown (13) that if one trys to make a spherical-optical-model fit to "pseudo-data" obtained from a vibrational nucleus this unphysical energy dependence emerges. Thus the reason for this strange E-dependence in  $\frac{59}{Co}$  may be due to the fact that this nucleus is a vibrator.

Also shown in Fig. (8) are the results for  $J_{WS}$ , and  $J_{V}$  and  $J_{W}$  that emerge from fitting the iower energy data. In these cases, the distributions in broad energy intervals were fitted using the geometrical parameters and spin-orbit interaction given in Table I. However, the data strongly suggest significant fluctuations and moreover the potential strengths varied with the energy grouping. For these reasons, the values obtained in the low-energy region were not used in determining the "best fit" values for  $J_{y}$  and  $J_{u}$  given in Table I.

In Fig. (9) we show the predictions for the total scattering cross sections based on this model for  ${}^{59}$ Co. The entire data base available from the National Nuclear Data Center, augmented by the results of the present work, were averaged (over 100 keV to 1.0 MeV, over 200 keV from 1-5 MeV and over 500 keV at higher energies) to smooth fluctuations and reduce the number of experimental points to manageable proportions. The model calculations agree with the experimental averages to within a few percent from 1.5 to 20 MeV. The calculated results are slightly larger than observation about 12 MeV, but pass directly through the precision 14 MeV values. <sup>(14)</sup> From 0.5 to 1.5 MeV the model predicts significantly higher average total cross sections than indicated by experiment. This may, in part, be attributed to the absence of self-shielding corrections to the data. Alternatively, the concept of the simple optical model may not be valid at these low energies and, for example, the existence of doorway states, which are known to occur in this mass-energy region, <sup>(15)</sup> should be included. Finally, the model gives an s-wave strength function of  $3.6 \times 10^{-4}$  in excellent agreement with the experimental value, <sup>(8)</sup>

Thus, once again we have found a model that gives a good representation of the data and extrapolates quite adequately out of the energy range for which it was originally designed - particularly with regard to the total cross section at higher energies.

#### Summary

From Table I it is apparent that guite different optical model parameters are needed for cobalt and yttrium. If one compares the imaginary potentials, one sees that the interaction strength needed for  $^{59}$ Co is approximately twice that for  $^{89}$ Y. The energy dependence of this potential for vttrium is what one would expect physically, that is, in the 0-10 MeV incident energy range the imaginary strength increases with E. However, for cobalt the reverse happens, the strength goes down as E increases. As we have said before, this unphysical energy dependence may be caused by our treatment of cobalt as a spherical nucleus whereas in actual fact it may be a vibrator. A second major difference is in the radius  $r_{\rm u}$ , of the two wells. For  $^{59}$ Co this radius can be taken to be energy independent and is smaller than the real radius,  $r_{\rm u}$ , whereas for yttrium r, has a marked E-dependence and in the 0-10 MeV incident energy range is always larger than r. Since the imaginary potential "mops up" those channel and deformation effects not explicitly included in the calculation, it is not surprising that it has a different character in the two regions.

Turning to the real potential, once more there is a large difference in the parameters required. The radius  $r_v$  for  $^{59}$ Co is about 7% larger than the values needed in  $^{89}$ Y and although for the former nucleus only a weak dependence of  $a_v$  on E is required, for the latter a quadratic energy behavior is indicated. Because  $J_{WS}$  is energy independent for both cobalt

141

and yttrium (see Figs. (5-b) and (8-a)) the entire energy variation of  $J_{11}$ is given by the second term in Eq. (12). Therefore, the difference in the energy dependence of  $J_{ij}$  in the two regions is due entirely to the difference in the imaginary potentials. Although  $J_{wS}$  is constant in energy for each of the nuclei studied, the numerical values differ considerably in the two cases. The values read from Figs. (5-b) and (8-a), however, cannot be directly compared becasue the contribution from the dispersion integral was calculated differently in the two cases. For  $^{59}$ Co J<sub> $_{
m D}$ </sub> was assumed to by <u>symmetric</u> about E<sub>F</sub>, the Fermi energy, whereas it is clear from the integration limits in Eq. (11) that this was not taken to be the case for  $^{89}$ Y. If one does take J<sub>u</sub> to be symmetric about E<sub>p</sub> for the yttrium calculation one finds that  $J_{n}(E)$  is decreased by about 20 MeV-fm<sup>3</sup> and this decrease is almost independent of E in the range 0-10 MeV. Thus instead of the value 410 MeV-fm<sup>3</sup> one would read from Fig. (5-b), the appropriate value if the analyses had been done in the same way, would be

$$J_{WS}(^{89}Y) \simeq 430 \text{ MeV-fm}^3$$
, (15-a)

and this is to be compared with the cobalt value

$$J_{WS}(^{59}Co) = 505 \text{ MeV-fm}^{-3}$$
 (15-b)

Thus it is clear that the concept of a global optical model is not useful if one wishes to make a detailed fit to high quality data over a large incident energy range. However, it is possible that a regional optical model can be used. In Table II we compare the results of a conventional optical model fit (Model I) made to the <sup>89</sup>Y and <sup>93</sup>Nb data<sup>(18)</sup> in the incident energy range 1.5-10 MeV. Unfortunately, these fits were made using different assumptions about the experimental uncertainties,  $\delta\sigma_{expt}$ , of Eq. (1). For yttrium, as we have discussed, we attempted to make a careful estimate of the errors involved whereas in the niobium case the uncertainty was assumed to be purely statistical. For our method of taking data this means that  $\delta\sigma_{expt} \sim (\sigma_{expt})^{1/2}$ .

It is evident from Table II that the parameters of the real Woods-Saxon potential are almost identical. On the other hand, the imaginary potentials seem to be quite different in their geometry. However, this may be artificial since in the niobium analysis  $\mathbf{r}_{W}$  and  $\mathbf{a}_{W}$ were not allowed to have an energy dependence. Since the volume integrals,  $\mathbf{J}_{\omega},$  of the two potentials are similar in magnitude, it may turn

out that when these restrictions are removed the results for the imaginary potentials in the two nuclei will be comparable. Finally, since the spin-orbit interaction plays only a small role in the elastic scattering angular distributions at these energies and in this mass region (i.e. the back angle minima are not as deep as in cobalt) the differences shown in Table II are probably unimportant.

Thus from a comparison of these two nuclei it appears that a regional optical model might be quite successful with perhaps minor changes in the imaginary potential (to take into accout the different neglected channels in going from nucleus to nucleus) being required if a very detailed fit to the data is attempted.

<u>Table I</u>

Parameter r <sub>v</sub> (fm)	59 <sub>Co</sub>	<sup>89</sup> Y	
	1.33	1.24	
a <sub>v</sub> (fm)	0.62 - 0.001E	0.1916 + 0.0936E - 0.0043E <sup>2</sup>	
J <sub>v</sub> (MeV-fm <sup>3</sup> )	490.22 - 3.27E	445.30 - 2.14E	
r <sub>w</sub> (fm)	1.275	1.5336 - 0.0255E	
a <sub>w</sub> (fm)	0.279 + 0.01412E	0.1661 + 0.0284E	
J <sub>w</sub> (MeV-fm <sup>3</sup> )	124.12 - 3.73E	55.73 + 2.00E	
r <sub>so</sub> (fm)	1.005	1.025	
a (fm) so	0.65	0.4	
V (MeV) so	5.5	5.75	

A comparison of the optical model parameters used in the cobalt and yttrium calculations when the real potential has a surface peaked component as predicted by dispersion relations.  $r_v$  and  $a_v$  refer to the

radius and diffuseness of the Woods-Saxon part of the real potential whereas  $J_{ij}$  is the volume integral of the total real potential of Eq. (12).

 $\boldsymbol{J}_{\mathrm{u}}$  is a complicated function of the laboratory energy, E, measured in MeV.

Kowever, in the range 1.5 - 10 MeV it can be approximated by the linear E-dependence given in this table.

T	a	b	l	e	1	1

Parameter	89 <sub>Y</sub>	93 <sub>Nb</sub>	
r <sub>v</sub> (fm)	1.24	1.25	
a (fm)	0.7033	0.70	
V (MeV)	49.21 - 0.42E	47.34 - 0.25E	
J (MeV-fm <sup>3</sup> )	455.64 - 3:89E	445.34 - 2.38E	
r <sub>w</sub> (fm)	1.5336 - 0.0255E	1.30	
a <sub>w</sub> (fm)	0.1661 + 0.0284E	0.47	
J <sub>w</sub> (MeV-fm <sup>3</sup> )	66.47	51.97 + 2.99E	
r (fm) so	1.025	1.25	
a <sub>so</sub> (fm)	0.4	0.7	
V (MeV)	5.75	6.0	

A comparison of the optical model parameters used in the yttrium and niobium calculations when the real potential is only a volume Woods-Saxon interaction. E is the laboratory energy measured in MeV.

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142
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Fig. 1. The angular distribution for elastic scattering of 8 MeV neutrons from <sup>89</sup>Y ( $\frac{1}{K}$  data points) and natural Zr ( $\bigoplus$  data points). The results are plotted as a function of the laboratory scattering angle,  $\theta$ , and  $d\sigma/d\Omega$  is given in barns/steradian. The solid line is the optical model fit to the yttrium data.



0.85 r  $a_{\rm v}(fm)$ Α 0.60 4 60.0 ( J<sub>v</sub>(MeV-fm<sup>3</sup>) В 410.0 90.0  $J_w(MeV-fm^3)$ 40.0 10 0  $E_{lab}(MeV)$ 

Fig. 2. Comparison of measured and calculated neutron differentialelastic scattering cross sections of  $^{89}$ Y. The measured values are indicated by data symbols. Curves in (a) show the result when a three parameter fit, in which  $a_v$ ,  $V_o$  and  $W_o$  were varied, was made to the data. In this fit  $r_v$ , the spin-orbit potential and the imaginary geometry were given by Eqs. (4) and (5). The curves in (b) are the results obtained when the optical model potential was parametrized by Eqs. (4), (5), and (8). Fig. 3. The behavior, as a function of laboratory energy, of the diffuseness,  $a_v$ , of the real potential and the volume integrals of the real,  $J_v$ , and imaginary.  $J_w$ , potentials for neutron scattering from yttrium. The line in each case is the best fit to the parameters, see Eq. (8) of the text.



Fig. 4. Comparison of measured and calculated total neutron cross sections of <sup>89</sup>Y. The experimental values, indicated by the curve, are taken from Ref. 7. The calculated results, represented by circular symbols, are the optical model predictions based on Eqs., (4), (5) and (8) of the text.



Fig. 5 The diffuseness,  $a_v$ , and volume integral,  $J_{WS}$ , of the real Woods-Saxon potential ( $V_{WS}$ (r.E) of Eq. (12)) as a function of labortory energy for neutron scattering from yttrium. Both a linear and quadratic (curve with "tick" marks) fit to the  $a_v$ data are shown. The error bars are assigned as discussed in the text and their magnitudes chosen to give a  $\chi^2$  per degree of freedom of unity for the quadratic fit to  $a_v$  and the constant value of  $J_{WS}$ .





Fig. 6. The behavior, as a function of laboratory energy, of the volume integral of the imaginary potential,  $J_{W}$ , and the total real potential,  $J_{V}$ , including the surface-peaked contribution for neutron scattering from yttrium.



Fig. 7. Comparison of the measured (symbols) and calculated (curves) differential-elastic-scattering cross sections of neutrons on cobalt. The optical model which includes the surface peaked real potential predicted by dispersion relations (see Eq. (12)) was used. The geometric parameters and spin-orbit strength are given in Table I. The fitting at each energy was done by minimizing  $\chi^2$  of Eq. (1) as a function of V<sub>0</sub> and W<sub>0</sub>.



Fig. 8. The behavior, as a function of laboratory energy, of the volume integrals of the real Woods-Saxon well,  $J_{WS}$ , the total real potential,  $J_v$ , (see Eq. 12)) and the imaginary potential,  $J_w$ , for neutron scattering from cobalt. The line in each case is a best fit to these quantities and the uncertainties are assigned as discussed in the text.



Fig. 9. Energy-averaged neutron total cross sections (data symbols) compared with the model calculations (curve) for scattering from cobalt. The experimental data represent the complete files of the National Nuclear Data Center, augmented by the results of the present measurements. The method of averaging is discussed in the text.

## 148 NEUTRON INDUCED REACTION CROSS-SECTIONSOF IRON IN THE ENERGY RANGE 1 TO 20 MeV : A WORK PROGRAMME

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### ABSTRACT

Iron is one of the main constituents of stainless steel which is used as a structural material in nuclear reactors. In fast and conceptual fusion and fusion-fission hybrid systems the primary energy range of neutron interaction lies between 1 and 20 MeV which opens up several reaction channels. The reaction cross-sections in this energy range are important for dosimetry, radiation damage, neutronics and safety studies of nuclear reactors. Keeping this in view Nuclear Data Section of International Atomic Energy Agency has sponsored a Research Co-ordination Programme on Methods for the Calculation of Fast Neutron Nuclear Data For Structural Elements.

Under this programme we propose to study (n,n'), (n,2n), (n,3n), (n,p), (n,np), (n,pn),  $(n,\infty)$ ,  $(n,n\alpha)$ ,  $(n,\alpha n)$  and  $(n,\alpha)$  reaction cross-sections. Besides these, total, elastic and discrete level inelastic scattering cross-sections, angular distributions of neutron production cross-sections, neutron emission spectrum and charged particle emission spectra for protons and alpha particles will also be estimated.

We propose to investigate the above mentioned neutron interaction cross-sections with multistep Hauser-Feshbach, Kalbach exciton, Blann's Geometry Dependent Hybrid, Weisskopf-Ewing evaporation and Brink-Axel giant dipole models.

A literature survey of the measured cross-section data of iron, optical model parameters used by other investigators for neutron, proton and alpha particles and energy level parameters has been made. Computer codes utilizing some of the above listed nuclear models have been commissioned and tested. A brief report will be presented on the planned evaluation work programme and some of the preliminary results obtained.

# TRANSFORMATION FORMULAS FOR LEGENDRE COEFFICIENTS OF DOUBLE-DIFFERENTIAL CROSS SECTIONS

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## ABSTRACT

Approximate analytical formulas have been derived for the transformation of Legendre coefficients of double-differential continuum cross sections of two-body nuclear reactions from the center-of-mass to the laboratory system. A difference with respect to the transformation of elastic-scattering angular distribution coefficients is that the accuracy depends not only upon the target mass, but also on outgoing energies. A fast code has been written to transform Legendre coefficients of neutron inelastic scattering cross-sections. This code has been used to check the results for some simple problems with analytical solutions. For more complicated problems in which the energy spectrum is either an evaporation spectrum or a spectrum obtained from a (pre-)compound model calculation comparisons have been made with a recently introduced numerical integration method. The results are quite satisfactory provided that the target mass or the outgoing energy is not too low.

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#### 1. INTRODUCTION

In this paper we consider two-body nuclear reactions of which the ejectile is emitted into a continuum. The double-differential cross sections for these processes are denoted by:

$$\frac{d^2 \sigma (E, \varepsilon, \Omega)}{d \varepsilon d \Omega} \text{ or } \frac{d^2 \sigma (E, \varepsilon, \mu)}{d \varepsilon d \Omega}$$

where E is the incident energy,  $\varepsilon$  is the emission energy and  $\Omega$  is the solid-angle direction at scattering angle 0 ( $\mu = \cos 0$ ). The doubledifferential reaction cross sections can be calculated with nuclear models such as pre-equilibrium exciton models (see e.g. the review in [1]). In most cases the results are conveniently expressed by a Legendre polynomial series in the center-of-mass system:

$$\frac{d^{2} \sigma(\epsilon_{c}, \mu_{c})}{d \epsilon_{c} d \Omega_{c}} = \sum_{k} \frac{2k+1}{4\pi} F_{k}^{c}(\epsilon_{c}) F_{k}(\mu_{c}) . \qquad (1)$$

In Eq. (1) we have dropped the incident energy dependence (E) of the cross section and the coefficients  $F_k$ ; the index c denotes that the quantities are given in the center-of-mass system (c.m.). From a comparison of calculated data with experimental results or for reactor cal-culations these data need to be expressed in the laboratory system (lab.):

$$\frac{d^{2} \sigma_{\ell} (\epsilon_{\ell}, \mu_{\ell})}{d \epsilon_{\ell} d \Omega_{\ell}} = \sum_{k} \frac{2k+1}{4\pi} F_{k}^{\ell} (\epsilon_{\ell}) P_{k} (\mu_{\ell}) . \qquad (2)$$

For elastic scattering or for scattering to discrete nuclear states the transformation of the differential cross section  $\frac{d \sigma_c}{d \Omega_c} (\mu_c)$  to  $\frac{d \sigma_\ell}{d \Omega_\ell} (\mu_\ell)$  is well-known, see for instance the recent review of Bersillon et al. [2]. In these cases the emission energy  $\varepsilon_c$  in the center-of-mass system is a function of the incoming c.m. energy and the reaction Q-value.

After emission the energy  $\varepsilon_{\ell}$  is determined by the kinematics of the reaction and has become a function of  $\mu_{\ell}$ , Q, E and the masses of the particles involved in the reaction process. One could also eliminate Q and consister  $\varepsilon_{\ell}$  as a function of  $\mu_{\ell}$ ,  $\varepsilon_{c}$ , E and the masses. In Eqs. (1) and (2) we consider  $\varepsilon_{c}$  and  $\varepsilon_{\ell}$  as continuous variables, implying that also Q is a continuous variable. The relations between  $\varepsilon_{c}$  and  $\varepsilon_{\ell}$  remain the same, of course. However, whereas in the elastic (and discrete-inelastic) scattering cases the value of  $\varepsilon_{\ell}$  as fixed, determined by  $\mu_{\ell}$  and Q, we may select any values of  $\varepsilon_{\ell}$  and  $\mu_{\ell}$  in Eq. (2) that are physically allowed. Since in the continuum description Q is an (implicit) variable the relation between Eq. (1) and Eq. (2) is basically different from the one between  $\frac{d \sigma_{c}}{d \Omega_{c}} (\mu_{c})$  and  $\frac{d \sigma_{\ell}}{d \Omega_{\ell}} (\mu_{\ell})$ .

So far there are only two papers, dealing with the conversion of Eq. (1) to Eq. (2). In [3] and [4] the problem is solved by straightforward numerical integration methods, Here, we propose to follow a method somewhat similar to the one used for elastic or discrete-inelastic scattering by following a Taylor-series expansion. However, the small parameter in the expansion ( $\beta$ ) is different because it is a function of both incoming and outgoing energy. The approximation will be shown to work well for small values of  $\beta$ , this means for not too small target masses and not too small outgoing laboratory energies. This has been checked against the numerical method of Gruppelaar et al. [3]. Advantages of the present method are that no iterative procedures are followed and that the approximative analytical formulas are easy to use and lead to very fast routines. This means that the method could be introduced directly into a nuclear model code for calculating double-differential cross sections.

In Section 2 the transformation problem is formulated by expressing the laboratory Legendre coefficients into a series expansion with coefficients T. These coefficients are evaluated in Section 3. Some numerical test calculations are discussed in Section 4. The conclusions are summarized in the last section.

150

## 2. FORMULATION OF THE TRANSFORMATION PROBLEM

In this section the following quantities are used:

E, = projectile energy in lab. system;

ε, = ejectile energy in lab. system;

ε = ejectile energy in c.m. system;

- $\mu_{g}$  = cosine of scattering angle  $\Theta_{\chi}$  in lab. system;
- $\mu_{c}$  = cosine of scattering angle  $\Theta_{c}$  in c.m. system;
- m = projectile mass;
- m' = ejectile mass;
- M = target mass;
- M' = residual nucleus mass.

The relation between Eqs. (1) and (2) can be written as:

$$\frac{d^{2} \sigma (\varepsilon_{\ell}, \mu_{\ell})}{d \varepsilon_{\ell} d \Omega_{\ell}} = J (\beta, \mu_{\ell}) \frac{d^{2} \sigma (\varepsilon_{c}, \mu_{c})}{d \varepsilon_{c} d \Omega_{c}}$$
(3)

where the Jacobian is given by [5]:

$$J(\beta, u_g) = (1 + \beta^2 - 2\beta u_g)^{-1/2}$$
(4)

with:

$$\beta = \sqrt{\frac{\mathbf{m} \cdot \mathbf{m}'}{(\mathbf{M} + \mathbf{m})(\mathbf{M}' + \mathbf{m}')}} \sqrt{\frac{\mathbf{E}_{g}}{\varepsilon_{g}}}$$
(5)

Note that as a rule of thumb  $\beta \ll 1$  if  $\varepsilon_{g} \gg E_{g}/M^{2}$ , i.e. usually for all emission energies except the very lowest. It is further noted that the Jacobian (4) has a more simple structure than the one used in elastic or discrete-inelastic scattering. For the relation between the energies and angles in the two systems it is found that:

$$\epsilon_{c} = \epsilon_{\ell} \left( 1 + \beta^{2} - 2\beta \mu_{\ell} \right) , \qquad (6)$$

$$\mu_{c} = (\mu_{\ell} - \beta)(1 + \beta^{2} - 2\beta\mu_{\ell})^{-1/2} = (\mu_{\ell} - \beta) J.$$
(7)

We set out to determine the Legendre coefficients  $F_k^{\ell}$  which according to their definitions and Eq. (3) are equal to:

$$F_{k}^{\ell}(\varepsilon_{\ell}) = 2\pi \int_{-1}^{1} \frac{d^{2} \sigma(\varepsilon_{c}, \mu_{c})}{d \varepsilon_{c} d \Omega_{c}} J(\beta, \mu_{\ell}) F_{k}(\mu_{\ell}) d \mu_{\ell}.$$
 (8)

This expression is calculated - in different ways - in [2] and [3]. Here we insert Eq. (1) into (8) to obtain:

$$F_{k}^{\ell}(\epsilon_{\ell}) = \sum_{k'}^{K'} \frac{2k'+1}{2} \int_{-1}^{1} F_{k'}^{c}(\epsilon_{c}) J(\beta, \mu_{\ell}) P_{k'}(\mu_{c}) P_{k}(\mu_{\ell}) d\mu_{\ell},$$
(9)

where K' is the maximum order of the c.m. coefficients. In contrast to the situation in elastic or discrete-inelastic scattering we cannot take  $F_k^c$ , ( $\varepsilon_c$ ) out of the integral, because  $\varepsilon_c$  depends upon  $\mu_p$ .

In principle, the above problem can be solved by computing the integral (9) <u>numerically</u>, cf. [3] and [4]. The central idea of the present paper is, however, that we can gain more insight into the transformation problem discussed here with the aid of analytical methods. Below we will demonstrate that it is possible to obtain very accurate analytical approximations to Eq. (9), and in some cases even exact results, by taking advantage of the orthogonality and recurrence properties of the Legendre polynomials combined with power-series expansions in the small parameter  $\beta$ .

Accordingly, we proceed by expanding the first factor of the integral

of Eq. (9),  $F_{k}^{c}$ ,  $(\epsilon_{c})$ , into a power series as follows:

$$\mathbf{F}_{\mathbf{k}}^{\mathbf{C}}, (\varepsilon_{\mathbf{c}}) = \sum_{n=0}^{N} \frac{d^{n} \mathbf{F}_{\mathbf{k}}^{\mathbf{C}}, (\varepsilon_{\ell})}{d \varepsilon_{\mathbf{c}}^{n}} \cdot \frac{(\varepsilon_{\mathbf{c}} - \varepsilon_{\ell})^{n}}{n!} .$$
(10)

Since  $(\varepsilon_c - \varepsilon_l)^n$  is of the order of  $\beta^n$  according to Eq. (6) and  $\beta$  is small, it is justified to truncate this series at a small number N. In addition, this is also acceptable if the energy dependence of  $F_k^c$   $(\varepsilon_c)$  is weak.

Insertion of Eq. (10) into Eq. (9) now leads to the following result:

$$F_{k}^{\ell}(\varepsilon_{\ell}) = \sum_{n=0}^{N} \sum_{k'=0}^{K'} T_{kk'}^{(n)}(\varepsilon_{\ell}) \frac{d^{n} F_{k'}^{c}(\varepsilon_{\ell})}{d \varepsilon_{c}^{n}}$$
(11)

with generalized transformation coefficients:

$$T_{kk'}^{(n)} = \frac{2k'+1}{2} - 1 \int^{1} \frac{(\epsilon_{c} - \epsilon_{\ell})^{n}}{n!} J(\beta, \mu_{\ell}) P_{k}, (\mu_{c}) P_{k}(\mu_{\ell}) d\mu_{\ell}.$$
(12)

For n=0 these coefficients have a similar shape as those for elastic or discrete-inelastic scattering, except that the expressions for J and  $\mu_c$  are different. The evaluation of Eq. (12) is performed in the next section. The derivatives in Eq. (11) can be calculated from the known functions  $F_{\nu}^{c}$ , which are usually given in tabular form.

If the angular distribution is isotropic in the c.m. system Eq. (11) reduces to:

$$F_{k}^{\ell}(\epsilon_{\ell}) = \sum_{n=0}^{N} T_{k,0}^{(n)} \frac{d^{n} F_{0}^{c}}{d \epsilon_{c}^{n}} (\epsilon_{\ell}) .$$
(13)

Only one term (N=0) is needed if the energy distribution is uniform:  $F_0^c(\epsilon_c) = c$ . For a triangular energy distribution two terms are needed. In case of a realistic energy distribution three or more terms are generally required, cf. Section 4.

#### 3. EVALUATION OF TRANSFORMATION COEFFICIENTS

First we note that Eq. (12) can be expressed in terms of  $T^{(0)}$  coefficients by the following recurrent expression:

$$T_{kk'}^{(n)} = \frac{\beta \varepsilon_{\ell}}{n} \left[\beta T_{kk'}^{(n-1)} - \frac{2(k+1)}{2k+1} T_{k+1,k'}^{(n-1)} - \frac{2k}{2k+1} T_{k-1,k'}^{(n-1)}\right]. (14)$$

This exact expression is easily derived by means of the following relation resulting from Eq. (6):

$$(\varepsilon_{c} - \varepsilon_{\ell})^{n} = \beta \varepsilon_{\ell} (\beta - 2\mu_{\ell})(\varepsilon_{c} - \varepsilon_{\ell})^{n-1}$$
(15)

and the recurrence formula:

$$\mu_{\ell} P_{k} (\mu_{\ell}) = \frac{k+1}{2k+1} \left[ P_{k+1} (\mu_{\ell}) + \frac{k}{k+1} P_{k-1} (\mu_{\ell}) \right].$$
(16)

For the evaluation of

$$T_{kk'}^{(0)} = \frac{2k'+1}{2} - 1^{\int_{-1}^{1} J(\beta, \mu_{\ell})} P_{k'}(\mu_{c}) P_{k}(\mu_{\ell}) d\mu_{\ell}$$
(17)

we will express the first two factors of the integrand in a power series in  $\beta$ . The Jacobian J as given in Eq. (4) appears to be identical to the generating function of the Legendre polynomials. Accordingly, we have:

$$J(\beta, \mu_{\ell}) = \sum_{n=0}^{\infty} P_n(\mu_{\ell}) \beta^n.$$
(18)

For the Legendre polynomial with argument  $\mu_c$  an expansion into a Taylor series in powers of  $(\mu_c - \mu_c)$  is followed:

$$P_{k}, (\mu_{c}) \approx \sum_{p} \frac{d^{p} P_{k}, (\mu_{\ell})}{d \mu_{c}^{p}} \frac{(\mu_{c} - \mu_{\ell})^{p}}{p!},$$
 (19)

The p-th order derivatives can easily be written a sum over lower-order legendre polynomials in  $\mu_{\ell}$  using standard recurrence relations. The factor  $(\mu_{c} - \mu_{\ell})$  can be expressed as a power series, by employing Eqs. (7) and (18):

$$(\mu_{c} - \mu_{\ell}) = \sum_{m=1}^{\infty} \frac{1}{m} (\mu_{\ell}^{2} - 1) P_{m}' (\mu_{\ell}) \beta^{m}$$
 (20)

The final step is to calculate the integral (17) by inserting Eqs. (18) to (20), applying the orthogonality property of the Legendre polynomials, and sorting with respect to the various orders in  $\beta$ . The actual evaluation is elementary but tedious. The result can be summarized in the following expression:

$$T_{kk}^{(0)} = \beta^{q} s (k, k') \left[ 1 - \beta^{2} \frac{(k-q)(k+q+1)}{2(q+1)} \times \frac{2K^{2} - 2(q-1)K - 3q - 1}{(2K+3)(2K-2q-1)} \right], \qquad (21)$$

with K = max (k, k'), q = |k - k'| and: S (k, k') = 1 for k = k', (22.a)

$$S(k, k') = {\binom{K}{q}} \frac{\pi^{-1}}{\pi} \frac{k+q-2i-1}{2K-2i+1} \quad \text{for } k > k', \quad (22.b)$$

$$S(k, k') = (-1)^{q} {K \choose q} \prod_{i=0}^{q-1} \frac{k+q-2i}{2K-2i-1}$$
 for  $k < k'$ . (22.c)

The correctness of this formula has been directly checked up to q = 5. It is seen that for any given pair of values k, k' = 0,1,2,... the matrix element  $T_{kk'}^{(0)}$  is of the form:

$$\beta \left| \mathbf{k} - \mathbf{k}' \right| \cdot \mathbf{S} \cdot \left[ 1 - a\beta^2 + 0 \left( \beta^4 \right) \right] \, .$$

Thus, the relative accuracy is up to the order  $\beta^3$ . However, for isotropy in the c.m. system only the coefficients  $T_{k,\ 0}^{(0)}$  are required and these results represent the exact solution:

$$T_{k0}^{(0)} = \beta^{k} / (2k + 1) .$$
 (23)

In general the c.m. distribution is isotropic or almost isotropic at low emission energies. This means that even if  $\beta$  is close to 1 the approximation (21) will in practice be quite good.

For the calculation of  $F_k^2(\varepsilon_k)$  the coefficients  $T_{kk}^{(n)}$  are required. These coefficients are of the order  $\beta^n$  or  $\beta \begin{vmatrix} k-k' \\ kk \end{vmatrix}$ . So, the number of terms N in Eq. (11) should be  $N = \begin{vmatrix} k-k' \\ k-k' \end{vmatrix} + 2$  to keep the relative accuracy equal to the order of  $\beta^3$ . In practice values of N = 3 or 4 are often sufficient to obtain a small error in  $F_k^2(\varepsilon_k)$ , certainly if the higher-order derivatives in Eq. (11) are small.

In simple cases there will be a maximum value of n = N, just because the highest-order derivatives are zero. Trivial examples are isotropy in the c.m. system (K' = 0) with energy distributions according to a constant (N = 0) or a linear increasing function (N = 1). In these cases the exact expressions are available [3, 4], which are reproduced with the present method.

#### 4. NUMERICAL TEST CALCULATIONS

A computer code has been written in which N is equal to 4. If the Legendre coefficients in the c.m. system are analytical functions their n-th order derivatives can be supplied in a subroutine. This has been

coded for some simple cases mentioned in the previous section. The numerical results are virtually the same as those obtained from the exact analytical results given in [3] and [4].

A somewhat more realistic test is to assume an evaporation energy distribution, still with isotropy in the c.m. system:

$$F_{0}^{c}(\varepsilon_{c}) = a \varepsilon_{c} \exp \left[-\varepsilon_{c}/kT\right],$$

$$F_{k>0}^{c}(\varepsilon_{c}) = 0.$$
(24)

Using the analytical functions for the derivatives in Eq. (13), calculations have been made for neutron-inelastic scattering on a mediumlight target (A = 50) at incident energy  $E_{\ell}$  = 15 MeV. For the nuclear temperature the value kT = 1 MeV was adopted. The results for the coefficients up to k = 3 are given in Table 1 for outgoing energies  $\varepsilon_{\ell}$ varying from 0.01 to 10 MeV. A comparison has been made with the results of the GROUPXS code described in [3]. For  $\beta < 0.7$  the differences between the two results given in Table 1 are mostly less than 1%.

We have made more test calculations also for the realistic energy and angular distribution calculated with the GRAPE nuclear model code [6]. For this purpose a subroutine with our expansion method was introduced in the GROUPXS code [3]. The results of these calculations were in quite good agreement with those of GROUPXS. However, for the numerical determination of the derivatives in Eq. (11) a rather fine emissionenergy grid is required. In fact this is also required for the numerical integration method employed in GROUPXS. Some results of this intercomparison are given in Figure 1 for continuum neutron-inelastic scattering on lead at  $E_{\chi} = 15$  MeV and  $\varepsilon_{\chi}$  up to about 9 MeV (at higher energies a discrete-level excitation description is followed). The values of  $\beta$  vary from 0.19 at 0.01 MeV to 0.006 at 9 MeV. In the GROUPXS calculation the Legendre polynomials in the c.m. system are given by points with a prescribed linear-linear interpolation scheme. In our method the (higher-order) derivatives of  $F_{\mu}^{C}$  are determined numerically. The small differences between the results of the two calculations should be ascribed to the representation of the Legendre polynomials by means of a discrete grid rather than by a continuous function. Therefore, it is difficult to say which method is "best", because the grid size actually determines the uncertainties in both calculations. For high values of  $\beta$  the present method fails, but this may be a less interesting energy region in many applications. The calculation time for our method is very short, about 10 times faster than that of the integration method [3].

#### 5. CONCLUSIONS

The transformation of Legendre coefficients of double-differential continuum cross sections from the c.m. to the lab. system can be written in the form of Eq. (11) with coefficients that can be calculated by means of Eq. (14) and (21). Eq. (11) contains the (higher-order) derivatives of the Legendre coefficents in the c.m. system, which should be determined numerically or - in simple cases - from analytical representations. The relative accuracy of the present method is of order  $\beta^3$ , provided that N in Eq. (11) is not too small (cf. discussion in Section 3). For isotropic scattering the results of Eq. (21) are exact (equal to Eq. (23)). The method can be applied for values of  $\beta$  (Eq. (5)) smaller than 1, i.e. for not too low masses or not too low emission energies. Still good results may be obtained for  $\beta$  close to 1, if the distribution is nearly isotropic in the c.m. system.

Some tests have been made for simple problems e.g. an isotropic evaporation spectrum in the c.m. system and for realistic energy-angle distributions obtained from (pre-)compound model calculations. The results have been compared with those of a numerical integration method [3]. The conclusions from these tests are very satisfactory within the domain of validity of the approximation. The present method as well as the integration method of [3] require a very fine emission-energy mesh for the c.m. coefficients.

The present method gives more insight into the transformation problem. It is also very fast, which is convenient for the calculation of multi-group transfer matrices. It could therefore be introduced into nuclear model codes with the advantage that the transformation of c.m. distributions could be computed not only for first-particle emission, but also for secondary particle emission. This perspective is quite important, since all kinematic information for the calculation is available during the model calculation, whereas this information is lost or incomplete after storing the results of the calculation. A fast subroutine based upon the present approach may be very useful to obtain inclusive double-differential cross sections of the total neutron emission, without the currently made assumption that the secondary neutron emission is isotropic in the laboratory system.

#### ACKNOWLEDGEMENT

154

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<u>Table 1.</u> Comparison of  $F_k(\varepsilon_{\ell})(k=0,1,2,3)$  between the present transformation method and that of [3]. The evaporation spectrum and isotropic angular distribution are assumed in c.m. system. The masses of the target A, incident particle a and outgoing particle b are 50, 1, 1 respectively. The nuclear temperature kT = 1.0 MeV is used. The incident energy is  $E_{\ell} = 15$  MeV.

e	β	F <sub>O</sub> (mb/MeV)		F <sub>l</sub> (mb/MeV)		F <sub>2</sub> (mb/MeV)		F <sub>3</sub> (mb/MeV)	
(MeV)		Present work	Ref. [3]						
0.01	0.759	7.591	7.590	-1.393	-1.393	-0.194	-0.194	-0.0557	-0.0557
0.05	0.340	31.74	31.74	-3.038	-3.037	-0.269	-0.269	-0.0358	-0.0358
0.1	0.240	59.27	59.27	-3.675	-3.675	-0.299	-0.299	-0.0278	-0.0278
0.5	0.107	196.0	195.9	0.0161	0.0162	-0.299	-0.300	-0.0184	-0.0184
1.0	0.0759	237.7	237.7	6.012	6.012	-0.0895	-0.0913	-0.0129	-0.0129
2.0	0.0537	175.4	175.4	9.396	9.396	0.237	0.235	0.00027	0.00025
3.0	0.0438	97.13	97.11	7.072	7.071	0.285	0.285	0.00676	0.00673
4.0	0.0380	47.82	47.81	4.215	4.215	0.214	0.214	0.00726	0.00724
5.0	0.0340	22.07	22.07	2.234	2.234	0.133	0.133	0.00544	0.00543
6.0	0.0310	9.779	9.779	1.103	1.103	0.0734	0.0737	0.00344	0.00344
7.0	0.0287	4.213	4.213	0.519	0.519	0.0379	0.0381	0.00197	0.00197
8.0	0.0268	1.778	1.778	0.236	0.236	0.0186	0.0186	0.00105	0.00105
9.0	0.0253	0.7385	0.7386	0.105	0.105	0.00881	0.00890	0.000534	0.000537
10.0	0.0240	0.3030	0.3030	0.0455	0.0455	0.00406	0.00410	0.000262	0.000263

Comparison of coefficients  $F_k^{\ell}(\epsilon_{\ell})$  for k = 1, 2 and 3 between results of the present work (full lines) and those of GROUPXS [3] (crosses). The dashed lines represent the c.m. coefficients  $F_k^{c}(\epsilon_{c})$ . These data were calculated [6] to obtain the angular distribution of neutrons emitted after scattering on Pb at 15 MeV incident energy.

Fig. 1.

Neutron production from 14-MeV neutron on 27A1

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#### Abstract

Calculations of 14.5 Mev neutron cross sections on 27Al were performed in the frame of Hauser-Feshbach theory, generalized optical model and the exciton model for preequilibrium emission contributions.

In order to achieve a better agreement between theory and experimental data the necessity of a microscopic level density was shown.

#### Introduction

Aluminium is known to be a difficult case for the application of usual nuclear modelling methods, becouse it is carachterized by a pretty low mass number and by a pretty large nuclear level spacing even at relatively higher excitation energies. In addition aluminium is also deformed. All this peculiarities indicate the necessity of a particularly careful analysis.

We first analysed avalaible resonance parameter schemes in order to determine the necessary average resonance parameters and then, by use of ad hoc level density parameter systematics, we determined the complete level density parametrization.

We assumed contributions from reaction mechanisms via compound nucleus, preequilibrium and direct collective inelastic scattering.

The IDA /l/ modular system of codes was used to produce the inherent total cross sections, energy spectra and angular distributions.

The methods adopted are brievly summarized and results are shown against experimental data and discussed.

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The nuclear modelling

The equilibrium contribution was calculated according to the Hauser-Feshbach theory while the preequilibrium contribution was determined by use of the exciton model of ref.2 with inclusion of angular momentum conservation as in ref.3.

At first we tried our calculations in spherical optical model approximation according to Becchetti and Greenless/4/ parameters and with p-h level density described according to the usual William's formula/5/. In fig.1 our pure preequilibrium calculations (dotted dashed line) are compared with the data measured at Gaussig/6/ (full line). In order to try to improve our theoretical results we performed calculations with inclusion of Fermi motion and refraction, and using generalized optical model according to the method and parametrization in ref.7. As the latter attempt was unsatisfactory as well, we performed unified exciton model caculations (dashed line) with the inclusion, in addition, of spin dependent transition rates. As one can see, in all cases, very clearly,, theoretical results always give a wrong trend. This could be improved by changing the transition matrix element constant fom the usual value of 190 to at least 400 as can be seen in fig.2 , dashed line.

This result seemed to us particularly unconvenient becouse if we had to use a different transition matrix constant for different targets our nuclear modelling would loose much of its reliability, expecially in consideration of those cases where measurements are not available.

On the other hand, the idea that Aluminium has somewhat isolated levels up to several MeV excitation energy induced us to consider the effect of different p-h level density approaches in our calculations.

A microscopic approach to p-h level density.

Recently a microscopic approach has been developed/8/,/9/ for the calculation of all p-h configurations and their spin and parity distributions. this method is based on combinatorial calculations of all possible p-h configurations which can be generated from a shell model spectrum of single particle states. In particular configuration energies are determined in the frame of the BCS theory.

In fig.3 the ratio is considered of the final to initial p-h level density for the two typical configurations dominating the neutron prequilibrium emission in 28A1. The dashed line gives the ratio calculated according to William formula when no pairing correction is introduced. The dotted dashed hystogram gives the ratio according to our microscopic approach, when the shell model basis is taken from SeegerHoward/10/. The full line histogram gives the same when the shell model basis is taken from Nix-Moller/11/.

From what one can see, one can make immediately a few very important observations. Microscopic calculations, much more realistic then William's formula, exhibit large fluctuations which directly come from the large spacings between Al nuclear levels. Such fluctuations will never be reproduced by any statistical approach like Williams' one. This nuclear structure effect, however, appears to depend on the adopted shell model basis. In particular the energy gap, as a sum of the shell and of the pairing gap, is 3 MeV according to Seeger-Howard and 5 MeV according to Nix-Moller. As a matter of fact this gap is rather important becouse it determines the threshold for the preequilibrium emissions and therefore can be checked experimentally.

Here below we present results of cross section calculations by use of microscopic p-h level density.

#### Results and discussion

In fig.4 results of our calculations are compared with experiment. We found 33 and 126 degrees two very significative angles. In this calculations we used the usual value of 190 for the transition matrix element costant. The dashed hystogram gives the collective inelastic scattering contribution, while the full line one gives the contribution to neutron emission from n=3 exciton configurations, according to Nix-Moller basis. As one can see the 5-MeV gap of fig. 3 implies a deep in the neutron emission cross section wich correspond exactly to the separation between direct inelastic and preequilibrium contributions. This deep is pretty close to the trend of the experimental data. Fig.3 and fig.4 well explain the failure of the previous calculations already shown in fig.1 in term of Williams' formula and the necessity of encreasing the transition matrix element costant in order to reproduce better the measurements. In fig.4 it also appear that the preequilibrium contribution is practically negligible at backward angles. For completeness in fig.5 we give the pure compound nucleus calculation (dotted hystogram) and the total cross section (dashed hystogram) as a sum of the 3 different reaction mechanisms assumed, the full line hystogram including the contributions of all other neutron emissions from multiple particles emission processes. Fig.5 indicates that, as expected compound nucleus contributions dominate at backward angles, while they are completely negligible at all angles above 10 MeV emitted neutron energy. Similar conclusions can be drawn from figs.6 and 7 where angle integrated energy spectra are shown. In fig.8 the full and the dashed line respectively give the n=3 exciton preequilibrium contribution according to Seeger-Howard and Nix-Moller basis respectively. The dotted line includes the n=5 exciton contribution, according to Nix-Moller. the latter contribution being not very important, also becouse it has a threshold of 10 MeV.

Calculation of total gamma-ray emission according to the same model parameterization and with inclusion of both equilibrium and preequilibrium contributions are given in contribution /11/, presented at this meeting.

#### Conclusions

From the above considerations we feel we can conclude that use of Williams' formula should be made with more caution becouse cases exist where this formula really does not hold at all. Using the latter formula in some cases would imply forcing the model parametization so that conclusions of more general validity would be prevented.

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Fig. 7 Total neutron emission spectrum at 14.5 MeV. Dotted Hystogram gives the pure equilibrium contribution. Full line gives the sum of all n,n and n,2n contributions from equilibrium, preequilibrium and direct-collective mechanisms. Dashed line represents the calculated cross sections when all other n-emission processes are included.



Fig. 8 Full line and dashed line gives n=3 contribution when using Nix-Moller or Seeger Howard shell models respectively. Dotted-dashed line gives the sum of n=3 and n=5 contributions according to Nix-Moller shell model

# OPTICAL-STATISTICAL CALCULATIONS OF THE CHROMIUM NEUTRON CROSS-SECTIONS

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## Abstract

The quality of  $\mathfrak{S}_t$  and  $\mathfrak{S}_{nn'}$  neutron cross-section description of  $5^2$ Cr in the E < 5 MeV region has been analyzed. The impact of uncertainties in the calculated transmission coefficients at low energies on nearthreshold cross-sections of compound-processes accompanied by a neutron emission has been discussed. It has been shown that the introduced energy dependence of a potential diffusivity makes it possible to describe a specific minimum in the chromium total cross-section at E ~0.8 MeV and to improve the description of  $\mathfrak{S}_{nn'}$ .

At neutron energies of several MeV, it becomes necessary to calculate transmission coefficients of emitted charged particles. To perform such calculations, the procedure is proposed to eliminate the uncertainty in the choice of optical potential parameter sets. It has been shown that the depth of a real part of the optical potential can be approximated by the linear function of a reduced particle-nucleus mass.

The neutron transmission coefficients, calculated using an optical model (OM), are the input data for calculation of compound cross-sections and uncertainties in  $T_\ell$  (E) can considerably complicate the parametrization of statistical models. For statically nondeformed nuclei of a medium mass, a spherical OM is a sufficiently reliable method for obtaining  $T_\ell$ . Near the threshold, the calculations of neutron-emission reaction cross-sections should consider the transmission coefficients at the exit channel at low energies, i.e. in the region where the OM calculation meets considerable difficulties.

Fig.1 presents the calculations of the total chromium crosssection with the sets of optical potential parameters suggested in Ref. [1-4]. It is seen that the potentials [2,4] fitted at E > 2 MeV fail to describe the  $\overline{\bigcirc}_{\tau}$  minimum in the 0.6-0.8 MeV region. At the same time, the Kawai potential [1] which decreases the cross-section in this region, underestimates  $\bigcirc_{\tau}$  at higher energies. It results from underestimation of the absorption crosssection, which is seen in Fig.2, where the curves obtained by use of the given potential parameters are compared with the elastic scattering cross-section data.

Apart from experimental data on the total and elastic scattering cross-sections of [2,5,6], Fig.1 and 2 give the CJD-2 evaluation [7] averaged over the 200 keV intervals.

An increase of the chromium total cross-section at energies exceeding 0.8 MeV seems to be explained by appearence of the inelastic scattering channels in this energy region. To take into consideration this process in OM, an attempt can be made to introduce a strong energy dependence of the depth of an imaginary potential of a step-like or more complicated form.

Alternatively, strong nuclear vibrational excitations can cause the washing-out of a nucleus surface which can be modeled by a change in the potential diffuseness.

To investigate the possibility of describing the neutron scattering by chromium nuclei in the B < 5 MeV region, the Pronjaev potential [8], suggested for iron, was taken as the starting set of optical potential parameters:

$$V_{R} = 52.16 - 0.36E MeV$$

$$W_{D} = 5.0 + 0.16E MeV$$

$$V_{so} = 6.2 MeV$$

$$T_{R} = r_{so} = r_{D} = 1.24 \text{ fm}$$

$$a_{R} = a_{so} = a_{D} = 0.48 \text{ fm}$$
(1)

As directly applied to the chromium, it fits the total crosssection at low energies and considerably underestimates it at E > 2 MeV.

Some versions of the energy dependence of potential parameters were verified. It was found that the introduction of the E-dependence for a diffuseness of the potential within the energy range up to 3.5 MeV seems to be optimal. In so doing, the diffuseness increases by the law:  $\alpha = \alpha_0 + \alpha_1 E$ , where  $\alpha_0 = 0.42$  fm,  $\alpha_1 = 0.067$  fm/MeV. At the energy of 3.5 MeV, diffuseness becomes equal to 0.62 and further remains constant.

162

The total and elastic scattering cross-sections calculated using the above mentioned potential parameters are presented by a solid line in Fig. 1 and 2. It is seen that the shape of curves agrees with an averaged evaluation of CJD-2 and experimental data over the whole energy region considered.

All the calculations are performed by the "ABAREX" code, where the spherical optical model and the Hauser-Feshbach-Moldauer statistical model are realized [17]. The inelastic scattering crosssection for the  $5^2$ Cr 2<sup>+</sup> (1.434 MeV) level is calculated for the potential parameters mentioned (Fig.3). The contribution of a direct excitation was calculated by the "ECIS-79"-code using the couple-channel method realized by Raynal [18]; and potential parameters of Ref. [19] with allowance for a 6-level coupling. It is to be noted that, according to the calculations, an account of two levels leads to the overestimation of  $G_{nn'}^{2^+dit}$  (by about 50-70% at E = 3.0 MeV).

Potential parameters with the energy dependence of diffuseness provide a better description both in the  $\overline{O}_{nn}$ ' maximum region and in the excitation function fall-off at E > 3 MeV. However, as seen from the figure, we failed to describe the Karatzas et al. threshold experimental data [15] using different potential parameters both in an absolute value and form. In this case, we seem to meet the principal limitations of the OM analysis of neutron scattering processes.

For structural materials beginning with the energy of some MeV, the (n,p), (n,  $\propto$ ), ( n,d) reactions become energetically feasible. Therefore, transmission coefficients of emitted charged particles should be calculated. However, the choice of suitable potential parameters faces some difficulties due to scarcity of experimental data, as well as to uncertainties of the V<sub>o</sub> R<sup>2</sup> type attributed to the OM formalism. As an example, we can take two sets of optical potential parameters for  $\propto$ -scattering by mediummass nuclei, that are widely used for calculations:  $V_{\rm R}$  = 50 MeV,  $r_{\rm R}$ = 1.7 fm,  $\alpha_{\rm R}$  = 0.567 fm recommended by Igo [9], and  $V_{\rm R}$ =185 MeV,  $r_{\rm R}$ = 1.4 fm,  $\alpha_{\rm R}$ =0.52 fm by McFadden [10]. At small differences in real part geometric parameters, the potential depths differ

almost fourfold, which indicates the principal contradiction between them and the fact that additional information has to be involved to remove it.

Such additional information might be the evidence about the interaction nature in the nucleus-particle system and, in particular. about the behaviour of a wave scattering function in the region of small Y . This problem is sufficiently well studied for the processes of mutual scattering of light nuclei on the basis of a resonating-group method [11]. As shown in Ref. [11], the existence of states forbidden by the Pauli principle is explained by a nodcharacter of the wave function with the nods position stable in a rather wide range of energies. This conclusion served as a basis for broad calculations and investigations of optical potentials for d = 4He, d = 3He, d = 2D, T = 3He, n = 4He systems [12-14]. that obtained thereby a microscopic substantiation. A principally new proof in such an approach was the statement that to describe successfully the scattering process, it is necessary that the interaction potential would give a correct structure of bound states of the system being not only permitted but also forbidden by the Pauli principle. The potential parameters for the given scattering systems are presented in Table 1 and for the first sight, they do not show certain regularities. However, if a plot of the potential real depth versus a reduced particle-target mass is drawn (see Fig.4), it turns out that this dependence can be approximated linearly:

$$V_0 = (67 \text{ }\mu - 13) \text{ MeV}, \text{ where } \mu = \frac{m_1 m_1}{m_1 + m_2} \text{ (a.e.m.)} (2)$$

For the scattering of nucleons by medium-mass nuclei, this formula gives the value of the potential depth of the order of 50 MeV. It agrees well with the calculations of the single-particle level structure using the Woods-Saxon potential and with the result of the empiric fitting for the neutron scattering description.

The potential real depth values calculated from formula (2) can serve as the starting data for precise determinition of the potential parameters when the total set of experimental data is described. Besides, such a calculation can serve as an additional criterium for selecting the one of numerous sets of parameters of potential having the radial Woods-Saxon dependence.

As seen, the formula leads to the potential of a substantial depth. So, its extrapolation into the region of  $\not{\alpha}$  -particle scattering by medium-mass nuclei (  $\mu = 3-4$ ) gives  $\nabla_R \sim 188-255$  MeV. This value contradicts to the data by Igo [9] and serves as a basis for selecting the McFadden potential parameters [10] to calculate transmission coefficients for  $\not{\alpha}$  -particle emission at the fast neutron interaction with chromium isotopes.

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Table 1.		Optical model potential parametrs obtained for
		description of the light mass systems scattering.

System Parame- ters	d - <sup>2</sup> D	n - <sup>4</sup> He	d- <sup>4</sup> He	d - <sup>3</sup> He	T-3He
V <sub>R</sub> , MeV	75.5	43.5	125.0	98.0	83.5
r <sub>R</sub> , fm	1.85	1.70	1,78	1.80	1.85
a, fm	0.71	0.65	0,66	0.70	0.71





Fig.2. The total elastic scattering cross-section for <sup>nat</sup>Cr and calculational results obtained with different sets of the optical potential parameters: notation the same as in Fig.1.

Experiment:  $\mathbf{I} = [2]$ ,  $\mathbf{A} = [5]$ ,  $\mathbf{A} = [6]$ ,  $\mathbf{e}$  = averaged evaluation of CJD=2[7].



Fig.3. The inelastic scattering cross-section for the first  $2^+$ level of  $5^2$ Cr (B=1.434 MeV). The calculations used transmission coefficients obtained with different sets of the optical potential parameters: the notation same as in Fig.1. Experiment: • -[15], = -[6],  $\Delta$  -[16],  $\circ$  -[2].



Fig.4. Depth of an optical potentials real part for describing the light system scattering process [12-14] as a function of the reduced mass system.

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