International Atomic Energy Agency

INDC(AUS)-7/G
~~Supplement~~
Full report.

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Technical Co-operation Interregional Project on Nuclear Data Techniques and Instrumentation (INT/1/018)

Report on a Training Course on Nuclear Data Evaluation and Processing Techniques

held at the

Nuclear Data Centre
Instituto de Estudos Avançados
Centro Técnico Aeroespacial
BR-12.200 São José dos Campos, S.P., Brazil

from 15 November - 17 December 1982

by B. Strohmaier
Institut für Radiumforschung und Kernphysik
University of Vienna
Boltzmanngasse 3
A-1090 Vienna

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

Reproduced by the IAEA in Austria
April 1983
83-02211

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G E N E R A L R E P O R T

1. Task

The subject of this IAEA lecturer's mission was Data Evaluation and Processing Techniques, in particular the theoretical aspects and the practical use of nuclear reaction model computer codes. The use of such codes for the evaluation of nuclear data to be applied in nuclear reactor neutronics calculations is one of the recently started activities of the Nuclear Data Centre of the Instituto de Estudos Avançados of the Centro Técnico Aeroespacial, and therefore this course aimed at training the staff there in methods of nuclear data evaluation based on nuclear model calculations. The full report including lecture notes is available from the IAEA Nuclear Data Section as supplement to this report.

2. The Institute

The Instituto de Estudos Avançados (IEAv) is one of the institutes which belong to the Centro Técnico Aeroespacial (CTA) and comprises departments for nuclear energy, laser, theoretical physics and computing. The other four institutes belonging to the CTA are concerned with aeronautic technology, aircraft engine structure, space activities (missiles) and research and development concerning aviation. The Nuclear Data Centre involves collaboration of the groups for nuclear energy, theoretical physics and computer science, and also will cooperate with an experimental physics department to be founded in connection with the construction of an electron linear accelerator which is expected to become operative in 1986. The IEAv is located in new buildings outside the CTA campus several kilometres from the centre of São José dos Campos.

3. Participants

The course was mainly addressed to the members of the evaluation group which is part of the department for theoretical physics and consists of Dr. Helio Dias, Ricardo Afonso

do Rego, Tobias Frederico, Milton Pereira Isidro Filho and Jairo Fiorentino. The latter four persons are students at the University of São Paulo. This evaluation group participated in the theoretical and the practical part of the course; the theoretical lectures, moreover, were attended by up to five (mostly graduate) persons belonging to the reactor physics group of the nuclear energy division or other departments of the IEAv.

4. Activities

The course was divided up into a theoretical and a practical part. Theory was presented in two lectures per day, 45 minutes each, starting at 8.15 and 9.15 a.m. The practical part consisted of more loosely organized "workshops" held on many days in the late morning and everyday in the afternoon. During these workshops all steps of the evaluation procedure were exercised by treating sample problems. The used computer codes ABACUS, IUPITOR and STAPRE had been installed at the CDC Cyber 170/750 at the IEAv already, more recent versions as well as small subsidiary programs for preparing input data and processing results I had brought with me. Advice was given with input preparation, output evaluation, comparison of the results to experimental data (partly brought with me in form of EXFOR listings) and parameter variation. A more detailed description of the problems treated in the workshops is given in the last part of the report. Besides that, the workshops also offered a possibility of discussing open questions in connection with the theoretical lectures. The contents of the lectures can be seen in the 2nd part of this report which consists of copies of the transparencies used. Such kind of lecture notes were also made during the course for all participants in order to give them the chance to go through the theory afterwards on their owns. This was necessitated by the fact that often an immediate understanding of the lectures seems to have been hindered by their problems with the English language as well as by deficiencies in their basic

physics knowlegde.
Besides the time devoted to direct collaboration with the participants, much work was invested in lecture preparation, program modifications, debugging of sample runs and searching for particular experimental and evaluation papers in the library. In this context it may be worth stating that the library, despite its being equipped with nuclear theory textbooks rather completely, suffers from a grave lack of papers published before 1976.

5. Further needs

In order to support the beginning activities regarding model code-based evaluations, further experts' guidance is desirable. One of the aims of such support should be to enable the members of the evaluation group to work more independently which is not the case up to now, due partly to lack of experience, partly to the fact that they are mainly students and not yet used to perform independent research work. Maybe, advice can be given in written form in the frame of correspondence, maybe some other form of contact can be established. The director of the IEAv, Dr. Reginaldo, as well as the head of the nuclear energy department, Dr. Nair, asked me to come back for several months in late 1983 or beginning of 1984. Also, one thinks of sending 1-2 members of the evaluation group abroad for further training in the field of nuclear data evaluation.
A further mission of an expert from the ENEA Centro di Calcolo in Bologna is expected for middle 1983.
A complementary valuable source of obtaining information and advice is of course the participation in relevant training courses. In particular, the "Workshop on Nuclear Model Computer Codes" (Jan./Feb. 1984, Trieste) and the "Course on Methods of Nuclear Data Evaluation and Processing" (middle of 1984, Vienna) would probably be a suitable and helpful continuation of the presently described course for each of its participants.

Theoretical part: Contents of lectures

I) INTRODUCTION TO THE THEORY OF ELASTIC AND INELASTIC SCATTERING AND NUCLEAR REACTIONS

1) Direct and compound reactions

processes that take place when two nuclei collide

calculate
- types of reaction products
- their frequencies
- their energies
- their angular distributions
- their spin states

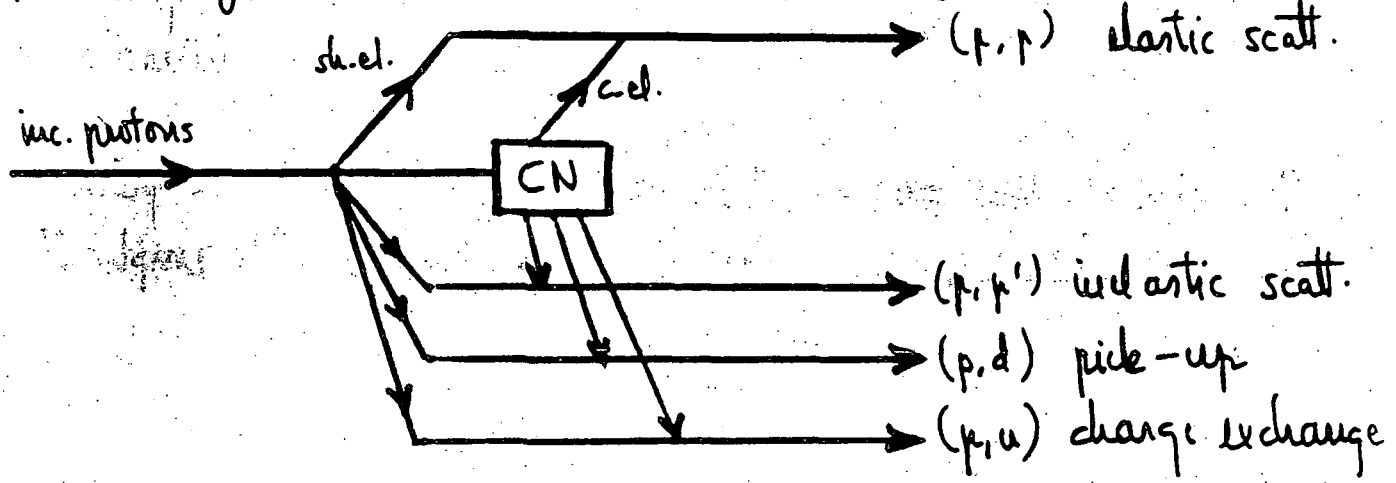
this information depends in many cases on structures of initial and final nuclei

→ comparison between XS's expected from various models of nuclear structure and experimental data can teach us about nuclear structure

example: proton incident on nucleus

$E_p \ll E_{Cb}$: interaction with Cb field of target nucleus only
Coulomb barrier → elastic scatt. acc. Rutherford's law

higher energy : interaction with nuclear field :



direct reactions pass from initial to final state without any intermediate state (CN stage)

character of the reaction depends on the structure of the target nucleus
light target → well spaced levels → XS's show resonance behaviour
heavier target → levels closely spaced, overlapping → resonance structure is averaged out and XS's vary more smoothly with energy

compound nucleus reactions — direct interactions

both processes may simultaneously contribute to the reaction in particular channel; cannot be distinguished experimentally
⇒ calculated XS's have to be combined before comparison to experimental data

electronic computers ⇒ gain in – accuracy !!
– time !!

practical calculations require approximations that cannot be rigorously justified
e.g.: inelastic scattering: truncate infinite set of coupled equations
⇒ account for this by allowing the coupling potentials to be complex
these potentials are adjusted to fit the experimental data
⇒ serve to cover up the deficiencies of the approximations
⇒ no longer derivable from microscopic theory of the interaction

The aim of the present treatment is to provide a path from general principles to practical calculations, with emphasis on the physical ideas.

2) Elastic scattering

basic task of nuclear reaction theory is to find solution of Schrödinger equation of the system that satisfies boundary condition

many-body Schrödinger equation practically impossible to solve

$\Rightarrow$ describe interaction between incoming particle and target nucleus by one body potential $V(r)$ (r ... separation)

form is considered later on

spinless neutral particle, spherical local <u>real</u> potential

C.M. system

$$\nabla^2\psi + \frac{2m}{\hbar^2}\{E - V(r)\}\psi = 0$$

requirement: in asymptotic region: incoming plane wave + scattered spherical wave

spherical polar coordinates, z axis = direction of inc. beam:

$$\psi \sim e^{ikz} + \frac{e^{ikr}}{r} f(\theta) \quad \text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

problem: calculate $f(\theta)$ for given $V(r)$

$\Rightarrow$ differential scattering XS $\quad \frac{d\sigma}{d\Omega} = |f(\theta)|^2$

expansion: $\psi = \sum_L \frac{u_L(r)}{r} P_L(\cos\theta)$

orbital angular momentum

$$\frac{d^2u_L}{dr^2} + \left[\frac{2m}{\hbar^2}\{E - V(r)\} - \frac{L(L+1)}{r^2}\right]u_L = 0$$

consider case of $L=0$: $\frac{d^2u_0}{dr^2} + \frac{2m}{\hbar^2}\{E - V(r)\}u_0 = 0$

large distances: $V(r)$ falls off more rapidly than r^{-1} $\Rightarrow$ may be neglected beyond a certain radius R

[not true for Cb potential $\rightarrow$ not considered at present]

general solution $\quad u_0 \sim \underbrace{A}_{\text{int. const.}} \sin(kr + \delta) \equiv A\frac{e^{-i\delta}}{2i}\left(e^{2i\delta}e^{ikr} - e^{-ikr}\right)$

since $u = r\psi$, this is $r\{\underbrace{\psi_{in}(L=0)}_{e^{ikz}(L=0)} + \psi_{out}(L=0)\}$

$L=0$ part of e^{ikz} is found from $e^{ikz} = \sum_{L=0}^{\infty}(2L+1)i^L j_L(kr)P_L(\cos\theta)$

as $e^{ikz}(L=0) = \frac{\sin kr}{kr} = \frac{1}{2ikr}\left(e^{ikr} - e^{-ikr}\right)$

$\triangleright$ $\psi_{out}(L=0) = \frac{u_0}{r} - \psi_{in}(L=0) =$

$$= \underbrace{\frac{Ae^{-i\delta}}{2ir}\left(e^{2i\delta}e^{ikr} - e^{-ikr}\right)}_{\psi} - \frac{1}{2ikr}\underbrace{\left(e^{ikr} - e^{-ikr}\right)}_{\psi_{in}}$$

ψ_{out} wholly outgoing $\Rightarrow$ no terms in e^{-ikr}

$\triangleright$ $\frac{Ae^{i\delta}}{2i} = \frac{1}{2ik}$

$$\psi_{out}(L=0) = \frac{1}{2ikr}\left(e^{2i\delta}-1\right)e^{ikr} = \frac{1}{r}e^{ikr}f_0(\theta)$$

$$f_0(\theta) = \frac{1}{2ik}\left(e^{2i\delta}-1\right)$$

for $L \neq 0$ similar: in asymptotic region $\left.\begin{matrix} V(r) \\ \frac{L(L+1)}{r^2} \end{matrix}\right\} \to 0$

$$\Rightarrow \frac{d^2u_L}{dr^2} + k^2 u_L = 0$$

general solution in L dependent form:

$$u_L \sim A\sin\left(kr - \frac{L\pi}{2} + \delta_L\right) = \frac{Ae^{-i\delta_L}}{2i}\left(e^{2i\delta_L}e^{i(kr-\frac{L\pi}{2})} - e^{-i(kr-\frac{L\pi}{2})}\right)$$

- $-\frac{L\pi}{2}$ arbitrary, as δ_L is a constant whose value is fixed later on by the integration in the nuclear region;
- $-\frac{L\pi}{2}$ is introduced so that $\delta_L \to 0$ as $V(r) \to 0$ for all L

part of e^{ikz} corresponding to certain L:

$$2i^L j_L(kr) \sim \frac{1}{ikr}\left(e^{ikr} - e^{iL\pi}e^{-ikr}\right)$$

$$\sim \frac{i^L}{ikr}\left(e^{i(kr-\frac{L\pi}{2})} - e^{-i(kr-\frac{L\pi}{2})}\right)$$

$$\psi^L_{out} = \psi^L - \psi^L_{in} = \frac{Ae^{-i\delta_L}}{2ir}\left(e^{2i\delta_L} e^{i(kr-\frac{L\pi}{2})} - e^{-i(kr-\frac{L\pi}{2})}\right) P_L(\cos\theta) -$$

$$-(2L+1)\frac{i^L}{2ikr}\left(e^{i(kr-\frac{L\pi}{2})} - e^{-i(kr-\frac{L\pi}{2})}\right) P_L(\cos\theta)$$

no terms in e^{-ikr} $\Longrightarrow$ $\frac{Ae^{-i\delta_L}}{2ir} = -(2L+1)\frac{i^L}{2ikr}$

L component of outgoing wave: $\frac{(2L+1)i^L}{2ikr} P_L(\cos\theta)(e^{2i\delta_L}-1)e^{i(kr-\frac{L\pi}{2})}$

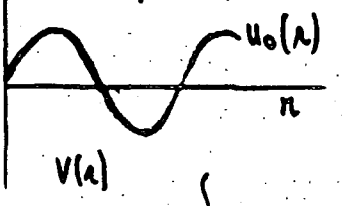
$$\boxed{\text{total scatt. amplitude}: f(\theta) = \frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)(e^{2i\delta_L}-1)P_L(\cos\theta)}$$

partial wave amplitude $\frac{1}{2i}(e^{2i\delta_L}-1)$

All the physical inform. is carried by the δ_L from the potential $V(r)$ to the XS:

Can be shown by consideration of the radial wave function $u_0(r)$:

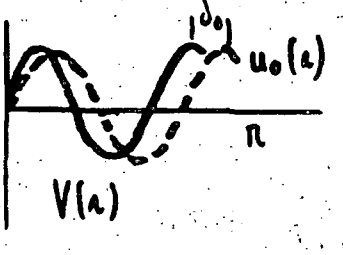
$V(r)=0 \Rightarrow \delta_L = 0 \Rightarrow$ sinusoidal



$V(r)<0$ (attractive) $\Rightarrow \delta_L \neq 0$

in the region of the potential: shorter wavelength

beyond the potential: same sinusoidal form as for $V(r)=0$, but shifted in phase by δ_0



similar for other partial waves

observed scattering is determined only by the asymptotic forms of the wave functions $\Rightarrow \delta_L$ carry all information from $V(r)$ to the observed scattering

usual for convenience: $e^{2i\delta_L} = S_L$ scattering matrix element

total elastic XS.: $\sigma_E = \int_{4\pi} |f(\theta)|^2 d\Omega = \frac{\pi}{k^2}\sum_L (2L+1)|1-S_L|^2$

3) Inelastic scattering

- simplest type of non-elastic interaction

XS may be calculated by perturbation theory expressions
↓
<u>not</u> sufficiently accurate when there is strong coupling between elastic and inelastic channels

then: solve coupled equations for the wave functions in all the reaction channels

Coupled channels theory

interaction of a neutral spinless particle with a nucleus that can be raised into a series of spinless excited states by the interaction

assumption: only elastic and inelastic scattering, no more complicated reactions

$T = -\frac{\hbar^2}{2m}\nabla_r^2$ kinetic energy of incident particle
↳ relative motion

$H(\xi)$ nuclear Hamiltonian (ξ ... all nuclear coordinates)

$V(\vec{r},\xi)$ interaction between incident particle and target nucleus

Schrödinger equation for whole system:

$$\{T - V(\vec{r},\xi) + H(\xi)\}\,\Psi(\vec{r},\xi) = E\,\Psi(\vec{r},\xi)$$

nuclear states defined by $H(\xi)\chi_\alpha(\xi) = \varepsilon_\alpha\chi_\alpha(\xi)$

χ_α complete, ON set $\Rightarrow$ $\Psi(\vec{r},\xi) = \sum_\alpha \psi_\alpha(\vec{r})\chi_\alpha(\xi)$

$$\{T - V(\vec{r},\xi) + H(\xi)\}\sum_\alpha \psi_\alpha(\vec{r})\chi_\alpha(\xi) = E\sum_\alpha \psi_\alpha(\vec{r})\chi_\alpha(\xi)$$

$$\sum_\alpha\{T - V(\vec{r},\xi) + \varepsilon_\alpha\}\psi_\alpha(\vec{r})\chi_\alpha(\xi) = E\sum_\alpha \psi_\alpha(\vec{r})\chi_\alpha(\xi)$$

multiply from the left with $\chi^*_{\alpha'}$, integrate over $d\xi$, use orthonormality:

$$(T - E - \varepsilon_\alpha)\psi_\alpha(\vec{r}) = \sum_{\alpha'}\psi_{\alpha'}(\vec{r})\underbrace{\int d\xi\,\chi^*_{\alpha'}(\xi)\,V(\vec{r},\xi)\,\chi_\alpha(\xi)}_{V_{\alpha\alpha'}(\vec{r})} \qquad (*)$$

remove angular coordinates by partial wave expansion:

$$\psi_\alpha(\vec{r}) = \sum_{LM} \frac{u_\alpha(r)}{r} Y_{LM}(\theta,\phi)$$

insert in eq. (*), multiply from the left with $Y_{L'M'}$, integrate over $d\Omega$:

$$\int Y_{L'M'}(\theta,\phi)(T-E_\alpha)\sum_{LM}\frac{u_\alpha(r)}{r}Y_{LM}(\theta,\phi) =$$

$$= \boxed{\int Y_{L'M'}(\theta,\phi)\sum_{\alpha'}\frac{u_{\alpha'}(r)}{r}\int Y_{LM}(\theta,\phi)\,V_{\alpha\alpha'}(\vec{r})\,d\Omega}$$

$$=: \frac{\hbar^2}{2m}W_{\alpha\alpha'}(r)$$

where $E_\alpha = E - \varepsilon_\alpha = \frac{\hbar k_\alpha^2}{2m}$

$$\Rightarrow \left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2\right)u_\alpha(r) = \sum_{\alpha'} W_{\alpha\alpha'}(r)\,u_{\alpha'}(r)$$

$$\boxed{\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2 - W_{\alpha\alpha}(r)\right)u_\alpha(r) = \sum_{\alpha'\neq\alpha} W_{\alpha\alpha'}(r)\,u_{\alpha'}(r)} \qquad (\mathcal{X})$$

→ set of coupled equations for the wave functions in the elastic and all the inelastic channels in the reaction being considered

<u>in principle</u>: if $V(\vec{r},\xi)$ and $H(\xi)$ known → set can be solved for all u_α
→ by application of appropriate boundary conditions elastic and inelastic XS's can be calculated

<u>in practice</u>: number of equations that can be solved is limited;
approximation: truncate set of equations, allow for the effect of not explicitly considered channels by letting $V(\vec{r},\xi)$ be complex

formalism may be extended to spin dependent interactions
⇒ calculation of polarizations and asymmetries for particles with spin

DWBA

CC theory : in principle exact calculation

in many cases sufficient to use a scattering matrix element that is exact in the limit of weak coupling between elastic and inelastic channels $\Rightarrow$ DWBA

incoming channel : α

outgoing channels : α', α

$S_{\alpha\alpha'}$: amplitude of the outgoing wave in the channel α' when a wave of unit amplitude is incident in channel α

asymptotic forms of the waves :

$$u_\alpha^\alpha(r) \sim e^{-i(kr-\frac{L\pi}{2})} - S_{\alpha\alpha} e^{i(kr-\frac{L\pi}{2})}$$

$$u_{\alpha'}^\alpha(r) \sim \qquad - S_{\alpha\alpha'} e^{i(kr-\frac{L\pi}{2})}$$

$u_\alpha^\alpha(r)$ satisfies the equation (*) :

$$\left\{\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2 - W_{\alpha\alpha}^\alpha(r)\right\} u_\alpha^\alpha(r) = \sum_{\alpha'\neq\alpha} W_{\alpha\alpha'}^\alpha(r)\, u_{\alpha'}^\alpha(r) \qquad (1)$$

consider reaction α that occurs when particles are incident in channel

$$\left\{\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2 - W_{\alpha\alpha}^\beta(r)\right\} u_\alpha^\beta(r) = \sum_{\alpha'\neq\alpha} W_{\alpha\alpha'}^\beta(r)\, u_{\alpha'}^\beta(r) \qquad (2)$$

From (1) :

$$\left\{\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2 - W_{\alpha\alpha}^\alpha(r)\right\} u_\alpha^\alpha(r) - \sum_{\alpha'\neq\alpha,\beta} W_{\alpha\alpha'}^\alpha(r)\, u_{\alpha'}^\alpha(r) = W_{\alpha\beta}^\alpha(r)\, u_\beta^\alpha(r) \qquad (1')$$

From (2) :

$$\left\{\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_\alpha^2 - W_{\alpha\alpha}^\beta(r)\right\} u_\alpha^\beta(r) - \sum_{\alpha'\neq\alpha,\beta} W_{\alpha\alpha'}^\beta(r)\, u_{\alpha'}^\beta(r) = W_{\alpha\beta}^\beta(r)\, u_\beta^\beta(r) \qquad (2')$$

multiply (1') by $u_\alpha^\beta(r)$ and (2') by $u_\alpha^\alpha(r)$ and subtract :

$$u_\alpha^\beta(r)\frac{d^2}{dr^2}u_\alpha^\alpha(r) - u_\alpha^\alpha(r)\frac{d^2}{dr^2}u_\alpha^\beta(r) - \Big[u_\alpha^\beta(r)\sum_{\alpha'\neq\alpha,\beta} W_{\alpha\alpha'}^\alpha(r)\, u_{\alpha'}^\alpha(r) - u_\alpha^\alpha(r)\sum_{\alpha'\neq\alpha,\beta} W_{\alpha\alpha'}^\beta(r)\, u_{\alpha'}^\beta(r)$$

$$= u_\alpha^\beta(r)\, W_{\alpha\beta}^\alpha(r)\, u_\beta^\alpha(r) - u_\alpha^\alpha(r)\, W_{\alpha\beta}^\beta(r)\, u_\beta^\beta(r)$$

Provided that [ ] = 0

$$\triangleright\ u_\alpha^\beta(r)\frac{d^2}{dr^2}u_\alpha^\alpha(r) - u_\alpha^\alpha(r)\frac{d^2}{dr^2}u_\alpha^\beta(r) = u_\alpha^\beta(r)W_{\alpha\beta}^\alpha(r)u_\beta^\alpha(r) - u_\alpha^\alpha(r)W_{\alpha\beta}^\beta(r)u_\beta^\beta(r) \quad (3)$$

integrate from 0 to ∞:

$$\left[u_\alpha^\beta(r)\frac{d}{dr}u_\alpha^\alpha(r)\right]_0^\infty - \int_0^\infty \frac{d}{dr}u_\alpha^\beta \cancel{\frac{d}{dr}u_\alpha^\alpha}\,dr - \left[u_\alpha^\alpha(r)\frac{d}{dr}u_\alpha^\beta(r)\right]_0^\infty + \int_0^\infty \frac{d}{dr}u_\alpha^\alpha \cancel{\frac{d}{dr}u_\alpha^\beta}\,dr$$

$$= -S_{\beta\alpha}e^+(-ike^- - ikS_{\alpha\alpha}e^+) - (e^- - S_{\alpha\alpha}e^+)(-ik)S_{\beta\alpha}e^+$$

left hand side of (3)

using asymptotic forms

$$= 2ikS_{\beta\alpha}e^+e^- = 2ikS_{\beta\alpha}$$

right hand side of (3):

1st term negligible due to $u_\alpha^\beta(r) \ll u_\alpha^\alpha(r)$ ← inelastic channels weakly coupled to elastic channel

$$\Rightarrow 2ikS_{\beta\alpha} = -\int_0^\infty dr\, u_\alpha^\alpha(r)W_{\alpha\beta}^\beta(r)u_\beta^\beta(r)$$

true for all channels β: $\beta \to \alpha$, $\alpha \to \alpha'$

$$\Rightarrow S_{\alpha\alpha'}^{LM} = -\frac{1}{2ik}\int_0^\infty dr\, u_{\alpha'}^{\alpha'}(r)W_{\alpha'\alpha}^{\alpha}(r)u_\alpha^\alpha(r)$$

DWBA expression for scatt. matrix element

[superscript LM on radial fcts. u should in fact carry this superscript

$$S_{\alpha\alpha'} = \sum_{LM} S_{\alpha\alpha'}^{LM}$$

total inelastic XS: $\boxed{\sigma_{\alpha\alpha'} = \frac{4\pi}{k^2}|S_{\alpha\alpha'}|^2}$

$$\boxed{S_{\alpha\alpha'} = -\frac{2m}{\hbar^2}\cdot\frac{1}{2ik}\int \psi_{\alpha'}(\vec{r})V_{\alpha\alpha'}(\vec{r})\psi_\alpha(\vec{r})\,d\vec{r}}$$

4) Nuclear Reactions

if incident energy > corresponding thresholds → many nuclear reactions can take place in addition to elastic and inelastic scatt.

apart from inelastic scatt. the coupling to non-elastic channels is weak enough for perturbation theory to be sufficient by accurate ⇒ general perturbation theory expansion for reaction amplitude

strong coupling
⇓

higher energies → more than 2 particles

sequential emission ⇒ successive application of the formalism of 2 particle reactions

simultaneous emission ⇒ reaction mechanism ?

for binary reaction:

if reaction time relative to transit time comparable — long :

direct interaction | precequilibrium decay | compound nucleus reaction

pertub. theory in above

in compound nucleus reactions:

many degrees of freedom excited, XS complicated function of energy

description of intermediate states not individual, but statistical (average values, correlation functions) → statistical model

compound nucleus = system formed from projectile and target nucleus, in statistical equilibrium

states whose excitation is determining for energy dependence of X

resonances: isolated, overlapping

- isolated resonances : Breit Wigner formula

$$\sigma_{ab} = \frac{\pi}{k_a^2} \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{(E-E_\mu)^2 + \frac{1}{4}\Gamma_\mu^2}$$

μ .. resonance

$\Gamma_\mu = \sum_c \Gamma_{\mu c}$

partial widths

$$\sigma_a^{comp} = \sum_b \sigma_{ab} = \frac{\pi}{k_a^2} \frac{\Gamma_{\mu a}\Gamma_\mu}{(E-E_\mu)^2 + \frac{1}{4}\Gamma_\mu^2}$$

$$\triangleright\ \sigma_{ab} = \sigma_a^{comp}(E) \cdot \frac{\Gamma_{\mu b}}{\Gamma_\mu}$$

• overlapping resonances:

contributions of many resonances interfere → fluctuations

Breit-Wigner-formula cannot be used

▷ above formula is taken over for average XS:

$$\langle \sigma_{ab} \rangle = \langle \sigma_a^{comp} \rangle \frac{\langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} \qquad \sum_c \langle \Gamma_{\mu c} \rangle = \langle \Gamma_\mu \rangle$$

averages with respect to μ

"independence of formation and decay"

Bohr's hypothesis

experimental evidence for Bohr's hypothesis: Ghoshal experiment

$$\frac{\langle \sigma_{ab} \rangle}{\langle \sigma_{ac} \rangle} = \frac{\langle \sigma_{db} \rangle}{\langle \sigma_{dc} \rangle}$$ for equal exc. en. of CN

now use: $k_a^2 \langle \sigma_{ab} \rangle = k_b^2 \langle \sigma_{ba} \rangle$ reciprocity ← time reversal invariance

for same exc. en. of CN

$$\frac{k_a^2 \langle \sigma_a^{comp} \rangle \langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} = \frac{k_b^2 \langle \sigma_b^{comp} \rangle \langle \Gamma_{\mu a} \rangle}{\langle \Gamma_\mu \rangle}$$

$$\frac{\langle \Gamma_{\mu a} \rangle}{k_a^2 \langle \sigma_a^{comp} \rangle} = \frac{\langle \Gamma_{\mu b} \rangle}{k_b^2 \langle \sigma_b^{comp} \rangle} = f(E, J, \Pi)$$ channel independent

$$\langle \Gamma_{\mu a} \rangle = k_a^2 \langle \sigma_a^{comp} \rangle \cdot f(E, J, \Pi)$$

$$\langle \sigma_{ab} \rangle = \langle \sigma_a^{comp} \rangle \frac{k_b^2 \langle \sigma_b^{comp} \rangle}{\sum_c k_c^2 \langle \sigma_c^{comp} \rangle}$$

definition: $T_a = \frac{k_a^2}{\pi} \sigma_a^{comp}$

$$\boxed{\langle \sigma_{ab} \rangle = \frac{\pi}{k_a^2} T_a \frac{T_b}{\sum_c T_c}} \qquad (*)$$

factors that characterize formation and decay are determined by the same quantities

transmission coefficients

observable XS: (*) summed over many channels → Hauser Feshbach formula

II) SPHERICAL OPTICAL MODEL CALCULATIONS

1) General description of the problem

Schrödinger equation : $\left[-\frac{\hbar^2}{\mu^2}\nabla^2 + V\right]\Psi = E\Psi$

$$\mu = \frac{m_i m_t}{m_i + m_t}$$

$$E = E_{lab}\cdot\frac{m_t}{m_i+m_t} \quad \text{C.M energy}$$

optical potential : $V = V_{coul}(r) + \underbrace{V_{CR}(r)}_{\text{central, real}} + i V_{CI}(r) + \{V_{SR}(r) + i V_{SI}(r)\}\hbar^2(\vec{J}\cdot\vec{L})$

inc. part. — rel. motion

$$\vec{J} = \vec{S} + \vec{L}$$

other terms have also been considered, seem to play a minor part

separation of the variables $\Rightarrow$ radial equation :

$$\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{k^2}{E}\Big[E - \big(V_{coul}(r) + V_{CR}(r) + i V_{CI}(r)\big) - \big(V_{SR}(r) + i V_{SI}(r)\big)\hbar^2\big(j(j+1) - l(l+1) - s(s+1)\big)/2\Big]\, u_l^j(r) = 0$$

$u_l^j(r)$ ... radial wave function, must satisfy the following boundary condition

- must vanish at the origin
- asymptotic form of the solution should in principle be matched to a plane wave plus an outgoing wave

in the actual case : solution is matched to a linear combination of regular and outgoing Coulomb wave functions at radius r_m beyond which the nuclear potential is sufficiently small :

$$u_l^j(r) = F_l(\eta, kr_m) + C_l^j\left[G_l(\eta, kr_m) + i F_l(\eta, kr_m)\right]$$

F ... regular, G ... irregular } normalized Coulomb wave functions

$$\eta = \mu\cdot\frac{zz'e^2}{\hbar k}$$

z ... incident, z' ... target } particle charge number

$$C_l^J = -\frac{i}{2}\left[\exp(2i\delta_l^J) - 1\right] = -\frac{i}{2}\left[\eta_l^J - 1\right]$$

phase shift absorption coefficient

total reaction cross section:

$$\sigma_R = \frac{4\pi}{(2s+1)k^2}\sum_{l=0}^{\infty}\sum_{J=|l-s|}^{l+s}(2J+1)\left\{\mathrm{Im}\, C_l^J - |C_l^J|^2\right\}$$

angular distributions : scattering amplitudes are expressed in terms of Legendre coefficients; expansion coefficients are functions of C_l^J

<u>Potential terms in radial Schrödinger equation:</u>

1) Coulomb pot.: $V_{coul}(r)$ usually taken to correspond to a constant charge density within the nucleus extending to a distance $r_c = R_c\, m_t^{1/3}$

$$V_{coul}(r) = \begin{cases} (ZZ'e^2/2r_c)(3 - r^2/r_c^2) & \text{for } r \le r_c \\ ZZ'e^2/r & \text{for } r \ge r_c \end{cases}$$

other forms suggested; in practice little effect on the final results

2) Central real nuclear potential : $V_{CR}(r)$, usually Saxon-Woods

$$V_{CR}(r) = V_0\left[1 + \exp(r - r_R)/a_R\right]^{-1}$$

$V < 0$ $r_R = R_R\, m_t^{1/3}$

for attractive potential

3) Central imaginary nuclear potential : $V_{CI}(r)$

- Volume absorption : Woods - Saxon

$$V_{CI}(r) = W_v \left[1 + \exp(r - r_I)/a_I \right]^{-1}$$

- Surface absorption :
  - Gaussian absorption : $V_{CI}(r) = W_s \exp\left[-((r - r_I)/b)^2 \right]$
  - Derivative absorption : $V_{CI}(r) = 4 a_I W_s \left[-\frac{d}{dr} \left(1 + \exp((r - r_I)/a_I) \right) \right]^{-1}$

$W_s, W_v < 0$ for an absorptive potential

$$r_I = R_I m_t^{1/3}$$

both forms of surface absorption have also been combined with a volume absorption

4) Spin orbit potential : usually assigned a Thomas factor :

$$V_{SR}(r) = V_{S0} \left(\frac{2}{\hbar^2 r} \right) \left(-\frac{d}{dr} \left[1 + \exp((r - r_R)/a_R) \right]^{-1} \right)$$

$$V_{SI}(r) = W_{S0} \left(\frac{2}{\hbar^2 r} \right) \left(-\frac{d}{dr} \left[1 + \exp((r - r_I)/a_I) \right]^{-1} \right)$$

Parameters of the model

geometrical parameters:

- R_C .... Coulomb radius parameter
- R_R ... real potential radius parameter
- R_I .... imag. -"- -"- -"-
- a_R .... real potential surface parameter
- a_I .... imag. -"- -"- -"-
- b .... Gaussian absorption width

dynamic parameters:

- V .... real potential depth
- W_v .... volume } absorption potential depth
- W_s .... surface } absorption potential depth
- V_{S0} ... real } spin-orbit potential depth
- W_{S0} ... imag. } spin-orbit potential depth

several of these parameters are usually related to each other

2) Comparison with experimental data

Comparison of the fits to the experimental data obtained with various sets of DM parameters may be given quantitatively by

$$\chi_\sigma^2 = \sum_{i=1}^{N} \left[(\sigma(\theta_i) - \sigma^x(\theta_i)) / \Delta\sigma^x(\theta_i) \right]^2$$

$\sigma^x(\theta_i)$ ... experimental differential XS at θ_i

$\Delta\sigma^x(\theta_i)$ ... experimental error

similar for polarization : χ_P^2

total χ^2 : $\chi^2 = \chi_\sigma^2 + \chi_P^2$

[spin 1 : $\chi^2 = \chi_\sigma^2 + \Sigma \chi_P^2$]

χ^2 criterion can be modified to take into account experimental uncertainties in the overall normalization of the data

→ divide data by renormalization factor λ which is chosen so as to minimize χ^2; permissible range $\Delta\lambda^x$ should be specified as an experimental uncertainty about a given value λ^x :

$$\chi_\sigma^2(\lambda) = \sum_i \left[\lambda\sigma(\theta_i) - \sigma^x(\theta_i)) / \Delta\sigma^x(\theta_i) \right]^2 + \left[\lambda - \lambda^x) / \Delta\lambda^x \right]^2$$

$$\chi_\sigma^2 = \min_\lambda \chi_\sigma^2(\lambda)$$

two further sources of errors in the experimental θ_i can also be included in the χ^2 criterion :

- detector width
- exp. uncertainty in the measured θ_i

Types of exp. data that may be used for comparison

— total cross section σ_t as fct. of inc. energy

— total elastic cross section σ_el —— " ——

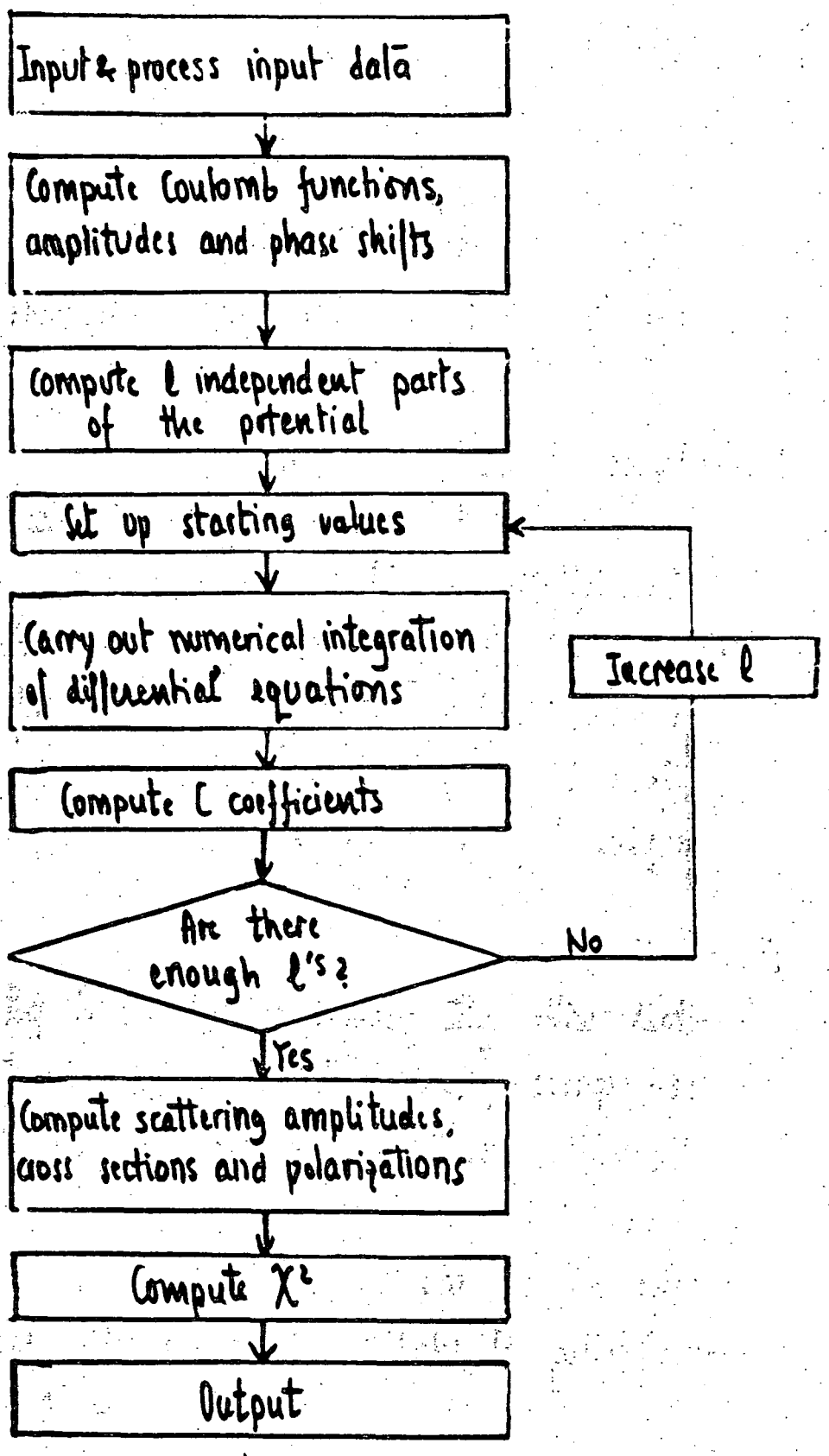
— reaction cross section σ_R —— " ——

— differential elastic cross section $\frac{d\sigma_el}{d\omega}$ as fct. of angle at various inc. energies

— polarizations $P(\theta)$ as fct. of angle at various inc. energies

— strength functions S_l (mostly S_0 and S_1); up to 1 eV

3) General flow chart of the program for a single run calculation



III) COUPLED CHANNELS OPTICAL MODEL CALCULATIONS

1) Introduction

inelastic scattering : involved interactions sometimes much stronger than in transmutation reactions

→ DWBA poor approximation

improvement — higher order BA → involved task
— CCC

Advantages of CCC :

- interaction is treated exactly within the channels considered ("to infinite order")
- certain low-lying states of collective nature (higher phonon state in vibrational nuclei ; higher members of rotational bands of deformed nuclei) cannot be excited in single step process → would require higher order BA

Formulation :

— start with quite general optical model potential (nonspherical)
— re-express potentials in some approximate ways, the way depending on the nature of the target => derive coupling terms between different channels
— solve set of coupled equations
— matching of solutions to asymptotic wave functions
=> S matrix elements
— compute XS's from S matrix elements

[If target nucleus well deformed and energy of incident particle sufficiently high → adiabatic approximation.]

2) The interaction potential

CCC required only if (direct or indirect) couplings between excited and ground state channels are strong, i.e. when the low lying states of the target nucleus have a strong collective nature

$$V(r,\theta,\phi) = -(V+iW)\frac{1}{1+\exp[(r-R)/a]}$$ real & vol. imag. : SW

$$-4iW_D\frac{\exp[(r-\bar{R})/\bar{a}]}{\{1+\exp[(r-\bar{R})/\bar{a}]\}^2}$$ surface imag. : der. SW

$$-V_{so}(\vec{\sigma}.\vec{l})\lambda_\pi^2\frac{1}{ar}\frac{\exp[(r-R)/a]}{\{1+\exp[(r-R)/a]\}^2}$$ spin-orbit : Thomas

$$+V_{coul}$$ Coulomb

if R and $\bar{R}$ independent of angle : spherical OM
if R and $\bar{R}$ dependent on angle : deformed OM
$\downarrow$
according to collective nature of target nucleus :

△ spherically symmetric, but susceptible to vibrations around spherical shape:

$$R = R_0\left(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right)$$

$$\bar{R} = \bar{R}_0\left(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right)$$

△ axially symmetric deformed nucleus :

$$R = R_0\left(1+\sum_{\lambda}\beta_\lambda Y_{\lambda 0}(\theta')\right)$$

$$\bar{R} = \bar{R}_0\left(1+\sum_{\lambda}\beta_\lambda Y_{\lambda 0}(\theta')\right)$$

θ' refers to body fixed system

$$\boxed{\begin{aligned} R_0 &= r_0 A^{1/3} \\ \bar{R}_0 &= \bar{r}_0 A^{1/3} \end{aligned}}$$

impractical to solve scattering problem subject to the above potential with these expressions for radii $\Rightarrow$ plausible approximations :

Vibrational nucleus :

$$f(r) = \{1+\exp[(r-R)/a]\}^{-1} = \{1+\exp[(r-R_0(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)))/a]\}^{-1}$$

$$g(r) = \exp[(r-\bar{R})/\bar{a}]\cdot\{1+\exp[(r-\bar{R})/\bar{a}]\}^{-2} =$$

$$= \{1+\exp[(r-\bar{R}_0(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)))/\bar{a}]\}^{-2}\cdot\exp[(r-\bar{R}_0(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}))/\bar{a}]$$

Notation: $\Sigma = \sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}$

$$e = \exp[(r-R_0)/a]$$

$$\bar{e} = \exp[(r-\bar{R}_0)/\bar{a}]$$

$$\triangleright\ f(r) = \{1+\exp[\frac{r-R_0}{a} - \frac{R_0}{a}\Sigma]\}^{-1} = \{1+e\cdot\exp[-\frac{R_0}{a}\Sigma]\}^{-1} = F(\Sigma)$$

expand around $\Sigma = 0$

$$F(\Sigma) = \{1+e.\exp[-\frac{R_0}{a}\Sigma]\}^{-1}$$

$$\frac{dF(\Sigma)}{d\Sigma} = e\,\frac{R_0}{a}\exp[-\frac{R_0}{a}\Sigma]\cdot\{1+e\exp[-\frac{R_0}{a}\Sigma]\}^{-2}$$

$$\left.\frac{dF(\Sigma)}{d\Sigma}\right|_{\Sigma=0} = e\,\frac{R_0}{a}(1+e)^{-2}$$

$$\frac{d^2F(\Sigma)}{d\Sigma^2} = -e\,\frac{R_0^2}{a^2}\exp[\quad]\cdot\{\quad\}^{-2} + 2e^2\frac{R_0^2}{a^2}\exp[\quad]\exp[\quad]\{\quad\}^{-3} =$$

$$= e\,\frac{R_0^2}{a^2}\exp[-\frac{R_0}{a}\Sigma]\cdot\left[-\{\quad\}^{-2} + 2e\exp[-\frac{R_0}{a}\Sigma]\{\quad\}^{-3}\right]$$

$$\left.\frac{d^2F(\Sigma)}{d\Sigma^2}\right|_{\Sigma=0} = e\,\frac{R_0^2}{a^2}\left[-(1+e)^{-2} + 2e(1+e)^{-3}\right] = e\,\frac{R_0^2}{a^2}(1+e)^{-3}(-1-e+2e) =$$

$$= e\,\frac{R_0^2}{a^2}(e-1)(1+e)^{-3}$$

$$F(\Sigma) = F(0) + \left.\frac{dF}{d\Sigma}\right|_{\Sigma=0}\cdot\Sigma + \frac{1}{2}\left.\frac{d^2F}{d\Sigma^2}\right|_{\Sigma=0}\cdot\Sigma^2 =$$

$$= (1+e)^{-1} + e\,\frac{R_0}{a}(1+e)^{-2}\Sigma + \frac{1}{2}e\,\frac{R_0^2}{a^2}(e-1)(1+e)^{-3}\Sigma^2$$

analogous for $g(r)$, with expansions for $f(r)$ and $g(r)$ in potentials, leads to :

$$V(r,\theta,\phi) = -(V+iW)(1+e)^{-1} - 4iW_D\,\bar{e}(1+\bar{e})^{-2} - V_{SO}(\vec{\sigma}\cdot\vec{l})(\lambda_\pi^2/ar)\,e\,(1+e)^{-2}$$
$$-\left\{(V+iW)\frac{R_0}{a}e(1+e)^{-2} - 4iW_D\frac{R_0}{a}\bar{e}(1-\bar{e})(1+\bar{e})^{-3}\right\}\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu} +$$
$$+\left\{(V+iW)\frac{R_0^2}{a^2}e(1-e)(1+e)^{-3} - 4iW_D\frac{\bar{R}_0^2}{2\bar{a}^2}\bar{e}(1-4\bar{e}+\bar{e}^2)(1+\bar{e})^{-4}\right\}\left(\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}\right)^2 +$$
$$+ V_{coul}$$

Use following relation:

$$\left(\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}\right)^2 = \sum_{\lambda'\lambda''}\frac{\sqrt{2\lambda'+1}\sqrt{2\lambda''+1}}{\sqrt{4\pi}\sqrt{2\lambda+1}}(\lambda'\lambda''00|\lambda 0)\sum_\mu Y_{\lambda\mu}\underbrace{(\alpha_{\lambda'}\otimes\alpha_{\lambda''})_{\lambda\mu}}$$

vector addition $\quad (\alpha_{\lambda'}\otimes\alpha_{\lambda''})_{\lambda\mu} = \sum_{\mu'\mu''}(\lambda'\lambda''\mu'\mu''|\lambda\mu)\,\alpha_{\lambda'\mu'}\alpha_{\lambda''\mu''}$

Specify Coulomb interaction:

$$V_{coul} = ZZ'\varepsilon^2\int\rho(r',\theta',\phi')\,|\vec{r}-\vec{r}'|^{-1}\,d\vec{r}' =$$
$$= 4\pi ZZ'\varepsilon^2\sum_{\lambda\mu}\int\rho(r',\theta',\phi')(2\lambda+1)\,r_<^\lambda r_>^{-(\lambda+1)}Y_{\lambda\mu}(\theta,\phi)Y^*_{\lambda\mu}(\theta',\phi')\,r'^2\,dr'\,d\theta'\,d\phi'$$

using expansion of $|\vec{r}-\vec{r}'|^{-1}$ in spher. harmonics

where $r_<^\lambda\, r_>^{-(\lambda+1)} = r^\lambda(r')^{-(\lambda+1)}\theta(r'-r) + r'^\lambda r^{-(\lambda+1)}\theta(r-r')$

charge distribution in the target is assumed to be constant within the ch radius $R_c(\theta',\phi')$ and zero outside:

$$\rho(r',\theta',\phi') = \frac{3}{4\pi R_c^3}\,\theta(R_c(\theta',\phi')-r')$$

const. radius $\quad$ vibration: $R_c(\theta',\phi') = R_c\left(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}\right)$

$$\triangleright\ \rho(r',\theta',\phi') = \underbrace{\frac{3}{4\pi R_c^3}\,\theta\left(R_c\left(1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta',\phi')\right)-r'\right)}$$

use this expression in the above integral

$$V_{coul} = \frac{ZZ'\varepsilon^2}{R_c^3}\sum_{\lambda\mu}\frac{Y_{\lambda\mu}(\theta,\phi)}{2\lambda+1}\int Y^*_{\lambda\mu}(\theta',\phi')\,\theta\left(R_c(\theta',\phi')-r'\right)\left[r^\lambda(r')^{-(\lambda+1)}\theta(r'-r) + r'^\lambda r^{-(\lambda+1)}\theta(r-r')\right]$$
$$\cdot\, r'^2\,dr'\,d\Omega' =$$

$$= \frac{3ZZ'\varepsilon^2}{R_c^3}\sum_{\lambda\mu}\frac{Y_{\lambda\mu}(\theta,\phi)}{2\lambda+1}\int_0^{\pi}d\theta'\sin\theta'\int_0^{2\pi}d\phi'\int_0^{R_c(\theta',\phi')}dr'\, r'^2\, Y^*_{\lambda\mu}(\theta',\phi')\cdot$$

$$\cdot\left[r^{\lambda}(r')^{-(\lambda+1)}\theta(r'-r)+r'^{\lambda}r^{-(\lambda+1)}\theta(r-r')\right]=$$

$$=\frac{3ZZ'\varepsilon^2}{R_c^3}\sum_{\lambda\mu}\frac{Y_{\lambda\mu}(\theta,\phi)}{2\lambda+1}\int_0^{\pi}d\theta'\sin\theta'\int_0^{2\pi}d\phi'\,Y^*_{\lambda\mu}(\theta',\phi')\Big\{\theta(R_c(\theta',\phi')-r)\int_r^{R_c(\theta',\phi')}dr'\,r^{\lambda}(r')^{-(\lambda+1)}+$$

$$+\theta(R_c(\theta',\phi')-r)\int_0^{r}dr'(r')^{\lambda+2}r^{-(\lambda+1)}+\theta(r-R_c(\theta,\phi))\int_0^{R_c(\theta',\phi')}dr'(r')^{\lambda+2}r^{-(\lambda+1)}\Big\}=$$

$$=\frac{3ZZ'\varepsilon^2}{R_c^3}\sum_{\lambda\mu}\frac{Y_{\lambda\mu}(\theta,\phi)}{2\lambda+1}\int d\Omega'\,Y^*_{\lambda\mu}(\Omega')\Big\{\theta(R_c-r)\frac{r^{\lambda}}{2-\lambda}\left[R_c(\Omega')^{-\lambda+2}-r^{-\lambda+2}\right]+\mathrm{II}+\mathrm{III}\Big\}$$

neglecting angle dependence of θ fct.

$$=\frac{3ZZ'\varepsilon^2}{R_c^3}\sum_{\lambda\mu}\frac{Y_{\lambda\mu}(\theta,\phi)}{2\lambda+1}\int d\Omega'\,Y^*_{\lambda\mu}(\Omega')\Big\{\frac{\theta(R_c-r)}{2-\lambda}\Big[r^{\lambda}R_c^{-\lambda+2}\Big(\Big(1+\sum_{\lambda'\mu'}\alpha_{\lambda'\mu'}\cdot Y_{\lambda'\mu'}(\Omega')\Big)^{-\lambda+2}-r^2\Big)\Big]+$$

$$+\mathrm{II}+\mathrm{III}\Big\}$$

leads to:

$$V_{coul}=\frac{ZZ'\varepsilon^2}{2R_c}\left[3-\frac{r^2}{R_c^2}\right]\theta(R_c-r)+\frac{ZZ'\varepsilon^2}{r}\theta(r-R_c)+$$

$$+\sum_{\lambda\mu}\frac{3ZZ'\varepsilon^2}{2\lambda+1}\left[r^{\lambda}R_c^{-(\lambda+1)}\theta(R_c-r)+R_c^{\lambda}r^{-(\lambda+1)}\theta(r-R_c)\right](\alpha_{\lambda\mu}Y_{\lambda\mu})+$$

$$+\sum_{\lambda\mu}\frac{3ZZ'\varepsilon^2}{2\lambda+1}\left[(1-\lambda)r^{\lambda}R_c^{-(\lambda+1)}\theta(R_c-r)+(\lambda+2)R_c^{\lambda}r^{-(\lambda+1)}\theta(r-R_c)\right]\cdot$$

$$\cdot\sum_{\lambda'\lambda''}\sqrt{\frac{(2\lambda'+1)(2\lambda''+1)}{4\pi(2\lambda+1)}}(\lambda'\lambda''00|\lambda 0)\sum_{\mu}(\alpha_{\lambda'}\otimes\alpha_{\lambda''})_{\lambda\mu}Y_{\lambda\mu}$$

$$V(r,\theta,\phi)=V_{diag}+V^{(v)}_{coupl}$$

vibrational

no $Y_{\lambda\mu}$ — linear or quadratic in $Y_{\lambda\mu}$

$$\triangleright\, V_{diag}=-(V+iW)(1+e)^{-1}-4iW_D\,\bar{e}(1+\bar{e})^{-2}-U_{SO}\frac{\lambda_\pi^2}{ar}(\vec{\sigma}\vec{L})\,e(1+e)^{-2}+$$

$$+\frac{ZZ'\varepsilon^2}{2R_c}\left(3-\frac{r^2}{R_c^2}\right)\theta(R_c-r)+\frac{ZZ'\varepsilon^2}{r}\theta(r-R_c)$$

$$V^{(v)}_{coupl}=\sum_{\lambda\mu}v^{(1)(v)}_{cp;\lambda}(r)\,\alpha_{\lambda\mu}Y_{\lambda\mu}+\sum_{\lambda_1\lambda_2}v^{(2)(v)}_{cp;\lambda}(r)\sqrt{\frac{(2\lambda_1+1)(2\lambda_2+1)}{4\pi(2\lambda+1)}}(\lambda_1\lambda_2 00|\lambda 0)\sum_{\mu}(\alpha_{\lambda_1}\otimes\alpha_{\lambda_2})_{\lambda\mu}$$

with:

$$U^{(1)(v)}_{(p;\lambda}(r) = -\left\{(V+iW)\frac{R_0}{a}e(1+e)^{-2} - 4iW_D\frac{\bar{R}_0}{\bar{a}}\bar{e}(1-\bar{e})(1+\bar{e})^{-3}\right\} + \frac{3ZZ'e^2}{2\lambda+1}\left\{r^\lambda R_c^{-(\lambda+1)}\theta(R_c-r) + R_c^\lambda r^{-(\lambda+1)}\theta(r-R_c)\right\}$$

$$U^{(2)(v)}_{(p;\lambda}(r) = (V+iW)\frac{R_0^2}{2a^2}e(1-e)(1+e)^{-3} - 4iW_D\frac{\bar{R}_0^2}{2\bar{a}^2}\bar{e}(1-4\bar{e}+\bar{e}^2)(1+\bar{e})^{-4} + \frac{3ZZ'e^2}{2\lambda+1}\left\{(1-\lambda)r^\lambda R_c^{-(\lambda+1)}\theta(R_c-r) + (\lambda+2)R_c^\lambda r^{-(\lambda+1)}\theta(r-R_c)\right\}$$

V_{diag} ... diagonal with respect to ang. mom. j of the projectile and eigenspin I of the target nucleus
= usual optical model potential

$V^{(v)}_{coupl}$ ... coupling potential between channels with different j and I

Rotational nuclei

Use $\left\{\begin{array}{l} R = R_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')) \\ \bar{R} = \bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')) \end{array}\right\}$ in expression for potential, expand potential in powers of $\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')$, leads to exactly the same expressions as for vibrational nucleus except that $\alpha_{\lambda\mu}$ and $Y_{\lambda\mu}(\theta,\phi)$ are replaced by β_λ and $Y_{\lambda 0}(\theta')$

Replace $Y_{\lambda 0}(\theta')$ by $\sum_\mu \mathcal{D}^\lambda_{\mu 0}(\theta_i)\, Y_{\lambda\mu}(\theta,\phi)$

in body fixed system — rotation matrix — Euler angles — in space fixed system

diagonal elements of coupling pot.: linear term has vanishing
-"- -"- for vibrational nucleus, nonvanishing for rotational nucleus

expanding potential in powers of $\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')$ and retaining a few of its leading terms may be a poor approximation when β_λ is large (~ 0.3) as is the case in many actual deformed nuclei

$\Rightarrow$ expansion of potential not in powers of $\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')$ but in terms of Legendre polynomials

for nuclear part:

$$V(\vec{r}) = -(V+iW)\left[1+\exp\left(\frac{r-R_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta'))}{a}\right)\right]^{-1} - 4iW_D \exp\left[\frac{r-\bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta'))}{\bar{a}}\right]\left\{1+\exp[\;]\right.$$

$$= \sum_{\lambda'} f_{\lambda'}(r)\, P_{\lambda'}(\cos\theta') = \sum_{\lambda'} f_{\lambda'}(r)\sqrt{\frac{4\pi}{2\lambda'+1}}\, Y_{\lambda' 0}(\theta') \quad (\varphi)$$

$$f_{\lambda'}(r) = 4\pi \int_0^1 Y_{\lambda' 0}(\theta')\, V(\vec{r})\, d\cos\theta' =$$

$$= -4\pi (V+iW)\int_0^1 d\cos\theta'\, Y_{\lambda' 0}(\theta')\left[1+\exp\left(\frac{r-R_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta'))}{a}\right)\right]^{-1} -$$

$$-4\pi\, 4iW_D \int_0^1 d\cos\theta'\, Y_{\lambda' 0}(\theta') \exp\left(\frac{r-\bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta'))}{\bar{a}}\right)\left[1+\exp\left(\frac{r-\bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta'))}{\bar{a}}\right)\right]$$

with $\lambda'=0$ this is diagonal part of nuclear pot.; add other terms (SO, Cb)

$$V_{diag} = \sqrt{4\pi}\int_0^1 \left\{\frac{-(V+iW)}{1+\exp[(r-R_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')))/a]} + \frac{-4iW_D \exp[(r-\bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')))/\bar{a}]}{\{1+\exp[(r-\bar{R}_0(1+\sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')))/\bar{a}]\}^2}\right\} d\cos\theta'$$

$$- V_{so}\frac{\hbar^2}{ar}(\vec{\sigma}\cdot\vec{\ell})\, e(1+e)^{-2} + \frac{Zz'e^2}{2R_c}\left(3-\frac{r^2}{R_c^2}\right)\theta(R_c-r) + \frac{Zz'e^2}{r}\,\theta(r-R_c)$$

Use $Y_{\lambda 0}(\theta') = \sum_\mu D^\lambda_{\mu 0}(\theta_i)\, Y_{\lambda\mu}(\theta,\phi)$ in (φ):

$$V(\vec{r}) = \sum_{\lambda'} f_{\lambda'}(r) \sum_\mu D^{\lambda'}_{\mu 0}(\theta_i)\, Y_{\lambda'\mu}(\theta,\phi)$$

with $\lambda' \neq 0$: coupling part of nuclear potential

$$V_{coupl} = \sum_{\substack{\lambda\mu \\ (\lambda\neq 0)}} \underbrace{v_{cp}^{(\lambda)(\lambda)}(r)}_{\text{rotational}}\, D^\lambda_{\mu 0}\, Y_{\lambda\mu}(\theta,\phi)$$

$$v_{cp}^{(\lambda)(\lambda)} \propto f_\lambda(r)$$

in particular:

$$v_{cp}^{(2)(c)}(r) = 4\pi \int_0^1 \left\{ \frac{-(V+iW)}{1+\exp[(r-R_0(1+\sum_{\lambda'}\beta_{\lambda'}Y_{\lambda'0}(\theta')))/a]} + \frac{-4iW_0 \exp[r-\bar{R}_0(1+\sum_{\lambda'}\beta_{\lambda'}Y_{\lambda'0}(\theta')))/\bar{a}]}{\{1+\exp[r-\bar{R}_0(1+\sum_{\lambda'}\beta_{\lambda'}Y_{\lambda'0}(\theta')))/\bar{a}]\}^2} \right.$$

$$* \, Y_{\lambda 0}(\theta') \, d\cos\theta'$$

(b part in coupling potential: power series expansion is sufficiently good approximation → as for vibrational nucleus except that $\alpha_{\lambda\mu} Y_{\lambda\mu}$ must be replaced by $\beta_\lambda D^{\lambda}_{\mu 0} Y_{\lambda\mu}$

3) The coupled equations

I_n, π_n, ω_n ... spin, parity and energy of nth target state, $n = 1, \dots N$.

coupled strongly (directly or indirectly) to ground state by V_{coupl}

incident particle: E_1 ... C.M. energy

energy of particle which leaves target in its nth state: $E_n = E_1 - \omega_n$

Consider channel corresponding to n^{th} state of target, particle spin $\vec{s}$, orb. ang. mom. $\vec{l}_n$, total ang. mom. $\vec{j}_n = \vec{s} + \vec{l}_n$

ang. mom. and parity of whole system:

$$\vec{J} = \vec{I}_n + \vec{j}_n \qquad \Pi = \pi_n (-)^{l_n} \qquad (◎)$$

with the interaction described by the coupling potentials, none of l_n, j_n, I_n, π_n or $(-)^{l_n}$ is a good quantum number, but J and Π are good

⇒ partial waves whose l_n and j_n satisfy (◎) for given $J\Pi$ are coupled together through coupling potential to form a set of coupled differential equations

number of (l_n, j_n) coupled to a given $J\Pi$: $n_c^{(n)}$

maximum possible number : $N_c^{(n)}$

for given I_n :

$N_c^{(n)} = I_n + 1$	if $s=0$	and I_n is an integer	
$= I_n + \frac{1}{2}$	$s=0$	I_n half odd integer	
$= 2I_n + 1$	$s=\frac{1}{2}$	all I_n	
$= 3I_n + 2$	$s=1$	I_n integer	
$= 3I_n + \frac{3}{2}$	$s=1$	I_n half odd integer	

total number of coupled partial waves for given $J\Pi$: $n_c = \sum_n^{N_s} n_c^{(n)}$

max. ——— " ——— $N_c = \sum_n^{N_s} N_c^{(n)}$

terminology :

"partial wave channel" ... particular $(l_n j_n)$

"n^{th} state channel" ..... $n_c^{(n)}$ values $(l_n j_n)$

in calculations : $J = J_{min}$ $(0$ or $\frac{1}{2})$ ... $J_{max} = I_1 + j_{max}$ for each Π

max. j_1 of the partial wave that gives non-negligible contribution to (elastic) scattering

Hamiltonian:

$$\mathcal{H} = T + \mathcal{H}_t + V(r,\theta,\phi) = T + \mathcal{H}_t + V_{diag} + V_{compl}$$

T : kinetic energy of inc. particle

$\mathcal{H}_t$: internal motion of the target

Schrödinger eq.: $\mathcal{H}\Psi = E_1\Psi$

E_1 : energy of inc. particle

total wave function: $\Psi = r^{-1} \sum_{J_n l_n j_n} R_{J_n l_n j_n}(r) \left(\mathcal{Y}_{l_n j_n} \otimes \Phi_{I_n} \right)_{JM}$

radial part of relative motion

$$= r^{-1} \sum_{J_n l_n j_n} R_{J_n l_n j_n}(r) \sum_{m_j M_n} (j_n I_n m_j M_n | J M) \mathcal{Y}_{l_n j_n m_j} \Phi_{I_n M}$$

where $\mathcal{Y}_{l_n j_n m_j} = \sum_{m_l m_s} (l\, s\, m_l\, m_s | j\, m_j)\, i^l\, Y_{l_n m_l}\, \chi_{s m_s}$

spin of projectile

angular part of rel. motion

target states $\mathcal{H}_t \Phi_{I_n M_n} = \omega_n \Phi_{I_n M_n}$ wave fct. of target in its nth state

— insert expressions for $\mathcal{H}$ and Ψ into Schrödinger equation
— multiply by $(\mathcal{Y}_{l_n j_n} \otimes \Phi_{I_n})^*_{JM}$ from the left
— integrate over all coordinates except r
— divide by E_n

$$\triangleright \left| \left(\frac{d^2}{d\rho_n^2} - \frac{l_n(l_n+1)}{\rho_n^2} - \frac{1}{E_n} V_{diag} + 1 \right) R_{J_n l_n j_n}(r) = \right.$$

$$= E_n^{-1} \sum_{n' l_{n'} j_{n'}} \langle (\mathcal{Y}_{l_n j_n} \otimes \Phi_{I_n})_{JM} | V_{coupl} | (\mathcal{Y}_{l_{n'} j_{n'}} \otimes \Phi_{I_{n'}})_{JM} \rangle R_{J_{n'} l_{n'} j_{n'}}(r)$$

$\rho_n = k_n r$

k_n ... wave number

set of n_c coupled equations,

quite general, holds irrespective of the nature of the projectile or the target

assumptions about nuclear structure only affect coupling matrix elements

evaluation of these is most crucial part of the calculations!

General form of coupling term:

$$V_{coupl} = \sum_{t,\lambda} v_\lambda^{(t)}(r)\,(Q_\lambda^{(t)} \cdot Y_\lambda)$$

t ... character of term with given rank

λ ... tensorial rank

$Q_\lambda^{(t)}$ ... operates only on the coordinates of the target nucleus

$$\langle (\mathcal{Y}_{lj} \otimes \Phi_I)_{JM} | V_{coupl} | (\mathcal{Y}_{l'j'} \otimes \Phi_{I'})_{JM} \rangle =$$

$$= \langle lj I | V_{coupl} | l'j' I' \rangle =$$

$$= \sum_{t,\lambda} v_\lambda^{(t)}(r) \langle I \| Q_\lambda^{(t)} \| I' \rangle \, A(lj I, l'j' I', \lambda J s)$$

reduced matrix element contains all the dynamics involved in the problem | geom factor (A matrix) from combination of Y in V_{coupl} with Y in wave functions; expressed by C J symbols

$\downarrow$

defined by:

$$\langle I M_I | Q_{\lambda\mu}^{(t)} | I' M_I' \rangle = \langle I \| Q_\lambda^{(t)} \| I' \rangle \frac{1}{\sqrt{2I'+1}} (I'\lambda M_I' \mu | I M_I)$$

Q Matrix B matrix

$\boxed{\text{Explicit form of reduced matrix elements for various cases}}$

A. Vibrational nucleus (even mass)

Comparing $V_{coupl} = \sum_{t,\lambda} v_\lambda^{(t)}(r)\,(Q_\lambda^{(t)} \cdot Y_\lambda)$

and $V_{coupl}^{(v)} = \sum_{\lambda\mu} v_{cp;\lambda}^{(1)(v)}(r)\, \alpha_{\lambda\mu} Y_{\lambda\mu} +$

$$+ \sum_{\lambda\lambda_1\lambda_2} v_{cp;\lambda}^{(2)(v)}(r) \sqrt{\frac{(2\lambda_1+1)(2\lambda_2+1)}{4\pi(2\lambda+1)}} (\lambda_1\lambda_2 00|\lambda 0) \sum_\mu (\alpha_{\lambda_1} \otimes \alpha_{\lambda_2})_{\lambda\mu} Y_{\lambda\mu}$$

leads to
$$\left.\begin{aligned} Q^{(1)}_{\lambda\mu} &= \alpha_{\lambda\mu} \\ Q^{(2)}_{\lambda\mu} &= \sum_{\lambda_1\lambda_2} \sqrt{\frac{(2\lambda_1+1)(2\lambda_2+1)}{4\pi(2\lambda+1)}}\,(\lambda_1\lambda_2 0 0|\lambda 0)(\alpha_{\lambda_1}\otimes\alpha_{\lambda_2})_{\lambda\mu} \end{aligned}\right\} \quad (o)$$

express operator $\alpha_{\lambda\mu}$ as sum of creation and annihilation operator:

$$\alpha_{\lambda\mu} = \beta_\lambda \frac{1}{\sqrt{2\lambda+1}}\left(b_{\lambda\mu} + (-)^\mu b^*_{\lambda-\mu} \right)$$

$|0\rangle$ no-phonon (ground) state

(a) one phonon state $|1; IM\rangle = b^*_{IM}|0\rangle$

(b) two phonon state $|2; IM\rangle = (1+\delta_{\lambda_1\lambda_2})^{-\frac{1}{2}}(b^*_{\lambda_1}\otimes b^*_{\lambda_2})_{IM}|0\rangle$

multipolarities of the 2 phonons

(c) three quadr. phonon state $|3; IM\rangle = \sum_{I'} N_I^{(I')}\left((b^*_2\otimes b^*_2)_{I'}\otimes b^*_2\right)_{IM}|0\rangle$ $\quad$ (w)

fractional parentage coefficients (= amplitudes of the different states with intermediate spin I')

Using (o) for the operators and (w) for the wave functions, one gets the following matrix elements $\langle I \| Q^{(t)}_\lambda \| I'\rangle$:

(i) Operators linear in α_λ

(a') Ground state $\leftrightarrow$ one phonon state (arbitrary λ):

$$\langle 0; 0 \| Q^{(1)}_\lambda \| 1; I\rangle = \delta_{\lambda I}\,(-)^I \beta_\lambda$$

phonon number $\quad$ spin

(b') One quadr. phonon state $\leftrightarrow$ two quadr. phonon state:

$$\langle 1; 2 \| Q^{(1)}_2 \| 2; I\rangle = \beta_2\left[2(2I+1)/5\right]^{\frac{1}{2}}$$

(c') Two quadrupole phonon state $\leftrightarrow$ three quadrupole phonon state:

$$\langle 2;I \| Q_2^{(1)} \| 3;I' \rangle = \frac{\beta_2}{\sqrt{10}} \sum_{I''} N_I^{(I'')} \Big(2\delta_{II''} (-)^{I+I'} \sqrt{2I'+1} + 4\sqrt{(2I+1)(2I'+1)(2I''+1)}\, W(222I';I''I) \Big)$$

(d') One octupole phonon state $\leftrightarrow$ quadr. oct. two phonon state:

$$\langle 1;3 \| Q_2^{(1)} \| \underbrace{2\otimes 3}_{\text{multipolarities, not phonon numbers}};I \rangle = \beta_2 [(2I+1)/5]^{\frac{1}{2}}$$

(e') One quadrupole phonon state $\leftrightarrow$ quadr. oct. two phonon state:

$$\langle 1;2 \| Q_3^{(1)} \| 2\otimes 3;I \rangle = \beta_3 (-)^I [(2I+1)/7]^{\frac{1}{2}}$$

(ii) Operators quadratic in α_λ

(a'') Ground state $\leftrightarrow$ two quadrupole phonon state:

$$\langle 0;0 \| Q_\lambda^{(2)} (\lambda_1=\lambda_2=2) \| 2;I \rangle = \beta_2^2\, \delta_{I\lambda} (2200|I0)/\sqrt{2\pi}$$

(b'') One quadrupole phonon state $\leftrightarrow$ three quadrupole phonon state:

$$\langle 1;2 \| Q_\lambda^{(2)} (\lambda_1=\lambda_2=2 \| 3;I \rangle = \beta_2^2 (2200|\lambda 0) \sum_{I''} N_I^{(I'')} * \left(2\delta_{I''\lambda} \sqrt{\frac{2I+1}{2\lambda+1}} + 4\sqrt{(2I+1)(2I''+1)}\, W(222I;I''\lambda) \right) / \sqrt{4\pi}$$

(c'') Ground state $\leftrightarrow$ quadrupole octupole two phonon state:

$$\langle 0;0 \| Q_\lambda^{(2)} (\lambda_1=2,\lambda_2=3) \| (2\otimes 3);I \rangle = \beta_2\beta_3\, \delta_{\lambda I} (2300|I0) (-)^{I+1} / \sqrt{4\pi}$$

(d'') One quadrupole phonon state $\leftrightarrow$ one octupole phonon state:

$$\langle 1;2 \| Q_\lambda^{(2)} (\lambda_1=2,\lambda_2=3) \| 1;3 \rangle = \beta_2\beta_3 (2300|\lambda 0)/\sqrt{4\pi}$$

Hermiticity: $\langle I \| Q_\lambda^{(t)} \| I' \rangle = (-)^{I-I'+\lambda} \langle I' \| Q_\lambda^{(t)} \| I \rangle$

▷ B matrix not hermitean

A matrix — " — (same property as B matrix above)

▷ coupling matrix hermitean, as it should be

When $\lambda_1 = \lambda_2$ in (0) : coupling term contributes nonvanishing diagonal elements:

(a''') Ground state : $\langle 0;0 \| Q_\lambda^{(2)}(\lambda_1=\lambda_2=2) \| 0;0\rangle = \beta_2^2 \delta_{\lambda 0}/\sqrt{4\pi}$

(b''') One quadr. ph. st.: $\langle 1;2 \| Q_\lambda^{(2)}(\lambda_1=\lambda_2=2) \| 1;2\rangle = \beta_2^2 (2200|\lambda 0)(2+5\delta_{\lambda 0})/\sqrt{4\pi}$

(c''') Two quadr. ph. st.: $\langle 2;I \| Q_\lambda^{(2)}(\lambda_1=\lambda_2=2) \| 2;I'\rangle = \beta_2^2 \frac{1}{\sqrt{4\pi}\,\lambda}(2200|\lambda 0) *$

$$* \left\{ \sqrt{5(2I+1)}\,\delta_{\lambda 0}\delta_{II'} + 4\sqrt{(2I+1)(2I'+1)(2\lambda+1)}\,W(2I2I';2\lambda) \right\}$$

B. Rotational nucleus

consider only the excitation of the states of the ground state rotational band (same internal structure as ground state, but additional rotation)

$$V_{coupl} = \sum_{t,\lambda} v_\lambda^{(t)}(r)\,(Q_\lambda^{(t)} Y_\lambda)$$

$$V_{coupl}^{(n)} = \sum_{\substack{\lambda\mu \\ \lambda\neq 0}} v_{cp}^{(\lambda)(n)}(r)\, D_{\mu 0}^{\lambda}\, Y_{\lambda\mu}(\theta,\phi)$$

$$\Rightarrow \langle l_j I | V_{coupl} | l' j' I' \rangle_{JM} = \sum_\lambda v_{cp}^{(\lambda)(n)}(r)\, B_\lambda(II')\, A(l_j I, l' j' I'; \lambda J s)$$

where $B_\lambda(I,I') = \sqrt{2I'+1}\,(I'\lambda K 0 | I K)$

projection of spin on body fixed axis

for the excitation of rotational states of bands or vibrational states (β and/or γ vibrations) : $B_\lambda(II')$ more involved

4) Scattering matrices and cross sections

Solve coupled equations for radial wave function $R_{JnLj}(r)$ } ⇒ S matrix
match at R_m to asymptotic solution

assumption : projectile and target initially both in polarized state
(unpolarized state included as special case)

amplitudes: $a^{(i)}_{m_s}$, $b^{(i')}_{M_A}$

i, i'... specify different spin ensembles when more than one ensemble is needed for the description of the pol. state

amplitudes of different ensembles do <u>not</u> interfere, amplitudes of one ensemble <u>do</u> interfere

A. Shape Scattering XS's and Polarizations

asymptotic form of wave fct.:

$$\Psi_{asym} = \frac{\sqrt{4\pi}}{r k_n \sqrt{v_n}} \sum_{(ii')m_s M_A} a^{(i)}_{m_s} b^{(i')}_{M_A} \sum_{LjJM} (L\,s\,0\,m_s | j\,m_s)(j\,I_A\,m_s\,M_A | J\,M) *$$

$$* \sum_{nL'j'} \Big[\sqrt{2L+1}\, \exp(i\sigma^{(n)}_L)\, \delta_{nn} \delta_{L'L} \delta_{j'j} F^{(n)}_L + \sqrt{2L'+1} \left(\frac{k_n}{k_m}\right)^{3/2} \exp(i\sigma^{(n)}_{L'}) *$$

$$* C_{Lj;nL'j'} (G^{(n)}_{L'} + i F^{(n)}_{L'}) \Big] (\mathcal{Y}_{L'j'} \otimes \Phi_{I_n})_{JM}$$

"scattering coefficients"

irreg. reg. Ch fcts. for orb. ang. mom. L' and energy E_n at $r = R_m$

$$\eta_n = \frac{m Z Z' e^2}{\hbar^2 k_n} \qquad m \text{... reduced mass}$$

$\sigma^{(n)}_L$ ... Ch phase shift

for uncharged projectile : $\eta_n = 0$

$\sigma^{(n)}_L = 0$

replace $F^{(n)}_L, G^{(n)}_L \longrightarrow k_n R_m \cdot j^{(n)}_L, k_n R_m n^{(n)}_L$

spher. Bessel Neumann

incident wave Ψ_{inc}: Ch distorted plane wave plus
Ch scattered wave

$$\Psi_{inc} = \frac{1}{\sqrt{v_1}} \Big\{ \exp\Big[i\big(k_1 z - \eta_1 \ln(2k_1|r-z|)\big) \Big\{ 1 - \frac{\eta_1^2}{i k_1 (r-z)} \Big\} + f_c(\theta) \frac{1}{r} \exp\Big[i\big(k_1 r - \eta_1 \ln(2k_1 r)\big) \Big] \Big\} *$$

$$* \sum_{(ii')m_s M_1} a^{(i)}_{m_s} b^{(i')}_{M_1} \chi_{s m_s} \Phi_{I_1 M_1}$$

add second terms of inc. and asympt. wave, noting the asymptotic behaviour of the Ch fcts.:

$$G_l^{(n)} \xrightarrow[r\to\infty]{} \cos \Sigma_l^{(n)}$$

$$F_l^{(n)} \xrightarrow[r\to\infty]{} \sin \Sigma_l^{(n)}$$

$$\Sigma_l^{(n)} = k_n r - \eta_n \ln(2k_n r) - \frac{l\pi}{2} + \sigma_l^{(n)}$$

$$\triangleright \quad \Psi_{scatt} = \sum_n \frac{\exp[i(k_n r - \eta_n \ln(2k_n r))]}{r\sqrt{v_n}} \sum_{(ii')m_s M_1} a^{(i)}_{m_s} b^{(i')}_{M_1} *$$

$$* \Big\{ f_c(\theta) \delta_{n1} \chi_{s m_s} \Phi_{I_1 M_1} + \sum_{l j l' j' J} \frac{4\pi}{k_n^2} \sqrt{2l'+1} \exp(2i\sigma_{l'}^{(n)}) C^{J}_{l j; n l' j'} *$$

$$* (l\, s\, 0\, m_s | j\, m_s)(j\, I_1\, m_s\, M_1 | J M)(Y_{l'j'} \otimes \Phi_{I_n})_{JM}$$

Shape scattering differential XS which leaves the target in its nth state

$$\boxed{\sigma_n^{(s)}(\theta,\phi) = \sum_{\underbrace{(ii')m_s' M_n}_{\text{summation over final states}}} \Big| \sum_{m_s M_1} a^{(i)}_{m_s} b^{(i')}_{M_1} \Big\{ f_c(\theta) \delta_{n1} \delta_{m_s m_s'} \delta_{M_1 M_n} + \sum_{l j l' j' J m_l m_{l'}} \frac{\sqrt{4\pi}}{k_n} \sqrt{2l'+1} *}$$

$$* \exp(2i\sigma_{l'}^{(n)}) C^{J}_{l j; n l' j'} (l\, s\, 0\, m_s | j\, m_s)(j\, I_1\, m_s\, M_1 | J M)(l'\, s\, m_{l'}\, m_{s'} | j'\, m_{j'}) *$$

$$* (j'\, I_n\, m_{j'}\, M_n | J M)\, Y_{l' m_{l'}}(\theta,\phi) \Big\} \Big|^2$$

depends in general on azimuthal angle ϕ

introduce an amplitude:

$$X_{m_s M_1, m_s' M_n}(\theta,\phi) = f_c(\theta)\,\delta_{n1}\,\delta_{m_s m_s'}\,\delta_{M_1 M_n} +$$

$$+ \sum_{l\,l'\,j'\,J\,m_l'\,m_j'\,M} \frac{\sqrt{4\pi}}{k_n}\sqrt{2J'+1}\,\exp(2i\sigma_{l'}^{(n)})\,C^{J}_{l\,j;\,n\,l'\,j'}\,(l\,s\,0\,m_s|j\,m_s)(j\,I_1\,m_s\,M_1|J\,M)$$

$$\times(l'\,s\,m_l'\,m_s'|j'\,m_j')(j'\,I_n\,m_j'\,M_n|J\,M)\,Y_{l'm_l'}(\theta,\phi)$$

$$\Rightarrow \boxed{\sigma_n^{(s)}(\theta,\phi) = \sum_{(ii')\,m_s'\,M_n} \Big|\sum_{m_s M_1} X_{m_s M_1;\,m_s' M_n}(\theta,\phi)\,a^{(i)}_{m_s}\,b^{(i')}_{M_1}\Big|^2}$$

Vector polarization also given as bilinear function of X

B. Total and Reaction Cross Sections

$$\sigma_{abs} + \sum_{n\neq 1}\sigma_n^{(s)} = -\frac{1}{v_1}\Big[-\oint \vec{j}\,d\vec{f}\Big]$$

prob. flux density

σ_{abs} ... compound nucleus XS

$\sum_{n\neq 1}\sigma_n^{(s)}$ ... direct inelastic XS

$$\sigma_{abs} + \sum_{n\neq 1}\sigma_n^{(s)} = \frac{\hbar}{2im}\int\Big[\psi_1\frac{\partial\psi_1^*}{\partial r} - \psi_1^*\frac{\partial\psi_1}{\partial r}\Big]_r\, r^2\,d\tau\,d\Omega$$

$\int d\tau$ ... integration and summation over internal coord.s

$\int d\Omega$ ... —"— over angular variables of rel. motion

$\sigma_{sh.el.}$ ... total shape elastic XS

$\sigma_t = \sigma_{abs} + \sigma_{sh.el.} + \sum_{n\neq 1}\sigma_n^{(s)} = \sigma_{abs} + \sum_n \sigma_n^{(s)}$ ... total cross section

if incident particle is charged: $\sigma_{sh.el.} \to \infty$

$\Rightarrow \sigma_t \to \infty$

$\Rightarrow$ consideration of $\sigma_{sh.el.}$ and σ_t has meaning only for neutral projectile

simplification of the expressions for σ_t and σ_{abs} by introducing

$$Z_{m_s M_1, m_s' M_1'; l'} = \sum_{l\,j\,J\,M\,m_l'\,m_j'} (l\,s\,0\,m_s|j\,m_s)(j\,I_1\,m_s\,M_1|J\,M)\,*$$

$$* \, C^{J}_{l\,j;\,1\,l'\,j'}\,(l'\,s\,0\,m_s'|j'\,m_s')(j'\,I_1\,m_s'\,M_1'|J\,M)$$

amplitude, intimately related to X

$$\Rightarrow \boxed{\sigma_t = \frac{4\pi}{k_1^2}\sum_{l'}(2l'+1)\left\{\mathrm{Im}\sum_{(ii')m_s m_s' M_s M_s'} a^{(i)}_{m_s} a^{(i)*}_{m_s'} b^{(i)}_{M_s} b^{(i)*}_{M_s'} Z_{m_s M_s; m_s' M_s'; l'}\right\}} \leftarrow \text{opt. theorem}$$

$$\sigma_{abs} + \sum_{n\neq 1}\sigma_n^{(s)} = \sigma_t - \int \sigma_s^{(s)}(\theta,\phi)\,d\Omega =$$

$$= \sigma_t - \frac{4\pi}{k_1^2}(2l'+1)\sum_{ii'j'J}\left|\sum_{m_s M_s} a^{(i)}_{m_s} b^{(i')}_{M_s}\sum_{lj}(l\,s\,0\,m_s|j\,m_s)(j\,I_s\,m_s\,M_s|J\,M)\,C^{J}_{lj;l'j'}\right|$$

cf. preceding section

C. Compound Contribution to the Differential Scattering XS

when energy of incident particle is low → add contribution of compound process to scattering XS to n^{th} state

Hauser Feshbach formalism

↓

XS as function of penetrabilities $T_l^{(n)}$ for various channels n and orb. ang. mom. l

$T_l^{(n)}$ computed from scattering coefficients $C_l^{(n)}$

spin orbit interaction $\Rightarrow C_{lj}^{(n)} \Rightarrow T_{lj}^{(n)}$

CCOM : $C^{J}_{lj;nl'j'}$ ▷ modify HF cross section:

$C^{J}_{lj;nl'j'}$ .... amplitude of outgoing wave in channel $nl'j'$ when there is an incoming wave in the channel $1\,lj$ with amplitude $1\exp(i\sigma_l^{(1)})$

defines penetrabilities in ground state channels

reduced scattering coefficients :

$C^{J}_{nlj;n'l'j'}$ ... amplitude of outgoing wave in channel $n'l'j'$ when there is an incoming wave in channel nlj with amplitude $1\exp(i\sigma_l^{(n)})$

Def.: generalized S matrix element $S^J_{nlj;n'l'j'}$

$$S^J_{nlj;n'l'j'} = \delta_{nn'}\delta_{ll'}\delta_{jj'} + 2i\sqrt{\frac{2l'+1}{2l+1}}\,\frac{k_c}{k_c'}\,C^J_{nlj;n'l'j'}$$

$$T^J_{nlj} = 1 - \sum_{n'l'j'} S^J_{nlj;n'l'j'}\, S^{J\,*}_{nlj;n'l'j'}$$ generalized transm. coeff.

Compound contribution to scattering XS leaving target in its nth state:

$$\boxed{\sigma_n^{(c)}(\theta) = \frac{\pi}{k_i^2}\sum_{ii'm_sM_i}(a^{(i)}_{m_s})^2(b^{(i')}_{M_i})^2\sum_J\Big[1/\sum_{nlj}T^J_{nlj}\Big] * \sum_{ll'j'(m)}(2l+1)(l\,s\,0\,m_s|j\,m_s)^2(j\,I_A\,m_s\,M_i|J\,M)^2 * (l'\,s\,m_l\,m_s'|j'\,m_j')^2(j'\,I_A\,m_j'\,M_n|J\,M)^2\,T_{nlj}\,T_{nl'j'}\,|Y_{l'm_l'}|^2}$$

independent on ϕ

T_{nlj} real

I. Adiabatic approximation (ACC)

requirements

- target well defined → exc. spectrum is closely that of an ideal rotational band
- inc. energy >> exc. energy of these rotational states
- interested only in excitation of ground state rotational band

coupling to all states of ground band is included automatically
⇒ quite accurate results with less complicated and faster calculations than with non-adiabatic coupled channels calcs. (NACC)

same potential as with NACC

$$R = R_0\Big(1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')\Big) \qquad \bar{R} = \bar{R}_0\Big(1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')\Big)$$

$$V^{(n)}_{coupl} = \sum_{\substack{\lambda\mu \\ (\lambda\neq 0)}} v^{(\lambda)(a)}_{cp}(r)\, \underbrace{Y'_{\lambda 0}}_{\text{with respect to body fixed system}}$$ don't transform to space fixed system

Denote by $\bar{m}_j$ the projection on the nuclear symmetry axis of the angular momentum j of a partial wave of the projectile

$$\triangleright\ \Psi = \frac{1}{r}\sum_{l j \bar{m}_j} R_{l j \bar{m}_j}(r)\, \underbrace{\mathcal{Y}'_{l j \bar{m}_j}}_{Y_{l m_l} \chi_{s m_s}}$$

<u>Coupled equation:</u>

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} - E^{-1} V_{diag} + 1\right) R_{l j \bar{m}_j} =$$

$$= E^{-1} \sum_{l' j'} \langle \mathcal{Y}'_{l j \bar{m}_j} | \sum_{\lambda} v^{(r)(\lambda)}_{cp}(r)\, Y'_{\lambda 0} | \mathcal{Y}'_{l' j' \bar{m}_j} \rangle R_{l' j' \bar{m}_j}$$

where $\rho = kr$

reason why the body fixed system was preferred is that otherwise there would be coupling between different $\bar{m}_j$ in addition to coupling of different j

<u>Coupling matrix:</u>

$$\langle \mathcal{Y}'_{l j \bar{m}_j} | \sum_{\lambda} v^{(a)(\lambda)}_{cp}\, Y'_{\lambda 0} | \mathcal{Y}'_{l' j' \bar{m}_j} \rangle =$$

$$= \sum_{\lambda} v^{(a)(\lambda)}_{cp} * \text{complete by geom. factor}$$

$\triangleright$ B matrix is replaced by c numbers which is unity

Asymptotic form of the wave function:

$$\Psi_{asym} = \frac{\sqrt{4\pi}}{r k_i \sqrt{v_i}} \sum_{(ii')m_s M_i} a^{(i)}_{m_s} b^{(i')}_{M_i} \sum_{l j} (l\, s\, 0\, m_s | j\, m_j)\, \underbrace{D_{m_s \bar{m}_j}}_{\text{space body}}(\theta_i) \sum_{l' j'} \sqrt{2l'+1}\, \exp(i\sigma^{(a)}_{l'})$$

$$* \left[\delta_{ll'}\delta_{jj'} F^{(i)}_{l'} + \underbrace{C^{\bar{m}_j}_{l j; l' j'}}_{\text{body}} (G^{(a)}_{l'} + i F^{(a)}_{l'})\right] \mathcal{Y}'_{l' j' \bar{m}_j}\, \Phi_{I M_I}$$

Important difference between ACC and NACC : in ACC no coupling of I_A and j ← ACC supposes that target nucleus is inert during the scattering process and thus carries no angular momentum dynamically

rotation fct. for transformation between space and body fixed system

scattered wave :

$$\Psi_{scatt} = \frac{1}{k_A\sqrt{v_A}} \exp(ik_A r - i\eta_A \ln 2k_A r) \sum_{(ii')m_s M_A} a^{(i)}_{m_s} b^{(i')}_{M_A} *$$

$$* \Big[f_c(\theta)\chi_{sm_s} + \frac{\sqrt{4\pi}}{k_A} \sum_{l_j l'_{j'} \bar{m}_j m'_j} \sqrt{2l'+1} \exp(2i\sigma^{(1)}_{l'}) C^{\bar{m}_j}_{l_j; l'_{j'}} (l\, s\, 0\, m_s | j\, m_s) *$$

$$* D^{j}_{m_s \bar{m}_j}(\theta_i) \, \mathcal{Y}^{m'_j}_{l'_{j'}} \Big] \Phi_{I_A M_A} =$$

$$= \frac{1}{k_A\sqrt{v_A}} \exp(ik_A r - i\eta_A \ln 2k_A r) \sum_{(ii')m_s M_A} a^{(i)}_{m_s} b^{(i')}_{M_A} *$$

$$* \Big[f_c(\theta)\chi_{sm_s} + \frac{\sqrt{4\pi}}{k_A} \sum_{l_j l'_{j'} \bar{m}_j m_s' m_l' m'_j} \sqrt{2l'+1} \exp(2i\sigma^{(1)}_{l'}) C^{\bar{m}_j}_{l_j; l'_{j'}} (l\, s\, 0\, m_s | j\, m_s) *$$

$$* (l'\, s\, m'_l\, m'_s | j'\, m'_j) \, D^{j}_{m_s \bar{m}_j}(\theta_i) \, D^{*j}_{m'_j \bar{m}_j} \, Y_{l' m'_l} \chi_{s m'_s} \Big] \Phi_{I_A M_A}$$

expand right hand side (except $\frac{1}{k_A\sqrt{v_A}} \exp(\ldots)$) in terms of eigenfunctions $\Phi_{I_n M_n}$ of the target => expansion coefficients give scattering amplitudes to leave the target in that particular state

note that $\underset{\text{space}}{\Phi_{I_n M_n}} = [(2I_n+1)/8\pi^2]^{\frac{1}{2}} \, \underset{\text{space}\ \text{body}}{D^{I_n}_{M_n K}(\theta_i)}$

K... projection of I_n to the nuclear symmetry axis

$$[\quad] \Phi_{I_A M_A} = \sum_{n m_s' M_A m_s'} \alpha_{n m_s M_A m_s'} \Phi_{I_n M_n}$$

$$\alpha_{n m_s M_A m_s'} = \langle \Phi_{I_n M_n} | [\quad] | \Phi_{I_A M_A} \rangle$$

leads to :

$$\Psi^{(ACC)}_{scatt} = \frac{1}{k\sqrt{v_a}} \exp(ikr - i\eta_1 \ln(2kr)) \sum_{n(ii')m_s M_1 m_s'} a^{(i)}_{m_s} b^{(i')}_{M_1} \alpha_{n m_s M_1 m_s'} \Phi_{I_n M_n} =$$

$$= \frac{1}{k\sqrt{v_a}} \exp(ikr - i\eta_1 \ln(2kr)) \sum_{n(ii')m_s M_1 m_s'} a^{(i)}_{m_s} b^{(i')}_{M_1} X^{(ACC)}_{m_s M_1; m_s' M_n} \chi_{s m_s'} \Phi_{I_n M_n}$$

with $X^{(ACC)}_{m_s M_1; m_s' M_n}(\theta,\phi) = f_c(\theta)\delta_{n1}\delta_{m_s' m_s}\delta_{M_n M_1} +$

$$+ \sum_{l j l' j' \bar{m}_j m_l' m_j'} \frac{\sqrt{4\pi}}{k_1}\sqrt{2l'+1}\, \exp(2i\sigma^{(1)}_{l'}) C^{\bar{m}_j}_{l j; l' j'} (l s 0 m_s | j m_s) *$$

$$* \sum_{J M_J} \Big[(-)^{\bar{m}_j - m_j} \sqrt{\frac{2I_1+1}{2I_n+1}} (I_1 J K 0 | I_n K)(I_1 J M_1 M_J | I_n M_n)(j j' \bar{m}_j - \bar{m}_j | J$$

$$* (j j' | m_s - m_j | J M_J)(l' s m_l' m_s' | j' m_j') Y_{l' m_l'}(\theta,\phi) \Big]$$

$X^{(ACC)}_{m_s M_1; m_s' M_1'}$ plays exactly the same role as $X_{m_s M_1; m_s' M_1'}$ in NACC

Expressions for XS's and polarizations derived for NACC can be used for ACC by replacing $X_{m_s M_1; m_s' M_1'}(\theta,\phi) \to X^{(ACC)}_{m_s M_1; m_s' M_1'}$

$$Z_{m_s M_1, m_s' M_1'; l'} \to Z^{(ACC)}_{m_s M_1, m_s' M_1'; l'} = \sum_{j l' j' \bar{m}_j m_l' m_j'} (l s 0 m_s | j m_s) C^{\bar{m}_j}_{l j; l' j'} *$$

$$* (l' s m_l' m_s' | j' m_j') \sum_{J M} \Big[(-)^{\bar{m}_j - m_j} (I_1 J K 0 | I_1 K) *$$

$$* (I_1 J M_1 M_J | I_1 M_1')(j j' \bar{m}_j - \bar{m}_j | J 0)(j j' m_s - m_j | J M_J)$$

Saving of computational time and core storage with ACC:

- Symmetry relations of X and Z under $\bar{m}_j \to -\bar{m}_j$
  $\Rightarrow$ coupled equation is needed to be solved for $\bar{m}_j > 0$ only
- number of coupled channels for given $\bar{m}_j$ (ACC) is smaller than for given J (NACC)
- number of systems of coupled equations to be solved is smaller with ACC than with NACC
- sizes of coupled equations to be solved (ACC) are unchanged if incident energy is fixed, irrespective of how high we go up in the excited states

IV) THE STATISTICAL MODEL FOR COMPOUND NUCLEUS REACTIONS AND PREEQUILIBRIUMDECAY

1) Compound nucleus model

A. Theory

In theoretical treatment of nuclear reactions : XS's expressed in terms of S matrix:

$$\sigma_{ab} = \frac{\pi}{k_a^2} |\delta_{ab} - S_{ab}|^2$$

general properties of S : unitarity $SS^\dagger = S^\dagger S = I$ (flux conservation)

symmetry $S^T = S$ (time reversal inv.)

theory of nuclear reactions aims at calculation of S matrix by solving Schrödingerequation for A particle system

from general reaction theories (particularly R matrix theory):

$$S_{ab} = S^0_{ab} - \underbrace{i \sum_\mu \frac{g_{\mu a}\, g_{\mu b}}{E - E_\mu + \frac{i}{2}\Gamma_\mu}}_{\text{resonance pole term}}$$

S^0_{ab} slowly varying function of energy, compared to 2nd term

for energy interval ΔE around E_0:

$$S_{ab} = \overline{S_{ab}} + S^{fl}_{ab} \qquad \overline{S_{ab}} = \frac{1}{\Delta E}\int_{E_0-\frac{\Delta E}{2}}^{E_0+\frac{\Delta E}{2}} dE\, S_{ab} \qquad \overline{S^{fl}_{ab}} = 0$$

averaging of unitary relation leads to relation between $\overline{S_{ab}}$ and S^{fl}_{ab}

$$\sum_c S_{ac} S^*_{bc} = \sum_c \overline{S_{ac}}\, \overline{S^*_{bc}} + \sum_c \overline{S^{fl}_{ac} S^{fl*}_{bc}} = \delta_{ab}$$

averaging of cross section :

$$\overline{\sigma_{ab}} = \frac{1}{\Delta E}\int_{E_0-\frac{\Delta E}{2}}^{E_0+\frac{\Delta E}{2}} dE\, \sigma_{ab}(E) = \frac{\pi}{k_a^2}|\delta_{ab} - \overline{S_{ab}}|^2 + \frac{\pi}{k_a^2}\overline{|S^{fl}_{ab}|^2} = \sigma^{dir}_{ab} + \langle \sigma^{fl}_{ab} \rangle$$

interpretation : σ^{dir}_{ab} : $\overline{S_{ab}}$ describes direct reactions

σ^{fl}_{ab} : S^{fl}_{ab} describes compound nucleus reactions

assumption : $\bar{S}_{ab}$ known from direct reaction model

aim of the statistical theory of cross sections : calculation of $\langle \sigma_{ab}^{fl} \rangle$ (and correlation fcts.) from $\bar{S}_{ab}$

Cases :

A) No direct reactions in non-elastic channels: $\bar{S}_{ab} = \delta_{ab} \bar{S}_{aa}$

$\bar{S}_{aa}$ from single channel optical model

transmission coefficients : $\frac{\pi}{k_a^2} T_a = \sum_b \langle \sigma_{ab}^{fl} \rangle = \frac{\pi}{k_a^2} (1 - |\bar{S}_{aa}|^2)$

$$T_a = 1 - |\bar{S}_{aa}|^2 \quad \text{with } 0 \le T_a \le 1$$

▲ Isolated resonances $\frac{\langle \Gamma_\mu \rangle}{D} \ll 1$

where $\langle \Gamma_\mu \rangle$ ... average width, D .... spacing } of res.s

$S_{ab}^0 = \delta_{ab} e^{2i\varphi_a}$ $\quad \varphi_a$ – phase shift for potential scattering

$g_{\mu a} = e^{i\varphi_a} \Gamma_{\mu a}^{\frac{1}{2}}$ in resonance pole term

▷ $S_{ab} = \delta_{ab} e^{2i\varphi_a} - i e^{i(\varphi_a + \varphi_b)} \sum_\mu \frac{\Gamma_{\mu a}^{\frac{1}{2}} \Gamma_{\mu b}^{\frac{1}{2}}}{E - E_\mu + \frac{i}{2}\Gamma_\mu}$ $\qquad \Gamma_\mu = \sum_c \Gamma_{\mu c}$

$$\bar{S}_{ab} = \delta_{ab} e^{2i\varphi_a} - e^{i(\varphi_a + \varphi_b)} \frac{\pi}{D} \underbrace{\langle \Gamma_{\mu a}^{\frac{1}{2}} \Gamma_{\mu b}^{\frac{1}{2}} \rangle_\mu}_{\langle \Gamma_{\mu a} \rangle_\mu \text{ since } \bar{S}_{ab} \text{ assumed to be diagonal}} = \delta_{ab} e^{+2i\varphi_a} \left(1 - \frac{\pi}{D} \langle \Gamma_{\mu a} \rangle\right)$$

$$T_a = 1 - |\bar{S}_{aa}|^2 = \underbrace{\frac{2\pi}{D} \langle \Gamma_{\mu a} \rangle}_{\ll 1} + \underbrace{\frac{\pi^2}{D^2} \langle \Gamma_{\mu a} \rangle^2}_{\text{negligible if } \langle \Gamma \rangle / D \ll 1}$$

Calculate $S_{ab}^{fl} = S_{ab} - \bar{S}_{ab}$

▷ $|S_{ab}^{fl}|^2$

▷ $\overline{|S_{ab}^{fl}|^2}$ $\quad$ average over ΔE

leads to

$$\langle \sigma_{ab}^{\#} \rangle = \frac{1}{\Delta E} \int_{E_0-\frac{\Delta E}{2}}^{E_0+\frac{\Delta E}{2}} dE \left\{ \frac{\pi}{k_a^2} \sum_\mu \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{(E-E_\mu)^2 + \frac{1}{4}\Gamma_\mu^2} + \text{resonance interference term} \right\} =$$

$$= \frac{\pi}{k_a^2} \left\{ \frac{2\pi}{D} \underbrace{\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle_\mu}_{\text{average over } \Delta E \,\hat{=}\, \text{ensemble average over resonance parameter}} + \mathcal{O}\left(\frac{\langle \Gamma_\mu \rangle^2}{D^2} \right) \right\}$$

$$\frac{\pi}{k_a^2} T_a = \sum_b \langle \sigma_{ab}^{\#} \rangle = \frac{\pi}{k_a^2} \frac{2\pi}{D} \langle \Gamma_{\mu a} \rangle$$

▷ $T_a = \frac{2\pi}{D} \langle \Gamma_{\mu a} \rangle \ll 1$ for isolated resonances
"weak absorption"

$$\sum_a T_a = \frac{2\pi}{D} \langle \Gamma_\mu \rangle \text{ due to } \sum_a \Gamma_{\mu a} = \Gamma_\mu$$

Rewrite $\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle_\mu$ in order to express XS' by means of T_a:

$$\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle = \frac{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} W_{ab}$$

$$W_{ab} = \left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle \frac{\langle \Gamma_\mu \rangle}{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}$$ "width fluctuation correction factor"

W_{ab} can be calculated if statistical properties of $\Gamma_{\mu a}$ are known
Closed form expression for W_{ab} if the following conditions are satisfied:

(i) $\langle \Gamma_{\mu a} \cdot \Gamma_{\mu b} \rangle = \langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle$ for $a \neq b$

(ii) $\Gamma_{\mu a}$ follows χ^2 distribution with ν_a degrees of freedom

▷ $$\boxed{W_{ab} = \left(1 + \frac{2}{\nu_a}\delta_{ab}\right) \int_0^\infty dt \prod_c \left(1 + \frac{2t}{\nu_c} \frac{\langle \Gamma_{\mu c} \rangle}{\langle \Gamma_\mu \rangle}\right)^{-(\frac{1}{2}\nu_c + \delta_{ac} + \delta_{bc})}}$$

for isolated resonances : $\nu_c = 1$ ... Porter Thomas distribution

Properties of W_{ab}:

$W_{aa} > 1$ ("elastic enhancement") $\xrightarrow{N\gg1} 3$ } where N is the # of open channels

$W_{ab} < 1$ for $a \neq b$ (in general); $\xrightarrow{N\gg1} 1$

▷ $$\boxed{\langle \sigma_{ab}^{fl} \rangle = \frac{\pi}{k_a^2} \frac{T_a T_b}{\sum_c T_c} W_{ab}}$$

$$\boxed{W_{ab} = \left(1+\frac{2}{\nu_a}\delta_{ab}\right) \int_0^\infty dt \prod_c \left(1+\frac{2t}{\nu_c}\frac{T_c}{\sum_{c'} T_{c'}}\right)^{-\left(\frac{\nu_c}{2}+\delta_{ac}+\delta_{bc}\right)}}$$

width fluctuation corrected Hauser Feshbach formula

▷ $\langle \sigma_{ab}^{fl} \rangle$ completely expressed in terms of $T_c = 1 - |\bar{S}_{cc}|^2$

▲ Overlapping resonances: $\frac{\langle \Gamma_\mu \rangle}{D} > 1$

[for neutrons incident on medium heavy nuclei: already at a few tens of keV]

$T_c \lesssim 1$ "strong absorption"

$\overline{|S_{ab}^{fl}|^2}$ cannot be described sufficiently simply to express it in terms of transmission coefficients

This is due to the fact that the condition $SS^\dagger = I$ causes complicated correlations between resonance parameters $\{E_\mu, g_{\mu c}, \Gamma_\mu\}$ for different μ ▷ exact calculation of average resonance interference term impossible

but "computer experiments" (Moldauer 1975) as evidence for validity of WF corrected HF formula also for overlapping resonances:

$$\boxed{\langle \sigma_{ab}^{fl} \rangle = \frac{\pi}{k_a^2} \frac{T_a T_b}{\sum_c T_c} \left(1+\frac{2}{\nu_a}\delta_{ab}\right) \int_0^\infty dt \prod_c \left(1+\frac{2t}{\nu_c}\frac{T_c}{\sum_{c'} T_{c'}}\right)^{-\left(\frac{\nu_c}{2}+\delta_{ac}+\delta_{bc}\right)}}$$ WF corrected HF formula

$T_c = 1 - |\bar{S}_{cc}|^2$ $\qquad \nu_c = 1 + \sqrt{T_c}$

Width factor $\xrightarrow{N\gg1} 2$ for $a = b$ ("elastic enhancement")

B) Direct reactions in non-elastic channels: $\overline{S_{ab}} \neq 0$ for $a \neq b$

Direct reactions between channels a and b lead to correlations between $\Gamma_{\mu a}, \Gamma_{\mu b}$ ▷ enhancement in channels which are coupled to the incident channel via direct reaction

$\overline{S_{ab}}$ from coupled channels optical model

transmission coefficients : $\frac{\pi}{k_a^2} T_a = \sum_b \langle \sigma_{ab}^{fl} \rangle = \frac{\pi}{k_a^2} \sum_b \overline{|S_{ab}^{fl}|^2} \underset{\text{unitarity}}{=} \frac{\pi}{k_a^2}\left(1 - \sum_b |\overline{S_{ab}}|^2\right)$

$$\triangleright \; T_a = 1 - \sum_b |\overline{S_{ab}}|^2$$

Generalization of transmission coefficients : transmission matrix P_{ab}

$$P_{ab} = \delta_{ab} - \sum_c \overline{S_{ac}}\, \overline{S_{bc}^*} = \sum_c \overline{S_{ac}^{fl}\, S_{bc}^{fl*}}$$

$$P_{aa} = T_a$$

In order to calculate $\langle \sigma_{ab}^{fl} \rangle$ in the case where $\overline{S_{ab}}$ is non-diagonal, diagonalize transmission matrix:

$$(UPU^\dagger)_{ab} = p_a \delta_{ab} \quad \text{Engelbrecht Weidenmüller Transf.}$$

unitary : $UU^\dagger = U^\dagger U = I$

Properties of transformed scattering matrix $S' = USU^T$:

i) $\overline{S'_{ab}} = \delta_{ab}\, \overline{S'_{aa}}$

ii) same statistical properties as scattering matrix of a problem with no direct reactions in non-elastic channels

▷ Procedure for calculating $\langle \sigma_{ab}^{fl} \rangle$:

1) determination of U by diagonalizing P

2) calculate XS^s from S'^{fl} :

$$\langle \sigma_{ab}^{fl} \rangle = \frac{\pi}{k_a^2} \sum_{cdef} U_{ca}^* U_{db}^* U_{ea} U_{fb}\, \overline{S'^{fl}_{cd}\, S'^{fl*}_{ef}}$$

3) Calculation of $\overline{S'^{H}_{cd} S'^{H*}_{ef}}$ by means of WF corrected HF formula

$$\langle \sigma^{H}_{ab} \rangle = \sum_c |U_{ca}|^2 |U_{cb}|^2 \langle \sigma'^{H}_{cc} \rangle + \sum_{d \neq c} \left[U^*_{ca} U^*_{db} (U_{ca} U_{db} + U_{da} U_{cb}) + \left(\frac{2}{\nu'_c} - 1\right)^{\frac{1}{2}} \left(\frac{2}{\nu'_d} - 1\right)^{\frac{1}{2}} U^*_{ca} U^*_{cb} U_{da} U_{db} \right] \langle \sigma'^{H}_{cd} \rangle$$

with $\langle \sigma'^{H}_{cd} \rangle = \frac{\pi}{k_c^2} \frac{T'_c T'_d}{\sum_e T'_e} \left(1 + \frac{2}{\nu'_c} \delta_{cd}\right) \int_0^\infty dt \prod_e \left(1 + \frac{2t}{\nu'_e} \frac{T'_e}{\sum_{e'} T'_{e'}}\right)^{-\left(\frac{\nu'_c}{2} + \delta_{ec} + \delta_{ed}\right)}$

$$T'_c = 1 - |\overline{S'_{cc}}|^2 \qquad \nu'_c = 1 + \sqrt{T'_c}$$

computer experiments (Moldauer 1975)

B. Subsidiary quantities

1) Particle transmission coefficients

$$T_\ell = 1 - |S_\ell|^2$$

if spin-orbit term : $T_{\ell j}$; $T_\ell = \sum_j \omega_{\ell j} T_{\ell j}$

weight, for $s = \frac{1}{2}$: $\frac{j+1}{2\ell+1}$

T_ℓ are needed for all incoming and outgoing channels in relevant energy range and for reasonable range of partial waves

also charged particles

— centrifugal barrier $\propto \ell(\ell+1)$

— weight in stat. model calcs. $\underbrace{(2\ell+1)\, T_\ell}_{\text{contr. to } \sigma_{abs}}$

2) <u>γ ray transmission coefficients</u>:

$$T_{\chi L}(\varepsilon_\gamma) = 2\pi\, \varepsilon_\gamma^{2L+1}\, \underbrace{f_{\gamma\chi L}(\varepsilon_\gamma)}_{\gamma \text{ ray strength function}}$$

type (M,E) multipolarity

— Weisskopf model : str. fcts. energy independent, values are calculated in a single particle picture

— Brink - Axel model : str. fcts. related to γ ray absorption XS

<u>for E1</u>:

$$f_{\gamma E1}(\varepsilon_\gamma) = \frac{1}{(\pi\hbar c)^2}\, g^J\, \frac{1}{\varepsilon_\gamma}\, \underbrace{\langle \sigma_{\gamma E1}^J(\varepsilon_\gamma)\rangle}_{\text{average photo-absorption XS}} \quad \text{"Brink hypothesis"}$$

statistical weight of comp. nucleus any. mom. J

for energy dependence of photo abs. XS Lorentz form is adopted:

$$\langle \sigma_{\gamma E1}^J(\varepsilon_\gamma)\rangle = \frac{1}{3}\, g_J\, \sigma_R\, \frac{(\Gamma_R \varepsilon_\gamma)^2}{(\varepsilon_\gamma^2 - E_R^2)^2 + \Gamma_R^2 \varepsilon_\gamma^2}$$

where E_R .... resonance energy

Γ_R .... — " — width

σ_R — peak cross section

for deformed nuclei : splitting of the E1 giant resonance
⇒ superposition of Lorentz curves

<u>other multipolarities</u>:

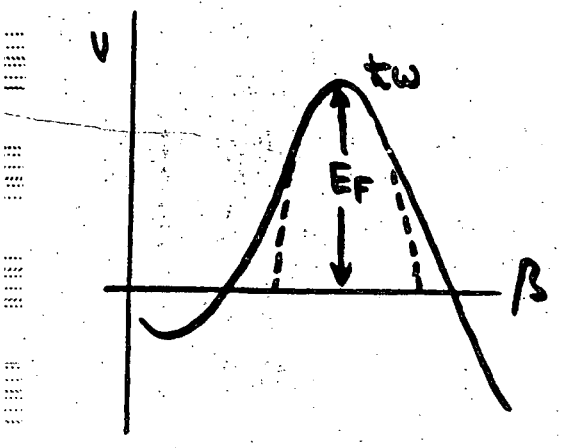
in principle same procedure, in practice information of giant resonances missing

normalization of $T_{\gamma L}$ such that exp. values of $\frac{\langle \Gamma_\gamma \rangle}{D}$ are reproduced

where $\langle \Gamma_\gamma \rangle$ ... average radiation width
D ... -"- resonance spacing } of s-wave neutron

if exp. data are lacking => use of systematics of str. fcts., normalization by fitting to exp. low energy neutron capture XS of neighbouring nuclei

3) Fission transmission coefficients



fission barrier, assumed to be one-dimensional
transmission coefficients for fission are related to transition states at saddle point deformation

a) single humped barrier

approximation : parabolic shape, height E_F, curvature $\hbar\omega$

$$P(E) = \left\{ 1 + \exp\left[\frac{2\pi}{\hbar\omega}(E_F - E) \right] \right\}^{-1} \quad \text{"penetrability"}$$

Hill Wheeler formula

fission transmission coefficient for CN states with (E, J, π) is the sum of contributions of all transition states with quantum numbers (J, π)

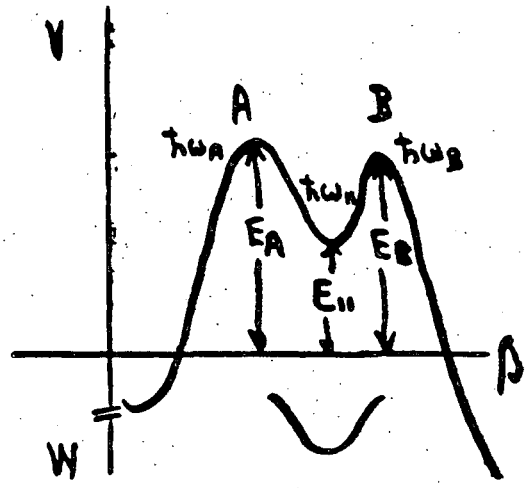
$$T_f(E, J, \pi) = \int_0^\infty dE' \, \rho_f(E', J, \pi) \left\{ 1 + \exp\left[\frac{2\pi}{\hbar\omega}(E' - E) \right] \right\}^{-1} \qquad (88)$$

where $\rho_f(E', J, \pi)$ ... density of transition states

barrier shape is assumed to be the same for all transition states

E' ... exc. energy referred to lowest transition state

b) double humped barrier



description by model of Back et al.
usually: three smoothly joined parabolae
"inner barrier" A: E_A, $\hbar\omega_A$
"outer barrier" B: E_B, $\hbar\omega_B$
"secondary minimum": E_{II}, $\hbar\omega_{II}$

definition of fission transmission coefficients has to allow for the following consequences of the secondary minimum in the potential energy surface:

i) damping in the 2nd well:
excitation of CN states by interaction of the fission motion with internal degrees of freedom: "damping" of the fission mode
accounted for by adding to real deformation potential a negative imaginary part of parabolic shape, located at position of 2nd well (see below)
solution of Schrödinger equ. ⇒ • directly transmitted flux $P_f^{AB}(E)$
= penetrability through combined barrier
• absorbed flux $\mathcal{A}^{AB}(E)$

P_f^{AB} describes 'direct' fission contr., $\mathcal{A}^{AB}$ provides 'indirect' fission
both show vibrational resonances at the positions of quasistatic levels in the 2nd minimum
relative magnitude of direct and indirect fission depends on strength of the absorptive potential: partial ↔ complete damping
no direct fission contr.

ii) intermediate class II structure:
coupling of CN states in 1st and 2nd well enhances indirect fission contribution near a state in 2nd well ("class II state")

in the limit of complete damping and smeared out class II structure (realized at higher incident energies):

$$T_f(E,J,\Pi) = \frac{T_f^A(E,J,\Pi)\, T_f^B(E,J,\Pi)}{T_f^A(E,J,\Pi) + T_f^B(E,J,\Pi)}$$

in this limit barriers act independently;
T_f^A, T_f^B calculated according to (88) (p.47)

4) <u>Level density</u>

= number of excited levels per unit energy

Δ phenomenological models for spherical nuclei:

<u>Fermi gas model</u>

independent particles, no residual interactions, equidistant spacing of the single particle states near the Fermi surface, saddle point approximation (concerns integration for Laplace transformation of grand canonical partition function)

— conventional shifted Fermi gas model (Gilbert & Cameron): consideration of odd-even effects by means of a pairing energy shift Δ_{pair}; i.e.: exc. energy is measured from a fictive ground state which is assumed to coincide with the actual ground state for odd nuclei and to be shifted upwards by the conventional pairing energies for odd mass and even nuclei

=> fictive ground state is determined by experimental mass differences, 1 free parameter ("a")

conv. shifted Fermi gas formula provides reasonable description of level density only for a rather small range of a few MeV around the excitation energy where a-parameter is adjusted, e.g. at neutron binding energy => underestimation below, overestimation above

— composed four-parameter formula (Gilbert & Cameron):
conv. shifted Fermi gas formula at higher exc. energies only
at low exc. energies constant temperature formula $C\exp(\frac{U}{T})$
both parts smoothly joined

— back shifted Fermi gas model:
ground state position as adjustable parameter $\Delta = \Delta_{pair} - \Delta_{BS}$
spin dependent level density:

$$\rho(U,J) = \frac{1}{24\sqrt{2}} \frac{2J+1}{\sigma^3 a^{1/4}} \frac{\exp[2(a(U-\Delta))^{\frac{1}{2}} - J(J+1)/2\sigma^2]}{(U-\Delta+t)^{5/2}}$$

where a ... "a-parameter"
t ... thermodynamic temperature : $U-\Delta = at^2 - t$
σ^2 ... spin cutoff parameter, describes spin distribution

$$\sigma^2 = \frac{I_{eff} \cdot t}{\hbar^2} = \eta \frac{I_{rigid} \cdot t}{\hbar^2} \quad \text{with} \quad \eta = \frac{I_{eff}}{I_{rigid}}$$

fitting procedure:

$$N_0 = \int_0^{U_0} \rho(U)\, dU = F(a, \Delta, A, U_0)$$

number of levels up to U_0, summed over all spins

$$\frac{2}{D_{l=0}} = \left\{ \begin{matrix} \rho(S_n + \frac{1}{2}\Delta E, I_t + \frac{1}{2}) + \rho(S_n + \frac{1}{2}\Delta E, I_t - \frac{1}{2}) \\ \rho(S_n + \frac{1}{2}\Delta E, 1/2) \end{matrix} \right\} = G(a, \Delta, A, S_n + \tfrac{1}{2}\Delta E, I_t) \text{ for } \begin{cases} I_t \neq 0 \\ I_t = 0 \end{cases}$$

$D_{l=0}$ ... spacing of $l=0$ resonances of $\underbrace{\text{one parity}}_{\text{for both parities : factor 2}}$, averaged over $[S_n, S_n + \Delta E]$

$F(\ldots)$ and $G(\ldots)$ each represent a curve in the (a, Δ) plane;
only (a, Δ) corresponding to their crossing point reproduce
N_0 and $D_{l=0}$ simultaneously

Δ... large negative for odd nuclei
slightly -"- for odd mass nuclei
moderately positive for even nuclei

$\Delta_{BS} = \Delta_{pair} - \Delta$
a-parameters } show shell effects

— BCS model for microscopic calc. of level density

in order to account for effect of shell structure and pairing on the energy dependence of the level density

not for "routine calculations" of XS's

— semi-empirical level density formulae : Kataria & Ramamurthy
Jensen
Ignatyuk

parametrization of shell effects in terms of shell correction to nucleus ground state mass
also account for pairing
- This type of parametrization is extremely useful for applications

Δ for deformed nuclei : enhancement of level density by rotational degree of freedom

Δ density of transition states in the continuum is calculated in the same way as level densities at equilibrium deformation ; excitation energy refers to the lowest transition state

2) Preequilibrium model (exciton)

starting from simple configuration the composite system is assumed to equilibrate through a series of two-body collisions and to emit particles from all intermediate states

exciton number : $n = p + h$

particles holes (no distinction between protons & neutrons)

state density $\omega(p,h,E) = \dfrac{g(gE - A_{p,h})^{p+h-1}}{p!\ h!\ (p+h-1)!}$

$$A_{p,h} = \frac{p^2 + h^2 + p - 3h}{4}$$

Pauli principle correction

g ... single particle state density

residual interactions : assumed to be energy conserving and two-body in nature => transitions $\Delta p = \Delta h = 0, \pm 1$

rates for these transitions :

$$\lambda_+(p,h,E) = \frac{2\pi}{\hbar} M^2\, \omega(p+1, h+1, E)$$

$$\lambda_0(p,h,E) = \frac{2\pi}{\hbar} M^2\, \omega(p,h,E)$$

$$\lambda_-(p,h,E) = \frac{2\pi}{\hbar} M^2\, \omega(p-1, h-1, E)$$

where M ... average matrix element:

$$M^2 = k\, A^{-3} E^{-1} \quad (\mathrm{MeV}^2)$$

or, more accurately :

$$\left.\begin{array}{ll}
M^2(n,E) = \dfrac{k'}{A^3 e}\left(\dfrac{e}{7\,\mathrm{MeV}}\right)^{\frac{1}{2}}\left(\dfrac{e}{2\,\mathrm{MeV}}\right)^{\frac{1}{2}} & e < 2\,\mathrm{MeV} \\
M^2(n,E) = \dfrac{k'}{A^3 e}\left(\dfrac{e}{7\,\mathrm{MeV}}\right)^{\frac{1}{2}} & 2 \le e < 7\,\mathrm{MeV} \\
M^2(n,E) = \dfrac{k'}{A^3 e} & 7 \le e \le 15\,\mathrm{MeV} \\
M^2(n,E) = \dfrac{k'}{A^3 e}\left(\dfrac{15\,\mathrm{MeV}}{e}\right)^{\frac{1}{2}} & 15\,\mathrm{MeV} < e
\end{array}\right\} e = \frac{E}{n}$$

Average rate of emission of particle of type ν with energy ε_ν:

$$\lambda_\nu^e(h,\varepsilon_\nu)\,d\varepsilon_\nu \equiv \lambda_\nu^e(p,h,E,\varepsilon_\nu)\,d\varepsilon_\nu =$$

$$= \frac{2s_\nu+1}{\pi^2\hbar^3}\,\mu_\nu\,\varepsilon_\nu\,\sigma_\nu(\varepsilon_\nu)\,R_\nu(p)\,\frac{\omega(p-p_\nu,h,E-B_\nu-\varepsilon_\nu)}{\omega(p,h,E)}\,d\varepsilon_\nu$$

from "detailed balance" (quasi equilibrium) $\Rightarrow$ justification ??

p_ν ... nucleon #
s_ν ... spin
μ_ν ... reduced mass
B_ν ... binding energy
} of particle ν

$\sigma_\nu(\varepsilon_\nu)$ ... inverse reaction XS (replaced by OM abs. XS)

$R_\nu(p)$ ... factor which takes account of distinguishability of partons from neutrons:

If p_ν nucleons are imagined to be chosen at random from among the p excited particles available, $R_\nu(p)$ is intended to give the probability that they have the right combination of protons and neutrons to make a particle of type ν:

$$R_\nu(p) = \left(\frac{Z}{A}\right)^{z_\nu}\left(1-\frac{Z}{A}\right)^{p_\nu-z_\nu}\binom{p_\nu}{z_\nu}$$

Z ... charge # of composite system
z_ν ... parton # of particle ν

<u>Nucleon induced reactions:</u>

a) nucleon emission: $R_\nu(p) = \frac{n\pm1}{n}$

$+$ ... if projectile & ejectile of same type
$-$ ... ——— " ——— diff. —"—

b) α particle emission: $R_\nu(p) = \frac{\varphi K_{n-1}^\alpha}{\varphi K_n^\alpha + (1-\varphi)K_n^\nu}$

φ ... α cluster preformation probability
$K_{n-1}^\alpha, K_n^\alpha, K_n^\nu$ ... tabulated constants
$p_\nu = 1 \leftarrow$ α cluster considered as 1 excition!

A) Master equation approach

$P(p,h,t)$ ... occupation probability = probability that the system will be found in a state with p particles and h holes at time t

differential equation describing the approach of the nucleus towards statistical equilibrium : master equation:

$$\frac{dP(p,h,t)}{dt} = P(p-1,h-1,t)\lambda_+(p-1,h-1,E) + P(p+1,h+1,t)\lambda_-(p+1,h+1,E) - $$
$$- P(p,h,t)\left[\lambda_+(p,h,E) + \lambda_-(p,h,E) + \sum_\nu \int_0^{\varepsilon_{\nu max}} d\varepsilon\, \lambda_\nu^e(p,h,E,\varepsilon)\right]$$

one such equation for each allowed class of p-h-configurations

at time $t=0$: initial particle and hole number : $\underbrace{P(p,h,0) = \delta_{pp_0}\delta_{hh_0}}_{\text{initial cond. for numer. integration}}$

spectra emitted up to equilibration time T:

$$\underbrace{\frac{d}{d\varepsilon_\nu}\sigma_\nu(\varepsilon_\nu,T)\,d\varepsilon_\nu = \sigma_{abs}\cdot\sum_p \lambda_\nu(p,h,\varepsilon_\nu)\,d\varepsilon_\nu \int_0^T P(p,h,t)\,dt}$$

PE component of the energy spectrum of particles of type ν

σ_{abs} ... comp. nucleus formation XS

T ... time when all states in the system are equally populated

B) Random walk approach

occupation probabilities are not considered as functions of time but as functions of the # of internal transitions that have already taken place

$b^{(k)}(n) \equiv b^{(k)}(p,h)$ ... population probability of the states of a p-h-configuration resulting from k internal transitions

$$b^{(k+1)}(n) = b^{(k)}(n+2)\frac{\lambda_-(n+2)}{\lambda(n+2)} + b^{(k)}(n)\frac{\lambda_0(n)}{\lambda(n)} + b^{(k)}(n-2)\frac{\lambda_+(n-2)}{\lambda(n-2)}$$

with $\lambda(n) = \lambda_-(n) + \lambda_0(n) + \lambda_+(n) + \lambda^e(n)$ where $\lambda^e(n) = \sum_\nu \int_0^{\varepsilon_{\nu max}} d\varepsilon_\nu\, \lambda_\nu^e(n,\varepsilon_\nu)$

initial population probability : $b^{(0)}(n) = \delta_{nn_0}$ i.e.: $b^{(0)}(p,h) = \delta_{pp_0}\delta_{hh_0}$

successive application of the above equation describes equilibration process.

With increasing k the ratio $\frac{b^{(k-1)}(n)}{b^{(k)}(n)}$ becomes independent of n and k

$\Rightarrow$ upper limit K for the number of internal transitions to be considered for PE decay ($\hat{=}$ equilibration time T) from following condition:

$$\left| \frac{b^{(k-1)}(n)}{b^{(k)}(n)} - Q^{(k)} \right| < .01 * Q^{(k)} \quad \text{for all } n \text{ and } k \geq K$$

$$\text{where} \quad Q^{(k)} = \frac{\sum_n b^{(k-1)}(n)}{\sum_n b^{(k)}(n)}$$

PE spectrum (part. type ν):

$$\frac{d\sigma_\nu^{pe}}{d\varepsilon_\nu} d\varepsilon_\nu = \sigma_{abs} \sum_{k=0}^{K} \sum_n b^{(k)}(n) \frac{\lambda_\nu^e(n,\varepsilon_\nu)}{\lambda(n)} d\varepsilon_\nu$$

Fraction q^{pe} of the initial population which survives PE:

$$q^{pe} = 1 - \sum_{k=0}^{K} \sum_n b^{(k)}(n) \frac{\lambda^e(n)}{\lambda(n)}$$

Closed form expressions for PE emission spectra result from "random walk equations" by neglecting the rates $\lambda_-(n)$ and $\lambda_0(n)$:

$$\frac{d\sigma_\nu^{pe}}{d\varepsilon_\nu} d\varepsilon_\nu = \sigma_{abs} \sum_{n=n_0}^{\bar{n}} D_n \frac{\lambda_\nu^e(n,\varepsilon,\varepsilon_\nu)}{\lambda_+(n) + \lambda^e(n)}$$

$$\underbrace{\bar{n} = \sqrt{2gE}}_{\text{most probable exc. \#}}$$

$$\underbrace{D_n = \prod_{n'=n_0+2}^{n} \frac{\lambda_+(n')}{\lambda_+(n') + \lambda^e(n')}, \quad D_{n_0} = 1}_{\text{"depletion factors"}}$$

V) SURVEY OF NUCLEAR MODEL COMPUTER CODES

1) Optical model (and equilibrium compound nucleus model)

Code Ref.	Features regarding optical model	Features regarding equilibrium CN model
CERBERO F. Fabbri et al., Rept. RT/FI(74) 36 (1974) Rept. RT/FI(77) 6 (1977)	spherical opt. pot., local, non-local and local equivalent of non-local pot.	binary reactions, emission of n, p, d, γ. WFC for continuum channels. Improvement of Gilbert-Cameron level density at low exc. en.
COMNUC/CASCADE C. Dunford, Rept. AI-AEC-12931 (1970)	spherical opt. pot.	XS's for (n,γ), (n,n'), (n,γn), (n,2n), (n,f), (n,n'f). Gamma-ray cascades. Single humped fission barrier.
CRAPONE F. Fabbri et al., Rept. RT-FI(77)3 (1977)	spherical opt. pot., local, non-local and local equivalent of non-local pot. Automatic search on total, differential elastic and abs. XS, s- and p-wave str. fcts. and scattering radius	
DWUCK-4 P.D. Kunz, unpubl.	DWBA method. Transfer reactions and inelastic scatt., optionally deformed opt. pot. for inelastic scatt.	
ELIESE-3 J. Igarasi, Rept. JAERI 1224 (1972)	spherical opt. pot., local and non-local pot. Automatic search on diff. el. XS's and polarizations (spin ½ and 1).	binary reactions. All types of XS's involving absorption and emission of n, p, d, α.
ERINNI F. Fabbri et al., Rept. RT/FI(77)4 (1977)	spherical opt. pot., local, non-local and local equivalent of non-local pot.	binary and ternary reactions: (x,a), (x,ab), (x,abc) where x can be n, p or α a and b can be n, p, α or γ, c can be n or γ

IUPITOR-1 T. Tamura, Rept. ORNL-4152 (1962)	deformed opt. pot., coupled channels calc. Variety of different coupling schemes for vibr. and rot. nuclei is provided for.	
PELINSCA C.A. Engelbrecht et al., Rept. PEL-202 (1974)	spherical opt. pot. Automatic search on total, diff. elastic and reaction XS's and polarizations (spin ½).	reactions of type (a,b) and (a,bγ) differential and integrated XS's for up to 33 levels of each residual nucleus. Decay γ angular correlations.
GENDA F. Perey, unpubl.	spherical opt. pot. Automatic search on total, diff. elastic and abs. XS's for different nuclei simultaneously.	
ECIS J. Raynal IAEA-SMR-9/8 (1972)	deformed opt. pot. Coupled channels calcs.	
SCAT 2 O. Bersillon Rept. CEA-N-227	spherical opt. pot., local pot. and local equivalent of non-local pot.	
ABAREX (new version of ABACUS) T.A. Moldauer, unpubl.	spherical opt. pot. (local)	elastic & inelastic scat., capture, fission. WFC

2) Preequilibrium and equilibrium CN model codes

Code Ref.	Features of the models	Decay modes	Calcd. quantities
ALICE - 80 M. Blann, Rept. COO-3494-29 (1975), Rept. UR-NSRL-181 (1981)	(geometry dependent) hybrid model, multi-step Weisskopf-Ewing with approx. treatment of ang. mom. Single humped fission barrier.	n, p, d, α, f Residual nuclei may be out of a grid, 11 mass units wide and 9 charge numbers deep.	Particle spectra, activation & production XSs, fission XS.
AMALTHEE O. Bersillon et al., Rept. NEANDC(E) 191 "L" (1977)	Exciton model, time integrated master equ. gives PE and equil. contribution. Approx. treatment of 2nd chance PE. No ang. mom. effects.	n, p, d, t, ^{3}He, α, γ Binary and ternary reactions. Inverse XSs as input.	Particle spectra
GNASH P.G. Young et al., Rept. LA-6947 (1977)	exciton model plus semi-empirical direct reaction contribution. Multi-step Hauser-Feshbach, no WFC, γ ray cascades, single humped fission barrier. Accepts dir. reaction input	n, p, d, t, ^{3}He, α, γ, f Several reaction paths in 1 run, involving up to 10 decaying nuclei.	Particle spectra, γ ray spectra, activation & production XSs, isomeric state XS fission XS.
HAUSER - 5 F.M. Mann, Rept. HEDL-TME 78-83 (1978)	exciton model plus semi empirical direct reaction contribution. Multi-step Hauser-Feshbach. Double humped fission barrier, compl. damping. Accepts dir. reaction input.	6 reaction pairs (including γ and f). Binary and ternary reactions.	Particle spectra, double diff. XSs for particles, activation XSs, fission XS.

PREANG J.M. Akkermans et al., Rept. ECN 60 (1979)	Exciton model, generalized for any. distrs. (Mantzouranis), time integrated master eqns. give PE and equil. contr. No ang. mom. effects.	n, p, d, t, ^{3}He, α Binary reactions only. Inverse XS^s are input.	Particle spectra, double diff. XS^s for particles.
PRECO-D C. Kalbach, unpubl.	Exciton model plus semi-empirical direct reaction, MSC and MSD contr. Weisskopf-Ewing. Single humped fission barrier. Phenomen. ang. distr. No ang. mom. effects.	n, p, α, f + 1 arbitrary particle. Binary reactions only. Inverse XS^s are input.	Particle spectra, double diff. XS^s for particles, fission XS.
STAPRE M. Uhl et al., Rept. IRK 76/01 + addenda	Exciton model for 1st chance particle, multi step Hauser Feshbach, γ ray cascades. Double humped fission barrier, partial or compl. damping.	n, p, d, α, γ, f Up to 6 emitted part., but one reaction path only. Transm. coeffs. are input.	Particle spectra, γ-ray spectra, activation XS^s, isomeric state XS^s, fission XS.
TNG1 C.Y. Fu, Rept. ORNL/TM-7042	Exciton model for 1st chance particle, considers ang. mom. Multi-step Hauser Feshbach, γ ray cascades. Accepts dir. reaction input.	n, p, α, γ Up to 3 emitted particles	Particle spectra, γ ray spectra, double diff. XS^s for particles. Act. XS^s isomeric state XS^s
PENELOPE G. Reffo et al., Rept. NEANDC(E) 222	Exciton model for 1st chance particle, considers ang. mom. and pairing in p-h-state densities. Multi step Hauser Feshbach.		

VI) ABACUS

1) Program operation

a) Possible problems

CLASS 1

calculates scattering by an optical potential

potential well is generated and the Schrödinger equation solved by partial waves.

Results:
- absorption coefficients $\eta_{lj} = e^{2i\delta_{lj}}$ (δ_{lj} ... phase shift)
- transmission —"— $T_{lj} = 1 - |\eta_{lj}|^2$
- partial reaction XS^s σ_{lj}

* for each l, j up to an l_{max} (← given as input or determined by an internal criterion)

- reaction cross section σ_{reac}
- total —"— σ_{total}
- shape elastic —"— σ_{shape}

} for neutral incident particles

- angular distributions $\frac{d\sigma}{d\omega}$
- polarization $P(\theta)$

} if desired; results in C.M. and lab. system

- for charged particles $\frac{d\sigma}{d\omega}_{Rutherford}$

Incident particle may have spin 0 or $\frac{1}{2}$

Procedure:

— internal solution by numerical integration of radial Schrödinger equation

— external —"— (beyond well cutoff) constructed from Bessel functions (neutral incident particle) or Coulomb functions (charged inc. part.)

— determination of 1 integration constant from $\lim_{r \to 0} u(r) \to 0$

— —"— of scattering matrix (absorption coefficient) from matching of logarithmic derivative at well cutoff

CLASS 2

computes a bound state radial wave function for a specific ℓ and j

same problem as Class 1 except — only real parts of pot. considered
— energy is such that particle is bound

Results: radial wave function
internal and external logarithmic derivative
number of nodes inside well
energy eigenstate of particular ℓ and j, if desired (by means of search)

Proceeding:

either: — numerical integration of radial Schrödinger equation to well cutoff or even further, if desired
— search for energy eigenstates

or: — construction of — " — (exponentially decreasing) from modified Hankel functions beyond well cutoff
— inward integration (numerical)

CLASS 3

Solution of Class 1 problem to obtain transmission coefficients plus Hauser Feshbach calculation of compound elastic and inelastic scattering cross sections

Results:
- partial inelastic scattering XS's for each excited level (compound) } without WFC
- compound elastic XS
- total elastic XS
- $\frac{d\sigma_{el}}{d\omega}$ shape, compound
- $\frac{d\sigma_{inel}}{d\omega}$ compound

Proceeding:

solution of scattering by opt. pot. as Class 1

then Hauser Feshbach calculation :

$$\langle \sigma_{ab} \rangle = \frac{\pi}{k_a^2} \sum_J g_a^J \frac{\sum_{lj} T_a^{lj} \sum_{l'j'} T_b^{l'j'}}{\sum_{c''l''j''} T_c^{l''j''}}$$

$\vec{l}, \vec{s}, \vec{I}_{tar} \rightarrow \vec{J}$

j coupling scheme : 1. $\vec{j} = \vec{l} + \vec{s}$
2. $\vec{J} = \vec{j} + \vec{I}_{tar}$ } (in ABACUS)

whereas in the channel spin coupling scheme : 1. $\vec{I}_{ch} = \vec{s} + \vec{I}_{tar}$
2. $\vec{J} = \vec{I}_{ch} + \vec{l}$

(in STAPRE)

CLASS 4

calculation of radial integrals

Results :

$$\int_0^\infty \mathcal{O}_1 u_{(1)} \mathcal{O}_2 u_{(2)} \dots \mathcal{O}_n u_{(n)} r^m r^{-n+2} dr$$

where $u_{(i)}$ ... partial radial wave functions of specified l, j and energy

$\mathcal{O}_i$ ... operators, that may be
- unity
- pot. well components $V_{re}, V_{im}, V_{so}, V_{coul}$
- diff. operators $\frac{d}{dr}$ or $\frac{d}{dr} \cdot \frac{1}{r}$

m ... input parameter

Proceeding:

- calculation of radial wave fct. in (separate) Class 1 and 2 runs
- calculation of radial integrals by numerical integration

b) Available well forms

Real:

for nuclear part:
- Saxon Woods
- modified Saxon Woods (squared off toward the interior square well)
- special form, given by special subroutine or point by point

for Coulomb part:
- Ch pot. resulting from uniform charge distribution inside the well, $\frac{1}{R}$ outside the well
- special form, given by special subroutine or point by point

Imaginary:
- same form as real nuclear potential
- Saxon Woods (with parameters different from real potential)
- surface Gaussian
- derivative of the real well form
- derivative of Saxon-Woods (with parameters different from real pt)
- linear combination of volume form (as real potential) and surface form
- special form given by special subroutine or point by point

Spin-orbit: real and/or imaginary
- Thomas form
- special form given by special subroutine or point by point

c) Comparison with experimental data

- Calc. for one set of parameters
- Parameter scan : variation of up to 5 parameters in one run
- Search : exp. data given as input, procedure seeking minimum χ^2 by a modified method of steepest descent (calculations at several values of one input parameter)

d) Modified versions (Vienna)

"ABACUSTL"

averaging over transmission coefficients with same l but different j

for $s=\frac{1}{2}$: $T_l(\varepsilon) = \frac{1}{2l+1}\left[l\, T_{l,j=l-\frac{1}{2}}(\varepsilon) + (l+1)\, T_{l,j=l+\frac{1}{2}}(\varepsilon)\right]$

[necessary if transmission coeffs. are used as input for STAPRE, because it uses channel spin coupling scheme]

"ABACUST"

use of Tepel formula to account for fluctuation of level widths

$\frac{1}{N(U,J,\Pi)} T_{j_0 l_0}(\varepsilon_0) T_{j_i' l_i'}(\varepsilon_i)$ in Hauser-Feshbach formula

with $N(U,J,\Pi) = \sum_{i,j_i'' l_i''} T_{j_i'' l_i''}$ is replaced by

$$\frac{1}{N_t(U,J,\Pi)} V_{j_0 l_0}(\varepsilon_0) V_{j_i' l_i'}(\varepsilon_i) \left\{ 1 + \delta_{i0}\delta_{jj_0}\delta_{l_i l_0}(W_{l_0 j_0} - 1)\right\} \qquad (1)$$

V_{jl} ... modified transmission coefficient

W_{lj} ... elastic enhancement

$$\langle \sigma_{ab}^{fl} \rangle = \xi_a \xi_b \quad \text{for } a \neq b \qquad (2)$$

$$T_a \underset{\substack{\uparrow \\ \text{neglecting } \frac{1}{k_a^2}}}{=} \sum_b \langle \sigma_{ab}^{fl} \rangle = \sum_{b \neq a} \xi_a \xi_b + \langle \sigma_{aa}^{fl} \rangle \qquad (3)$$

Elastic enhancement $\langle \sigma_{aa}^{fl} \rangle = \xi_a^2 W_a \qquad (4)$

Ansatz $\xi_a = V_a X^{-\frac{1}{2}}$ where $X = \sum_c V_c$

Using this ansatz in eq. (3): $T_a = \sum_b \langle \sigma_{ab}^k \rangle = \xi_a^2 W_a + \xi_a \sum_{b \neq a} \xi_b$

$$T_a = \frac{V_a^2}{X} W_a + \frac{V_a}{X^{\frac{1}{2}}} \sum_{b \neq a} \frac{V_b}{X^{\frac{1}{2}}}$$

$$= \frac{V_a^2}{X} W_a + \frac{V_a}{X^{\frac{1}{2}}} \Big(\underbrace{\sum_b \frac{V_b}{X^{1/2}}}_{X} - \frac{V_a}{X^{1/2}} \Big)$$

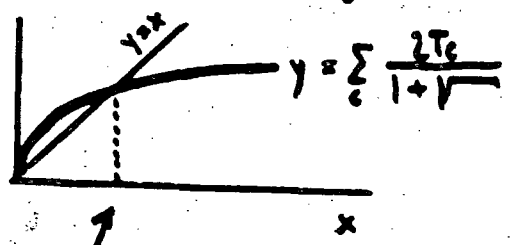
$$= \frac{V_a^2}{X} W_a + \frac{V_a}{X} (X - V_a)$$

$$\underbrace{\frac{V_a^2}{X}(W_a - 1) + V_a = T_a}$$

quadratic equation for V_a, can be solved for known T_a and W_a

$$V_a = \frac{2T_a}{1 + \sqrt{1 + \frac{W_a - 1}{X} T_a}}$$

Determination of X: since $X = \sum_c V_c \implies X = \sum_c \frac{2T_c}{1 + \sqrt{1 + (W_a - 1) X^{-1} T_a}}$



find solution numerically

Elastic enhancement factor must be given.

Empirical relation for it:

$$W_a = 1 + \frac{2}{1 + \sqrt{T_a}} \rightarrow \begin{cases} 3 & T_a \ll 1 \text{ weak absorption} \\ 2 & T_a \to 1 \text{ strong } - \text{"} - \end{cases}$$

<u>Approximation</u> (used in ABACUST):

$$\frac{V_a}{\sum_c V_c} \approx \frac{T_a}{\sum_c T_c}$$ need not calculate X

$$\Rightarrow V_a = \frac{T_a}{1 + \frac{T_a}{\sum_c T_c}(W_a - 1)}$$

above relation $W_a = 1 + \frac{2}{1+\sqrt{T_a}}$ results also from this approximation

This approximation does not conserve the normalization exactly.

e) list of routines

Main ABACUS

Sr. AUTO automatic sequencing (searches and scan)

Sr. CALC for cont. state calcs. and control of bound state calcs.

Sr. EDIT edit of radial wave fct.

Sr. ETA phase shifts and radial wave fct. normalization

Sr. BESL spherical Bessel fcts.

Sr. COUL Coulomb wave functions

Sr. COULA — " — special subroutine

Sr. PSUBL Legendre polynomials and derivatives

Sr. FWDINT integration of Schrödinger equation in well

Sr. WELLS generation of potential wells

Sr. WREAD

Sr. WELR
Sr. WELI
Sr. WELS
Sr. WELC
} dummy to be replaced by special sr.s generating { real, imag., spin-orbit, Coulomb } well

Sr. BOUND calc. of bound state radial wave function

Sr. HNKL (modified) Hankel functions

Sr. HFESH Hauser Feshbach compound elastic and inelastic with avg. distr.

Sr. FWXINT integration beyond well cutoff

Sr. BKWINT — " — (inward) beyond well cutoff

Sr. NUIN1 integrand development (for integration)

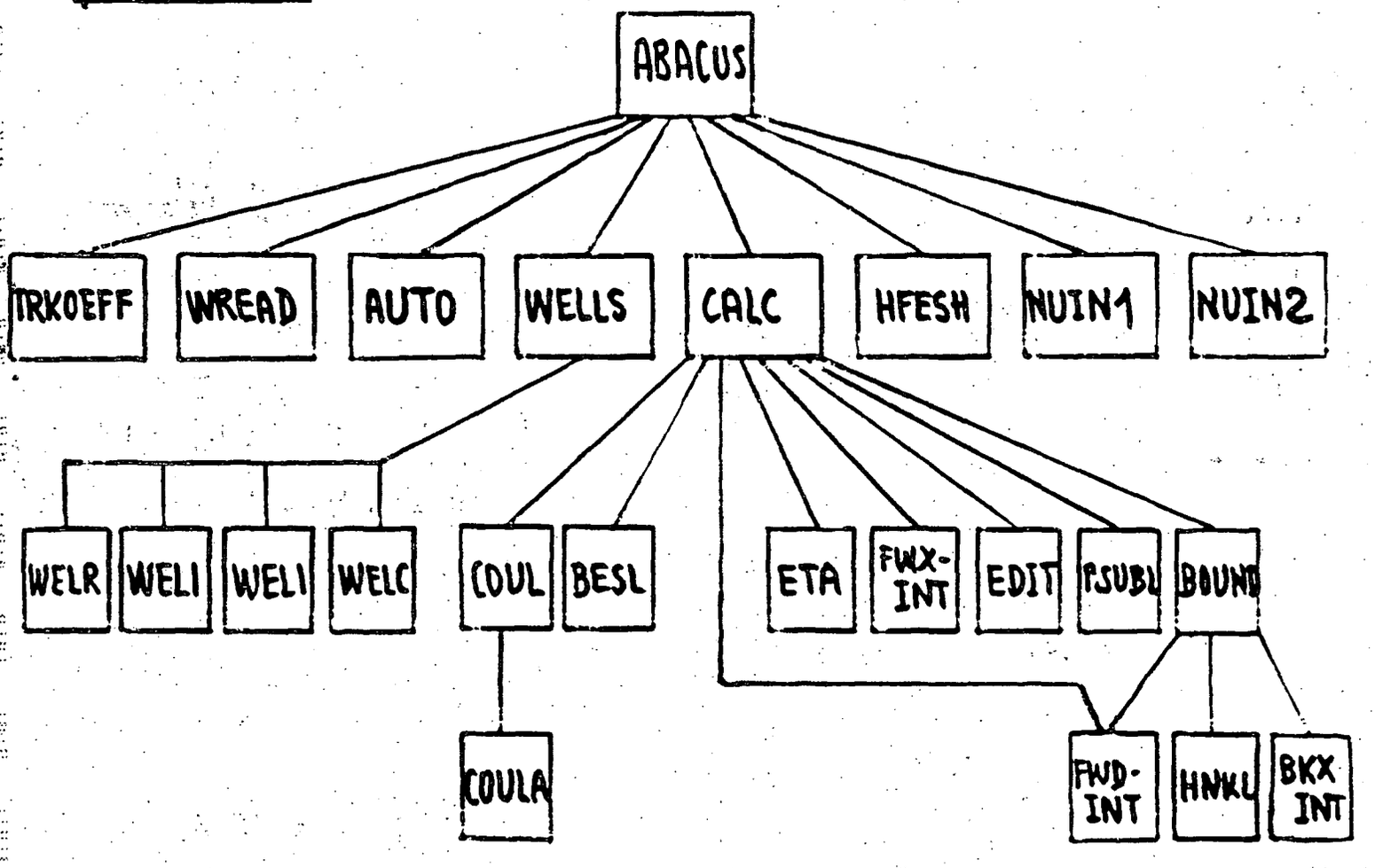
Sr. NUIN2 numerical integration

Fct. CLEB Clebsch-Gordan coefficients

Fct. RACAH Racah coeffs.

[Sr. TRKOEFF averaging of transmission coefficients] Hauser

f) Flow chart



2) Input

Control # 1 .. start of new problem

2 ... Call Trkoeff if Abacustl, Class 1, KT2 ≥ 1, else EXIT

Title

KLASS Class of problem to be calculated

KT1 (Class 3, 4)

Control # for whether or not the well parameters are retained unchanged for all levels (Class 3) or for all radial wave fcts. (Class 4)

KT2 (Class 3, Class 1 if Abacus II)
Control # for print/punch of T_ℓ

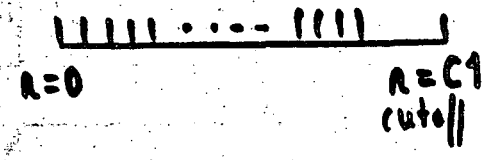
NOE (Class 3) : # of energy levels including ground state, ≤ 25

NOW (Class 4) : # of wave functions in integrand, ≤ 6

MM (Class 4) : power of r appearing in integrand of radial integral

KRE
KIM
KSO
KCL
} (all classes) control # for forms of various parts of pot. well

KPTS1 (all classes) : # of mesh points at which there is a potential acting (other than $\frac{1}{r}$ Cb pot.); determines integration interval



KPTS1-1 intervals

≤ 500

KPTS2 (optional, Class 1, 2, 3) : # of mesh points at which a wave function will be calculated. For Class 1 and 3 KPTS 2 > KPTS1 unnecessary
(optional, Class 4) : # of mesh points over which integration is to be performed

Control # for angles at which ang. distr. will be calcd.

KP1 (Class 1, 3) : Output printing control (XS's, ang. distr's, pot's)

KP2 (Class 1, 2, 4) : —— " —— (wave fcts.)

KP3 (operative only with search or scan)
control # concerning input of exp. data and χ^2 calc

KP4 (operative only with search or scan)
control # for suppressing print in dependence on χ^2 value

KAUTO (all classes) : search and scan control
(operative only with search or scan)

KK1 dimension of parameter space searched or scanned

NOV (operative only with search or scan)
# of values of specified parameter at which calcs. are made to compute a single χ^2

NOA (Class 1, 3)
number of angles calcd. (equally spaced with respect to angle ~ cosine) or given as input
Ignored if exp. data are supplied; then define angle ≤ 150

KP5 (Operative only if KP2 $\neq 0$): wave fct. print control

KP6 (all classes): well and well parameters print control

KP7 Control number for special search ("SCHIFFER")

AIN (optional): mass of incident particle

RC (– " –): radius of charge distribution

KP8 depending on value of KP7: punch control for any. distr. or control for calc. of scaling factors for special search

ZZP charge product

ANO mass of target nucleus

VRE, VIM, VIVOL, VSR, VSI } well depths (MeV); imag. ignored for Class 2

KTRLW input control for additional well parameters

VRE1, VRE2, VIM1, VIM2 } real & imag. well depth energy dependence

VX1, VX2, VX3 } additional parameters for special well subroutines (KRE, KIM, KSO, KCL = 8)

C1 well cutoff (fm)
required for KRE = ϕ, 1, 8, 9; for KRE = 2 - 7 C1 is set internally

R1
A1
R2
A2 } real and imag. pot. geometrical parameters

C2 volume fraction of imag. pot.; $0 \leq C2 \leq 1$

How to input combined volume & surface imag. potential:

1. $\underbrace{VIM}_{\text{total imag. pot. depth}} \neq 0$, $C2 \neq \phi$

   vol. part = C2 * total imag. pot. (obtained from VIM considering energy dependence)

   surf. part = tot. imag. pot − vol. part

2. $\underbrace{VIM}_{\to \text{surf.}} \neq 0$, $\underbrace{VIVOL}_{\to \text{vol.}} \neq 0$, $C2 = \phi$ (ignored if $\neq \phi$)

   VIS = preliminary surf. term (obtained from VIM considering en. dep.)

   VIV = — " — vol. term (— " — VIVOL — " —)

   $C2 = \dfrac{VIV}{VIV + VIS}$

   surface = prel. surface * (1 - C2) } program internal renormalization
   volume = prel. volume * C2

   ⇒ in order to use values VIM_{actual}, $VIVOL_{actual}$, one has to multiply them and the parameters for the energy dependence by $\dfrac{(VIVOL + VIM)_{actual}}{VIM_{actual}}$ in order to obtain these values after the internal renormalization

C0 wave function cutoff (fm)
necessary only if KPTS2 ≠ KPTS1

For class 4, CO is the upper limit of integration

$CO < C1$: $\frac{CO}{KPTS2-1} = \frac{C1}{KPTS1-1}$ [±1] same mesh interval

$CO > C1$: ——— // ——— not necessary ⇒ mesh interval beyond C1 may be different from that between $r = 0$ and C1

KTRLR Input control for radii
(actual radii or r_0 in $r = r_0 A^{1/3}$)

Point by point potential wells (for KRE, KIM, KSO, KCL = 9)
for each potential : set of KPTS1 cards

E energy of inc. particle (Class 1, 3) or binding energy (Class 2) (MeV)

LC lab./CM control

EJJ } ℓ, specification of partial wave to be printed/punched (Class 1, 3)
ELL } or bound state to be computed (Class 2)

LMAX (Class 1, 3) max. orb. ang. mom.
internal criterion checks sufficiency of number of ℓ's

KOP (Class 3) ang. distr. control (operative only if KP1 ≠ 0)

EJQ } (Class 3) { spin } of ground state of the target nucleus
PIQ } { parity }

Energy level cards (Class 3, 4)
Class 3 : NOE − 1 cards, one for each of the excited levels
Class 4 : NOW cards, one for each bound state

Angles (or cosines) list (Class 3)
for ang. distr.s for excited levels

Further comments on the input parameters

Integration parameters

Accuracy of numerical integration is determined by

- # of mesh points (KPTS1)
- cutoff (C1)
- reduced mass μ (calcd. from AIN, ANO)
- energy (E)

Integration in terms of variable $x = Kr$

let $E' = |E_{CM} - V|$

$$\Rightarrow \Delta x = 0.22 \sqrt{\mu E'} \frac{C1}{KPTS1-1}$$

values must be chosen so that $\Delta x \ll 1$ radian

Search and scan control

Types of search and scan procedures :

a) <u>single parameter search</u> : one parameter varied to obtain a match between one of the calculated quantities and a given comparison value for that quantity (KAUTO = 1)

b) <u>parameter space scan</u> : 1 - 5 parameters varied and calcs. performed for each set of parameters (KAUTO = 2)

c) <u>minimum χ^2 search</u> : 1 - 5 parameters varied to obtain min. χ^2 with respect to comparison values given as input (KAUTO = 3 or 4)

additional input necessary

Comparison with experimental values

Calculation of χ^2:

$$\chi^2 = \sum_{n=1}^{NOV} \left(\sum_i w_i \left(\sigma_i^{calc} - \sigma_i^{exp}\right)^2 + \frac{1}{N} \sum_j^N \omega_j \left(d\sigma_j^{calc} - d\sigma_j^{exp}\right)^2 \right)$$

not ang. distr. — ang. distr.

w_i, ω_j ... weights, determined by the code (KAUTO = 3) or given as input (KAUTO = 4)

sum is taken over the NOV values of one of the parameters

additional input necessary

Changes between problems

If new problem is identical in all respects to previous one but for changes in a few parameters, following procedure may be used:

- parameters which are relevant to class and well types can be changed
- control card entries and levels (class 3) and wave fcts. (class 4) may not be changed

* by "change cards" (change control #, control # for parameter changed, new value)

3) Output

Comprehensiveness depends on values of output control parameters

Minimum output comprises well parameters and results

self explanatory

Useful:

— check of well parameters

— when performing a search, review variation of χ^2 and of parameters during the course of the search ("local minimum"?)

— when comparing data "externally" (plot or by hand)

1. be aware of the meaning of σ_{reac}:

in ABACUS: σ_{reac} is the total compound nucleus reaction XS so it comprises comp. el. scattering also

better nomenclature: $\sigma_{abs} = \sigma_{comp.el.} + \sigma_{reac}$

total comp. nucleus reaction XS

XS for non-elastic comp. nucleus reactions

2. use the following relations for potential scattering radius and strength fcts.:

$$S_l = \frac{1}{2\pi}\sqrt{\frac{E_0}{E}}\,\frac{1}{P_l}\,\frac{(l+1)\,T_{l,j=l+1/2} + l\,T_{l,j=l-1/2}}{2l+1}$$

Str. fcts.

$$\left.\begin{aligned} P_0 &= 1 \\ P_1 &= \frac{(kR)^2}{1+(kR)^2} \end{aligned}\right\}$$ penetration factors

$E_0 = 1$ eV

R ... radius of real pot.

$$R' = \sqrt{\frac{\sigma_{sh.el.}(E_0)}{4\pi}}$$ potential scattering radius

VII) IUPITOR

1) Program description

a) Types of problems

Solution of scattering problem by means of CCC

- spin of projectile 0, ½, 1 (0, ½ for ACC)
- target nucleus of some collectivity of either even or odd A
  - vibrational (spherical) — rotational (deformed)
- for deformed target nucleus: NACC or ACC
- ——— " ——— : excitation of states belonging to higher (vibrational) bands can be considered (NACC only)
- inclusion of Cb excitation
- form factor either real (RFF) or complex (CFF)
- up to six states can be coupled at one time
- up to 30 partial waves can be coupled at one time (up to 25 — " —, if projectile energy becomes negative in some excited channels)
- $l_{max} = 69$
- computation of diff. XS's for up to 100 angles for any number of states (up to 35 angles if polarized beam or target); computation of total and reaction XS and s- and p-wave str. fct (only diff. cl. and total XS for ACC)
- if projectile is a neutron, its energy in some excited channels can be negative
- automatic plot of theoretical and experimental diff. XS's and polarizations

b) Modified versions

KARLSRUHE

△ Automatic search routine for fitting experimental data:

χ^2 minimizing routine in order to minimize the sum

$$S = \sum_{i,n}\left(\frac{\sigma^{(n)}_{exp}(\theta_i) - \sigma^{(n)}_{calc}(\theta_i)}{0.1 * \sigma^{(n)}_{exp}(\theta_i)}\right)^2 + \sum_{i,m}\left(\frac{P^{(m)}_{exp}(\theta_i) - P^{(m)}_{calc}(\theta_i)}{0.1}\right)^2$$

overall error of 10%

$\left.\begin{matrix} n \\ m \end{matrix}\right\}$ number of exp. $\left\{\begin{matrix}\text{cross sections} \\ \text{polarizations}\end{matrix}\right\}$ in set

additional input required

△ Improvement of rotational model treatment

- nucl. pot.: inclusion of terms with $\lambda = 8$ (Legendre expansion)
- Ch pot.: —"— —"— up to 2nd order (Taylor —"—)

VIENNA (on the basis of KARLSRUHE version)

△ Integration of differential XS's with respect to angle

$$\sigma_n^{(s)} = \int_{4\pi} \sigma_n^{(s)}(\theta,\phi)\, d\cos\theta\, d\phi =$$

$$= \frac{4\pi}{k_n^2} \sum_{(ii')} \sum_{\substack{m_s M_s \\ m_s'' M_s''}} \sum_{l_1 l_2 j_1 j_2 l' j' J} (2l'+1)\, |\exp(2i\sigma_l^{(n)})|^2\, a^{(i)}_{m_s}\, b^{(i')}_{M_s}\, C^{J\,*}_{l_1 j_1; n l' j'} (l_1 s\, 0\, m_s | j_1 m_s)(j_1 I_1 m_s M_s | J$$

$$* a^{(i)}_{m_s''}\, b^{(i')}_{M_s''}\, C^{J}_{l_2 j_2; n l' j'} (l_2 s\, 0\, m_s'' | j_2 m_s'')(j_2 I_1 m_s'' M_s'') J M$$

Δ Extraction of transmission coefficients :

$$T^J_{1lj} = 1 - \sum_{n'l'j'} \left| S^J_{n'l'j';1lj} \right|^2 =$$

$$= 1 - \sum_{n'l'j'} \frac{2l'+1}{2l+1} \frac{k_1^2}{k_{n'}^2} \left| \delta_{1n'} \delta_{ll'} \delta_{jj'} + 2i\, C^J_{1lj;n'l'j'} \right|^2$$

$$T_{lj} = \sum_{J=|I-j|}^{I+j} g^J T^J_{1lj} \Big/ \left(\sum_J g_J \right) \quad \text{where} \quad g_J = \frac{2J+1}{(2I_1+1)(2s+1)}$$

$$\triangleright\ T_{lj} = \frac{2s+1}{2j+1} \sum_J g^J T^J_{1lj}$$

for $s = \frac{1}{2}$: $T_l = \frac{1}{2l+1} \left(l\, T_{l,j=l-1/2} + (l+1)\, T_{l,j=l+1/2} \right)$

c) List of routines

Serial #

1 Main IUPITOR reads input cards and outputs them immediately

2 { Sr. CCCTRL control of coupled channels calcs., fixes basic quantities and calls subroutines
Sr. NLJJJK set up nlj of the partial waves coupled together for given JΠ

3 { Sr. FLGLCH, Sr. FLGLNG } Cb fcts. for { pos. / neg. } energy projectiles at matching radius

4 Sr. POTENT computes potentials that appear in the coupled equation

5 { Sr. COUPLE solves coupled equations (after geometrical part has been prepared by AMATRX and BMATRX)
Sr. RANGE exponent shift for reals (Karlsruhe)
Sr. BMATRX < || || > } coupling matrix element
Sr. AMATRX AMATRX = AMATRX * BMATRX }

6 { Sr. SMATRX constructs matching equations (using solution obtained with COUPLE)
Sr. SIMLEQ solves matching equations ⇒ C matrix elements

7 { Sr. XSEC partial summations of C matrix elements (NACC)
Sr. ACCSAB ——— " ——— (ACC)

8 { Fr. CROSPL rest of summation of C matrix elements to obtain cross sections (with help of CMMMFC, BFCTOR)
Fr. CMMMFC, Fr. BFCTOR } take part in summations for computing XS^s

9 { Sr. OUTPUT outputs the obtained results
Sr. PLOTER automatic plot of exp. and calcd. XS^s and polarizations

Sr. RAC7 Racah
Sr. CLEB Clebsch Gordan } coefficients

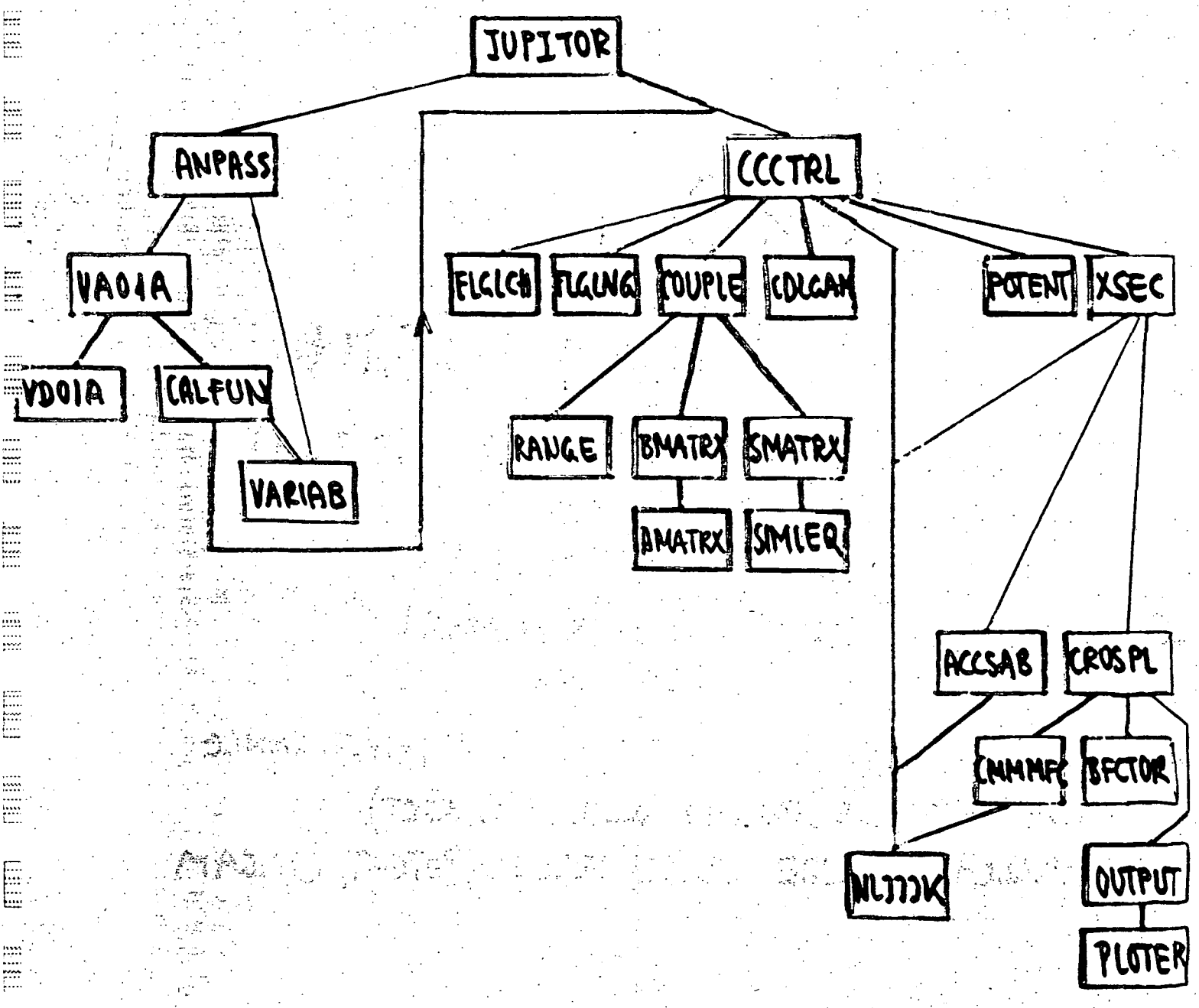
Sr. DOTEST check of whether index out of range (Karlsruhe)

Sr. ANPASS
Sr. VARIAB
Sr. CALFUN
Fct. CBRT
Fct. CDLGAM
Sr. VA01A
Sr. VDC1A
} Karlsruhe search procedure

Fct. W3JS Wigner 3J symbols

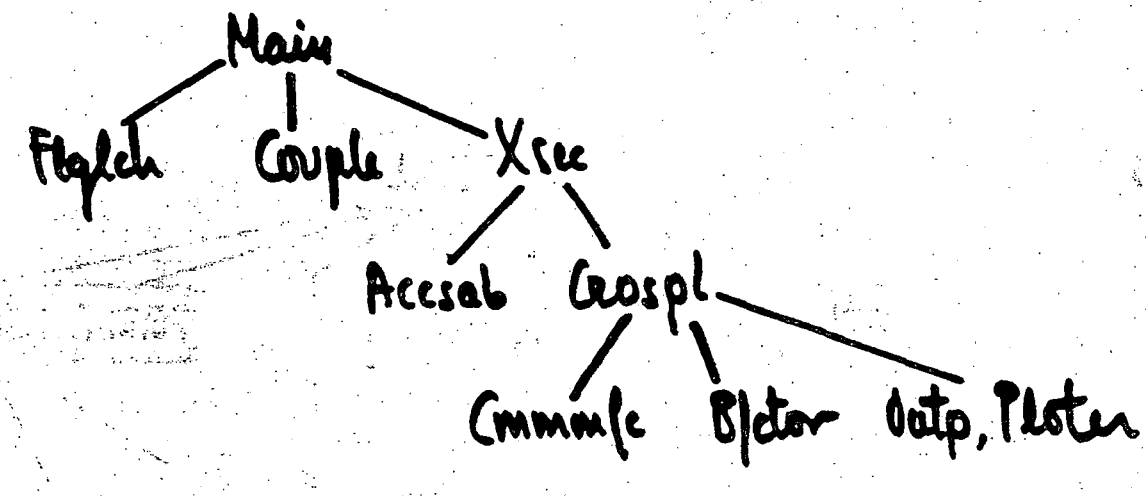
Sr. TRANS transmission coefficients (Vienna)

d) Flow chart



Note : CBRT, CLEB, DOTEST, RAC7, W3J5 are not contained in the flow chart. They are called by many of the above routines.

e) Implementation




```
SUBXS  TREE  CROSPL-(CMMMFC,BFCTOR,OUTPUT)
OUTPUT INCLUDE  OUTPUT, PLOTER
XSCT TREE XSEC-(ACCSAB,CROSPL)
COUP TREE COUPLE-(BMATRX,SMATRX)
SMATRX INCLUDE  SMATRX,SIMLEQ
BMATRX INCLUDE  BMATRX,AMATRX,RAC7,RANGE
IUP TREE IUPITOR-(FLGLCH,COUP,XSCT)
FLGLCH INCLUDE  FLGLCH,FLGLNG,POTENT,CDLGAM
```

f) Remarks on the numerical calculations

Dependence of various XS^s on parameters and $\underbrace{\text{scheme of coupling}}$

— set of states between the strong coupling is considered

— type of coupling

Notation : if imag. terms in $v^{(1)(v)}_{cp;\lambda}$, $v^{(2)(v)}_{cp;\lambda}$, $v^{(2)(r)}_{cp}$ are neglected : RFF (real form factor), otherwise CFF

takes only about half the comp. time

Standard set of OM parameters (used for this investigation)

Nucleons < 30 MeV : F. G. Perey, Phys. Rev. 131 (1963) 745

$r_0 = \bar{r}_0 = r_c = 1.25$ fm $\qquad a = 0.65$ fm

$\bar{a} = 0.47$ fm $(A<150)$ $\qquad \bar{a} = 0.76$ fm $(A>150)$

$V_{so} = 7.5$ MeV $\qquad W = 0$

V, W_D } varied, starting point: { $(52.2 - 0.3E)$ MeV; 11.5 MeV (← without coupling

Studies of dependence on parameters and coupling scheme

(i) comparison vibrational – rotational, same A and Z (^{156}Gd, in reality def.)

CFF

$0^+ - 2^+ - 4$

in matrix el.: $0^+ - 2^+$ 1 qu.ph.
$2^+ - 4^+$ —"— } same β_2
$0^+ - 4^+$ 2 qu.ph.

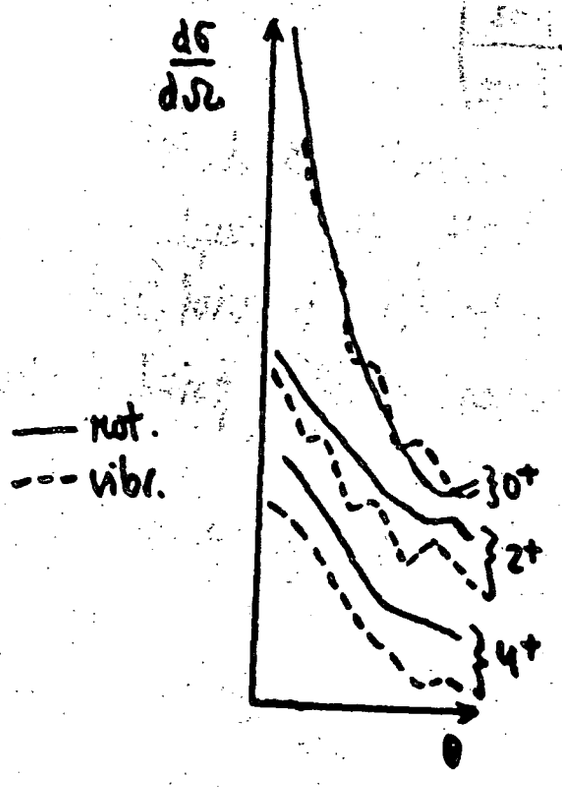
"ideal vibrator"

$\beta_2 = .2$

CFF, ACC

$\lambda' = 2$ highest order of def. in expansion of radius

$\beta_2 = .32$



- structure of XS is much more pronounced in vibrational case than in deformed case
- use of different β_2 in vibrational case leaves structure unchanged, but changes magnitude (not shown in figure)

(ii) vibrational nucleus : dependence of elastic scattering on coupling of higher states :
coupled calculation with $W_D = 7.5$ MeV almost coincides with uncoupled calculation with $W_D = 9.5$ MeV
=> about 20% of the absorptive potential observed in the (pure) elastic case is accounted for by the coupling to the 2^+ state (where $\beta_2 = .2$)

=> <u>fitting procedure vibr. nuclei</u> :
- global potential as starting point
- adjust V, W_D (or. V_{so}) to fit exp. diff. cl. XS's
- $0^+ - 2^+$ coupling with reduced W_D (20%), adjust β_2 to fit data
- couple to two phonon states :
  - increase the above β_2 by ~10% since coupling to 2 ph. st. reduces XS of 1 ph. st.
  - adjust β_2 values for coupling between 1 ph. st. – 2 ph. st's by fit to XS curve

$$\frac{B\,(E2;\,0 \leftrightarrow 2)}{B\,(E2;\,2 \leftrightarrow 1)} = \left(\frac{\beta_{02}}{\beta_{21}}\right)^2$$

red. electric transition probability

ratio is measure of how badly the simple harmonic nature of the vibration is violated
→ important from the nuclear structure point of view

(iii) rotational nucl. : dependence of elastic scattering on coupling of higher states :

NACC, $\underbrace{\text{Legendre expansion}}$ of potential

diag. part contains $V_{cp}^{(\lambda=0)(r)}(\lambda)$ which is a fct. of $\sum_{\lambda'} \beta_{\lambda'} Y_{\lambda' 0}$

diag. pot. not the same if $\beta_2 = 0$ or $\neq 0$
→ elastic scattering XS is fct. of β_2 even if there is no coupling to higher state

⇒ adjustment of W_D does not compensate for coupling
⇒ no step by step parameter adjustment procedure

This does not matter for ACC, since one has to solve coupled equation, irrespective of how many states are considered

(iv) a) vibrational nucl. : dependence of 1 ph st. XS on W_D and coupling scheme :

$0^+ - 2^+ - 3^- - 3^-$

1 qu. ph. 1 oct. ph. 1 qu. ph., 1 oct. ph.

consider XS of 1st 3^- state :

- RFF - CFF affects position of maxima and minima
  → CFF preferable
- cutting off 2nd 3^- state ⇒ 1st 3^- increased
- assuming $0^+ - 3^-$ coupling ⇒ —— " ——
  although 2^+ and 1st 3^- coupled only indirectly through separate coupling to ground state
  but : $0^+ - 2^+$ coupling accounts for ~20% of the absorption
  ⇒ leaving out 2^+ st. similar to change in W_D, and can in fact be compensated by it

b) vibrational nucl.: comparison of $0_0^+ - 2_1^+ - 0_2^+ - 2_2^+ - 4_2^+$ coupling to separate coupling $0_0^+ - 2_1^+ - 0_2^+$ and $0_0^+ - 2_1^+ - 4_2^+$

$\Rightarrow$ two ph. st. XS's ~10% larger with separate coupling

$\Rightarrow$ separate calcs. can cause ~5% error in β_2 values

$\Rightarrow$ β_2 values depend on coupling scheme

this ambiguity could be removed if a sufficiently large number of states could be coupled and it is assumed that the same WD can be used in all the channels

large number of states impossible with presently available computers $\Rightarrow$ effect of neglected coupling to the possible higher excited states is taken into account phenomenologically by using larger values of WD in the higher excited coupled states than are used in the lower coupled states: "fudging"

(v) rotational nucl.: dependence of various XS's on coupl. scheme RFF, $\underbrace{\text{NACC} - \text{ACC}}$, same parameters

large difference (in magnitude) for exc. states of ground band

If requirements of ACC ("ideal rotational band" $\leftarrow$ low excitation energies of exc. states, relatively high exc. energy) are fulfilled, ACC results are more accurate than those of NACC, if in NACC not all states are coupled, because in ACC coupling of all members of grd. st. band is accounted for automatically

(vi) rotational nucl.: comparison power series expansion - Legendre exp.

ACC ... drastic differences between the two calculations, although somewhat better if one goes to higher order in power series expansion and $\lambda = 4$ in Legendre expansion

NACC ... even worse

=> power series expansion should not be used for well deformed nuclei

(vii) rotational nucleus, ACC, comp. protons - neutrons

for neutrons: • oscillations in elastic XS
• 2^+ XS much larger

(viii) magnitude of V_{SO}:

if it turns out that one can put $V_{SO} = 0$ without loosing much accuracy of the result => assume spin = 0, at least for parameter search => saving of comp. time

not to be used for polarizations, of course

2) Input

KTRL(N), N = 1, ...28 control numbers, specify different uses of the program

KTRL(1) = { 0 target even A
1 —"— odd A

KTRL(2) > 0 range of reals is limited to exp(KTRL(2)) in COUPLE (Karlsruhe)

KTRL(3) = { 0 only diff. XS's
1 diff. XS's, total reaction XS's, s & p wave str. fcts. } are computed
2 total, reaction XS's, s & p wave str. fcts.

KTRL(4) = 1 vibr. nucl. : contribution of coupling terms quadratic in α to diagonal potential are considered

KTRL(5) = 1 parameter search is performed, with additional data (Karlsruhe)

KTRL(6) = { 1 direct Cb exc. ; 2 direct and multiple Cb exc. } added for rotational nucl., Legendre expansion (KTRL(11)=

KTRL(7) = 1 ACC

KTRL(8) = { 1 both projectile and target initially polarized ; 2 only projectile — " — ; 3 only target nucleus — " — }

KTRL(9) = { 1 ; 2 } ranges of JJ and K are restricted by { KEXCOM(5,6,7) ; KEXCOM(5,6) }

JJ or $\bar{m}_j$; K π

usually : JJ = 1, ... JJJMAX

where : • for vibr. nucl. & rot. nucl. with NACC (KTRL(7)=0)

JJ = J+1 if J integer

JJ = J+½ if J half odd integer

JJJMAX smallest integer $\geq l_{max} + J_1 + s + 1$

• rot. nucl. with ACC (KTRL(7) = 1):

JJ = $\bar{m}_j$+1 if $\bar{m}_j$ integer

JJ = $\bar{m}_j$+½ if $\bar{m}_j$ half odd integer

JJJMAX smallest integer $\geq l_{max} + s + 1$

whereas : { JJ = KEXCOM(5), ... KEXCOM(6) ; K = KEXCOM(7) only considered parity } if KTRL(9) = 1

{ JJ = KEXCOM(5), ... KEXCOM(6) ; no restriction of parity } if KTRL(9) = 2

KTRL (10) unassigned

KTRL (11) = 1 Legendre expansion of potential (not. nucl.)

KTRL (12) = 1 CFF

KTRL (13) = 1 Cb exc. is added

KTRL (14) to (16) unassigned

KTRL (17) = 1 theoretical elast. diff XS's are divided by Rutherford XS

KTRL (18) ≠ 0 Engelbrecht - Fiedeldey potential (Vienna)

KTRL (19) = 1 $(\vec{\sigma}.\vec{I})$ interaction is added (not. nucl., RFF only)

KTRL (20) to (24) unassigned

KTRL (25) ≠ 0 computation of transmission coefficients (Vienna)

KTRL (26) unassigned

KTRL (27) = 1 segmentation option of original IUPITOR, splitting calc. in two runs. With KTRL (27) = 1 it is assumed that C matrices were computed in previous run)

KTRL (28) unassigned

KEXCOM (N), N = 1, ... 14 control parameters:

KEXCOM (1) unassigned

KEXCOM (2) number of mesh points (within matching radius) } if no Cb exc. (KTRL(13) = 0)

[default: IFIX [(max($r_0 A^{1/3}$ + 10a))/DX]]

of real, vol. im., surf. im.; so

matching radius

mesh size

KEXCOM (3) unassigned

KEXCOM (4) ≠ 0 number of redefinition of number of meshpoints if Cb exc. is considered (KTRL (13) ≠ 0)

Previous number of meshpoints increased by KEXCOM (4); this corresponds to increase of matching radius with respect to "coupling radius" up to which nucl. pot. is const.

KEXCOM (5) lower } limit for JJ summation if KTRL(9) ≠ 0
KEXCOM (6) upper }

KEXCOM(7) solely considered parity if KTRL(9) = 1

KEXCOM (8) to (11) unassigned

KEXCOM (12) spin of two qu. ph. state to which the even core is excited, if target is odd A vib. nucleus (ground state spin 1/2) (INTYPE = 5)

KEXCOM (13) number of three phonon states to be included in the calc. if the target is even A vibrational nucleus (only 0 or 1 allowed presently)

KEXCOM (14) number of partial waves ($l_{max}+1$)

KTLOUT (N), N = 1, ... 28

KTLOUT (2n-1) = 1 small } output from routine with "serial number" n
KTLOUT (2n) = 1 extended } (see "list of routines")

EXTCOM (N), N = 1, ... 10 "extra common"

presently unused, useful if program is modified such that communication of a quantity from a routine to another is needed, and this quantity is to be given as input data

IICPLE number of coupled states in the target (if ACC is used (KTRL(7) = 1) IICPLE has to be = 1)

INTYPE, INTMAX control numbers specifying type of coupling

Cases:

INTYPE=2 even vibr. nucl., no quadrupole multi-phonon states considered

INTYPE=2, INTMAX=1 : 1) SCOM (spherical) if IICPLE=1
2) $0^+ - I^\pi$ coupling if IICPLE ≠ 1
one ph. st. with natural parity ($0^+, 1^-, 2^+, \ldots$)
$\beta_\lambda \rightarrow$ VCOUPL(1)

INTYPE=2, INTMAX=2 : $0^+ - 2^+ - 3^-$ coupling
1 qu. ph. 1 oct. ph.
$\beta_2 \rightarrow$ VCOUPL(1)
$\beta_3 \rightarrow$ VCOUPL(2)
[seems to be in error]

only terms linear in α cons.

INTYPE=2, INTMAX=5 : 1) $0^+ - 2^+ - 3^-$ coupling if IICPLE=3
also terms quadratic in α are included
$\beta_2 \rightarrow$ VCOUPL(1) } used in lin. terms $\langle 0;0 \| \| 1 \rangle$
$\beta_3 \rightarrow$ (2) }
$\beta_2 \rightarrow$ (3) } used in quadr. terms $\langle 1;2 \| \| 1;3 \rangle$
$\beta_3 \rightarrow$ (4) }

2) $0^+ - 2^+ - 3^- - I^-$
quadrup. octup. 2 ph. st. ($1^-, 2^-, \ldots, 5^-$)
$\beta_2 \rightarrow$ VCOUPL(1) } used in lin. terms $\langle 0;0 \| \| 1;\lambda \rangle$
$\beta_3 \rightarrow$ (2) }
$\beta_2 \rightarrow$ (3) } used in lin. terms $\langle 1;\lambda \| \| 2;I \rangle$
$\beta_3 \rightarrow$ (4) } and in quadr. terms $\langle 1;\lambda_1 \| \| 1;\lambda_2 \rangle$

INTYPE = 3 even vibrational nucleus, quadr. multi-phonon states considered

1) $0_0^+ - 2_1^+ - I_2^+$ $(I_2^+ = 0_2^+, 2_2^+ \text{ or } 4_2^+)$ with IICPLE = 3

2) $0_0^+ - 2_1^+ - I_2^+ - I_2'^+$ $(I_2^+, I_2'^+$ any combination of $0_2^+, 2_2^+, 4_2^+)$
or $0_0^+ - 2_1^+ - I_2^+ - I_3^+$ *) $(I_2^+ = 0_2^+, 2_2^+ \text{ or } 4_2^+;$ $I_3 = 0,2,3,4,6)$
} with IICPLE = 4

3) $0_0^+ - 2_1^+ - 0_2^+ - 2_2^+ - 4_2^+$
or $0_0^+ - 2_1^+ - I_2^+ - I_2'^+ - I_3^+$ *) $(I_2, I_2', I_3$ same as above)
} with IICPLE = 5

4) $0_0^+ - 2_1^+ - 0_2^+ - 2_2^+ - 4_2^+ - I_3^+$ *) with IICPLE = 6

Corresponding β's :

Notation : β_{02} grd. st. – 1 qu. ph. st.
β_{2I} 1 qu. ph. st. – 2 qu. ph. st.
β'_{0I} grd. st. – 2 qu. ph. st.
β''_{0I} grd. st. – 1 ph. st., but appears in matrix element grd. st. – 2 qu. ph. st., so it describes one ph. admixture in 2 qu. ph. st.

Input:	$\beta_{02} \rightarrow$	VCOUPL(1)		$\beta_{24} \rightarrow$	VCOUPL(6)
	$\beta_{20} \rightarrow$	(2)		$\beta'_{04} \rightarrow$	(7)
	$\beta'_{00} \rightarrow$	(3)		$\beta''_{00} \rightarrow$	(8)
	$\beta_{22} \rightarrow$	(4)		$\beta''_{02} \rightarrow$	(9)
	$\beta'_{02} \rightarrow$	(5)		$\beta''_{04} \rightarrow$	(10)

---

*) requires KEXCOM (13) = 1
and a 2nd card with coupling potentials:

$\beta_2 \rightarrow$ VCOUPL(11) used in linear term $\langle 2;I \| \quad \| 3;I' \rangle$
$\beta_2 \rightarrow$ VCOUPL(12) –"– quadr. term $\langle 1;2 \| \quad \| 3;I \rangle$

INTYPE = 4 deformed nuclei (make KTRL(11) = 1 ... Legendre exp.)

INTYPE = 4, INTMAX = 1 (NACC or ACC)

only one term of Legendre expansion of pot. ($\lambda = 2$) considered

$\beta_2 \rightarrow$ VCOUPL (1)
ev. $\beta_4 \rightarrow$ VCOUPL (2) } belong to Legendre exp. of radii !

INTYPE = 4, INTMAX = 2 (NACC or ACC)

Legendre expansion up to $\lambda = 4$

$\beta_2 \rightarrow$ VCOUPL (1)

$\beta_4 \rightarrow$ VCOUPL (2)

INTYPE = 4, INTMAX = 3 (NACC)

odd A target, spin-spin interaction considered (KTRL(19) = 1, do not make KTRL(12) = 1 (CFF))

$V_{SS} \rightarrow$ VCOUPL(3)

INTYPE = 4, INTMAX = 4 (NACC, ACC; Karlsruhe)

Legendre expansion up to $\lambda = 8$

for Cb pot. same treatment as for nuclear part (unlike INTMAX = 1,2, where there is power series exp. for Cb pot.)

KTRL (6) = 1 in Cb pot. only terms linear in β_λ (direct Cb exc.)

KTRL (6) = 2 — // — also quadr. terms (direct & multiple Cb exc

INTYPE = 5 odd A vibrational nucleus

INTYPE = 5, INTMAX = 1

core excitation is restricted to one phonon (quadr. or octupole)

target ground state spin $I_1 \leq 9/2$

$\beta_\lambda \rightarrow$ VCOUPL(1) for coupling grd.st. - 1st exc.st. } concern same
$\beta_\lambda \rightarrow$ (2) — // — grd.st. - 2nd exc.st. } core exc.

INTYPE = 5, INTMAX = 2

core excitation up to two phonon states (quadrupole)

requires target g.s. spin $I_1 = 1/2$

only one target state may have a 2 ph. core, together with 3 states with 0 and 1 ph. cores:

$\underset{0\,ph.}{1/2} - \underbrace{\underset{1\,qu.ph.}{3/2} - 5/2} - \underset{2\,qu.ph.:\ I = 1/2, \ldots 9/2}{I}$ with IICPLE = 4

β_2	→	VCOUPL (1)	
β_{2I_c}	→	(2)	
β'_{0I_c}	→	(3)	
c *)	→	(4)	if 1st and 2nd 3/2 states are considered to be a mixture of 1 and 2 ph. states: $\psi_1 = a\,\lvert 1\rangle \pm c\sqrt{1-a^2}\,\lvert 2\rangle + \ldots$
a(3/2)**)	→	(7)	
sign(3/2)	→	(8)	$\psi_2 = -a\,\lvert 2\rangle \pm c\sqrt{1-a^2}\,\lvert 1\rangle + \ldots$
a(5/2)**)	→	(9)	
sign(5/2)	→	(10)	

---

*) $|c| \leq 1$ accounts for the case that $|1\rangle$ and $|2\rangle$ do not exhaust ψ_1 and ψ_2

**) $\sqrt{1/2} \leq a \leq 1$

<u>INTYPE=6</u> case A rotational nucleus, excitation of vibrational bands are to be considered

requires additional cards with states of the considered bands (≤ 7. (see KEXCOM(21) - (27))

β_2 → VCOUPL(1) gd. band

η_1 → (3) } strengths of the excitation of the $\leq$ six exc. bands

⋮

η_6 → (8)

In Appendix A of Jupiter manual

ISTRTW 2* projectile spin

NANGLR number of angles for which diff. XS's and polarizations are comput.

IIXCAL number of states for which diff. XS's are computed

NACC: { IIXCAL = IICPLE usually
{ IIXCAL < IICPLE if inc. energy < exc. en. of an exc. state

ACC : IIXCAL > IICPLE = 1 usually

IIXPLT number of states for which th. & exp. diff. XS's are to be machine plotted

IIXPLT $\leq$ IIXCAL

IIPCAL } same for polarizations
IIPPLT } IIPPLT $\leq$ 2

KANGRD control number for angles θ_{CM}

=1 angles given as input

=0 smallest angle and increment given as input, θ_{CM} equidistant

[KEXCOM(N), N=21, ...27 additional bands, if vibrational states of deformed even nucleus are to be considered (INTYPE=6)]

(IIREAD(N), KPRITR(N), QVALUE(N)), N=1, ... N_c
spin (+½, if A odd), parity, energy of nth target state
N_c ... IICPLE or IIXCAL, resp.
NACC ACC
certain rules for the order of appearance of these states (cf. IUPITOR manual)

ELAB laboratory system energy of the projectile in MeV
PMAS mass of the projectile in amu or pmu depending on AMUPMU
TMAS mass of the target
CHARGE charge product
XMES1 meshsize h_1 } used in differential equation integration
XMES2 meshsize h }
[in integration : $h_1, 2h_1, 4h_1, \ldots, h, 2h, 3h, \ldots$ are used
$\Rightarrow h_1 = \frac{h}{2^k}$ (k integer)]

AMUPMU control number for mass unit
=0 atomic } — " —
=1 proton }

ANGLER(N) CM angles in degree
N=1, ... NANGLR, if KANGRD=0
N=1,2 (min θ, increment), if KANGRD=1

SGMEXP(N,I), POLEXP(N,I) exp. XS^S and polarizations for plot (Tamura) or search (Karlsruhe)
angle angle
state, I=1,...IIXPLT≤6 state, I=1,...IIPPLT≤2

Angles and amplitudes of polarized states (only if KTRL(8) ≠ 0)

VSX depth of real pot.

WSX —"— vol. imag. pot.

WSF —"— surf. —"—

VSO —"— spin orbit pot.

WC(N), N=1,...6 "fudge" factors for the strength of vol. and/or surf. imaginary potential (no fudging 1.0)

DFN, RZERO diffuseness, radius of real pot.

DFNW, RZEROW —"— vol. imag.

DFNS, RZEROS —"— surf. —"—

DFNSP, RZROSP —"— spin orbit pot.

} all diffuseness ≠ 0 !

RZEROC radius parameter of Cb pot. (>0 also for neutrons!)

[RONE, RONEW, RONES } r_1^s in Engelbrecht Friedrich pot. (Vienna) ($R = r_0 A^{1/3} + r_1$)]

VCOUPL(N), N=1,...10 quantities related to coupling, see INTYPE, INTMAX

KREAD1 control number for continuation of input

=1 new problem

=2 next input starts with incident energy

=3 —"— potential depths

Number of exp. points = NANGLR * (IIXPLT + IIPPLT)

N number of variable parameters

MA max. number of complete sets of calcs. (MA ≥ N+4)

IP print control number

ES step size parameter

} (Karlsruhe search)

3) Output

Notation :

SGTOTL ... σ_t , total cross section

REACCR ... $\sigma_t - \sigma_{sh.el.} = \sum_{n \neq 1} \sigma_n^{(s)} + \sigma_{abs}$

"reaction cross section" in the sense that it gives the cross section for all processes apart from shape el. scatt., different from both meanings of "σ_{reac}" mentioned on p. 74

STRGFS, STRGFP ... S_0, S_1 , strength functions for $l=0$ and 1

in fact, $S_l = \lim_{E \to 0} \frac{1}{2\pi} \frac{T_l}{P_l}$

therefore, even if S_l refers to $E_0 = 1\,eV$ due to the factor $\sqrt{\frac{E}{E_0}}$ (cf. p. 74), S_l may differ when calculated at different energies E, if constancy is not yet reached

[S_0, S_1 in JUPITOR output refer to 1 eV]

VIII.) STAPRE

1) Program operation

a) Possible problems

— calculation of energy averaged cross sections of particle induced nuclear reactions in the frame of the statistical model
- activation cross sections
- population cross sections of isomeric states
- production XS's for γ rays from low excited levels
- energy spectra for all emitted particles
- γ-ray production spectra

— up to 6 emitted particles and γ rays (sequential evaporation)
— angular momentum and parity conservation
— width fluctuation correction
— preequilibrium decay (1st step)

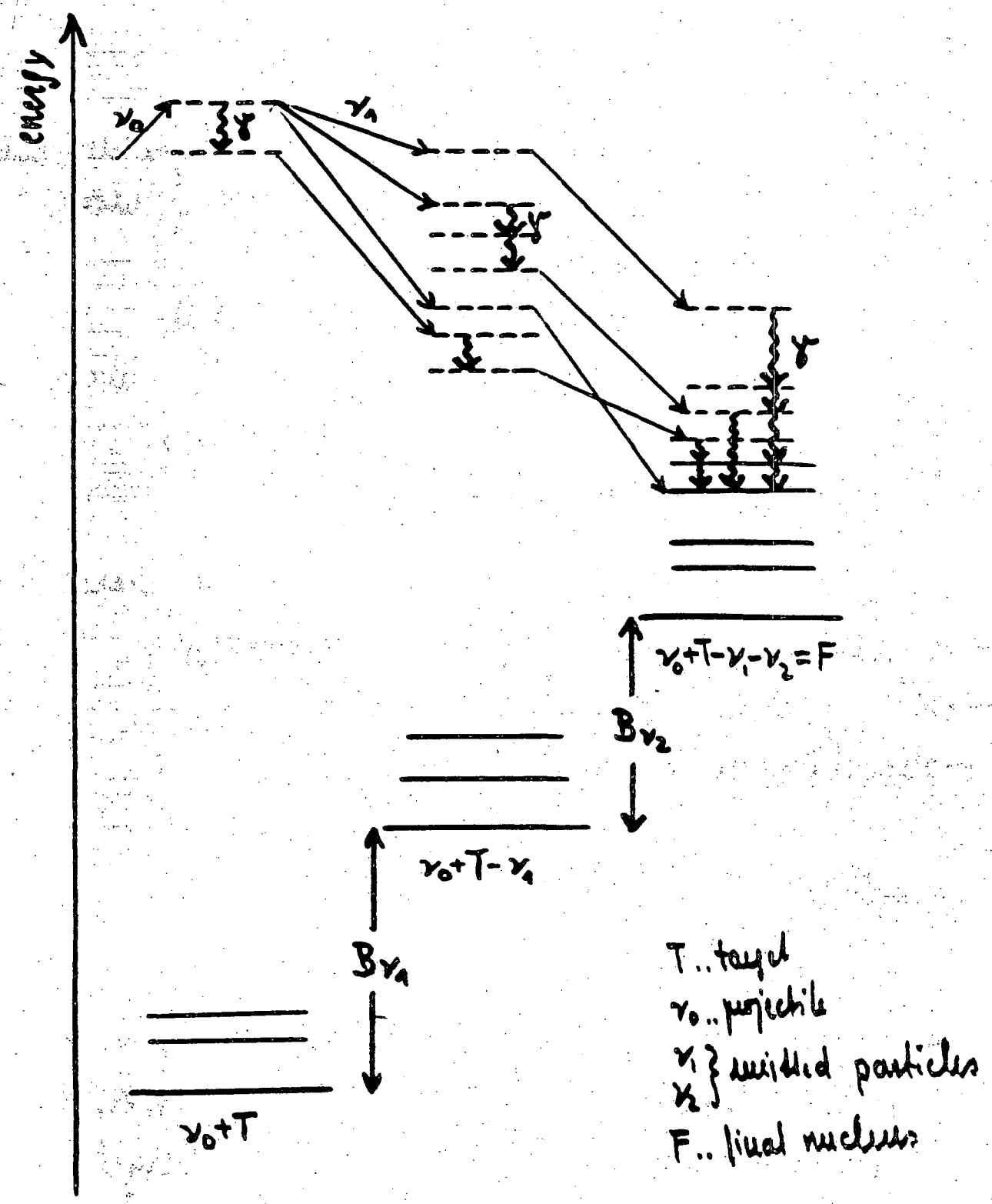
b) Formalism

Notation

i^{th} compound nucleus (CN) = nucleus resulting from emission of $i-1$ particles of a specified sequence $\nu_1, \nu_2, \nu_3 \ldots$:
1st CN : composite system of projectile + target
2nd CN : after emission of one particle $\nu_1 \ldots$

$WB_i(E,J,\pi)\Delta E$ ... primary population of states with exc. energy in interval ΔE around E, ang. mom. J, parity π of ith CN

$T(\nu_0, \nu_1 \nu_2 \gamma) F$



$\overline{WB}_i(E,J,\pi)\Delta E$ ... population of states E,J,π of ith CN after γ-ray cascades

$\frac{\partial\sigma^{pre}_{\nu_1}}{\partial\varepsilon_1} d\varepsilon_\nu$ ... presquilibrium contribution to emission spectrum of 1st particle (cf. p. 55)

q^{pre} ... fraction of the initial population which survives presquilibrium

$\left.\begin{array}{l}\frac{\partial\sigma^{HF}_{\nu_1}}{\partial E'}(E',J',\pi')\Delta E' \\ \frac{\partial\sigma^{HF}_{\gamma}}{\partial E'}(E',J',\pi')\Delta E'\end{array}\right\}$ Hauser Feshbach contribution to 1st emission step for $\left\{\begin{array}{l}\text{part.}\\ \gamma\text{ rays}\end{array}\right.$

$$\frac{\partial\sigma^{HF}_{\nu_1}}{\partial E'}(E',J',\pi')\Delta E' = \frac{\pi}{k^2}\sum_{J\pi} g_J \frac{\sum_{s_0 l_0} T_{\nu_0 l_0} \sum_{s_1 l_1} T_{\nu_1 l_1}}{N_1(E,J,\pi)} W^{J\pi}_{\nu_0 s_0 l_0, \nu_1 s_1 l_1} \rho_{\nu_1}(E',J',\pi')\Delta E'$$

$$\frac{\partial\sigma^{HF}_{\gamma}}{\partial E'}(E',J',\pi')\Delta E' = \frac{\pi}{k^2}\sum_{J\pi} g_J \frac{\sum_{s_0 l_0} T_{\nu_0 l_0} \sum_{\chi l} T_{\gamma\chi l}}{N_1(E,J,\pi)} \rho_\gamma(E',J',\pi')\Delta E'$$

$\uparrow$

limit of infinite number of open channels, non-elastic processes $\Rightarrow W \to 1$

$N_i(E,J,\pi)$ ... Hauser Feshbach denominator of ith CN

$$N(E,J,\pi) = \sum_\nu \sum_{J'\pi'} \sum_{sl} \int_0^{E-B_\nu} d\varepsilon_\nu\, T_{\nu l}(\varepsilon_\nu)\, \rho_\nu(E-B_\nu-\varepsilon_\nu, J',\pi') +$$
$$+ \sum_{J'\pi'} \sum_{\chi l} \int_0^{E} d\varepsilon_\gamma\, T_{\gamma\chi l}(\varepsilon_\gamma)\, \rho_\gamma(E-\varepsilon_\gamma, J',\pi') +$$
$$+ \int_0^\infty dE'\, \rho_f(E',J,\pi)\left\{1+\exp\left[\frac{2\pi}{\hbar\omega}(E'-E)\right]\right\}^{-1}$$

$\left.\begin{array}{l}\rho_\nu(E',J',\pi')\\ \rho_\gamma(E',J',\pi')\end{array}\right\}$ — " — of CN resulting from $\left\{\begin{array}{l}\text{part.}\\ \gamma\text{ ray}\end{array}\right\}$ emission

$\rho_f(E',J,\pi)$ ... transition state density

$W^{J\pi}_{\nu_0 s_0 l_0, \nu_1 s_1 l_1}$ ... width fluctuation correction factor

Continuation of HF & PE model

$$WB_1(E,J,\Pi)\,\Delta E = q^{pre}\,\frac{\partial\sigma_\gamma^{HF}}{\partial E}(E,J,\Pi)\,\Delta E \quad \text{for } 1^{st} \text{ chance } \gamma \text{ ray em.}$$

$$WB_2(E,J,\Pi)\,\Delta E = \left\{ q^{pre}\,\frac{\partial\sigma_{\nu_1}^{HF}}{\partial E}(E,J,\Pi) + \frac{\partial\sigma_{\nu_1}^{pre}}{\partial E}\,\frac{\frac{\partial\sigma_{\nu_1}^{HF}}{\partial E}(E,J,\Pi)}{\sum_{J'\Pi'}\frac{\partial\sigma_{\nu_1}^{HF}}{\partial E}(E,J',\Pi')} \right\}\Delta E$$

for 1st chance particle em.

since PE model J independent: for each J, PE contribution is weighed with relative share of this J in equilibrium → ??

later chance particle emission

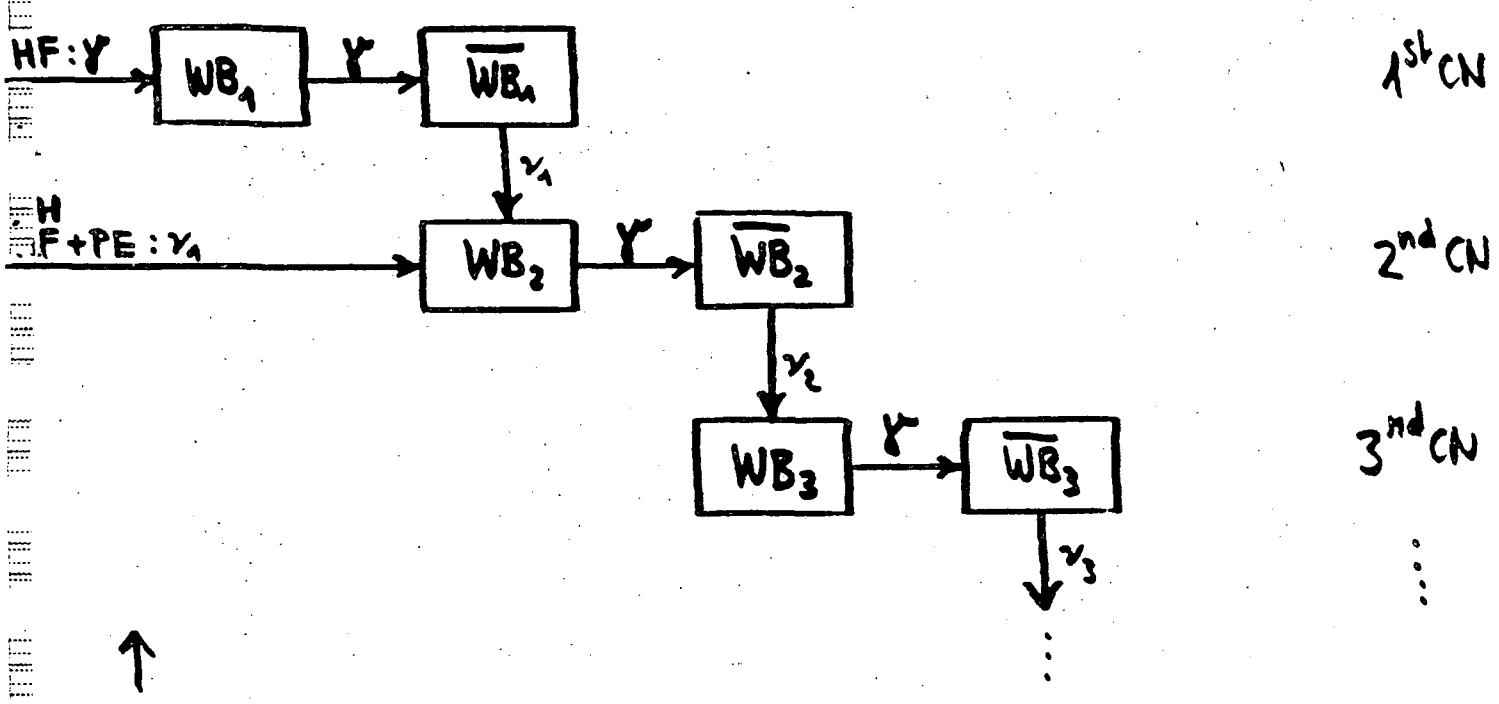
evaporation of ith particle from i^{th} CN with population $\overline{WB}_i(E,J,\Pi)\Delta E$ leads to population $WB_{i+1}(E',J',\Pi')\Delta E'$ of $(i+1)^{th}$ CN:

$$WB_{i+1}(E',J',\Pi')\,\Delta E' = \sum_{J\Pi}\int_{E'+B_{\nu_i}}^{E_{max}} dE\;\overline{WB}_i(E,J,\Pi)\;\frac{\Gamma_{\nu_i}(E,J,\Pi;E',J',\Pi')}{\Gamma_i(E,J,\Pi)}\,\rho_{\nu_i}(E',J',\Pi')\,\Delta E'$$

where $$\frac{\Gamma_{\nu_i}(E,J,\Pi;E',J',\Pi')}{\Gamma_i(E,J,\Pi)} = \frac{1}{N_i(E,J,\Pi)}\sum_{l_i s_i} T_{\nu_i l_i}(E-E'-B_{\nu_i})$$

$\Gamma_i(E,J,\Pi)$ ... total width of states E,J,Π of ith CN

Schematic representation :

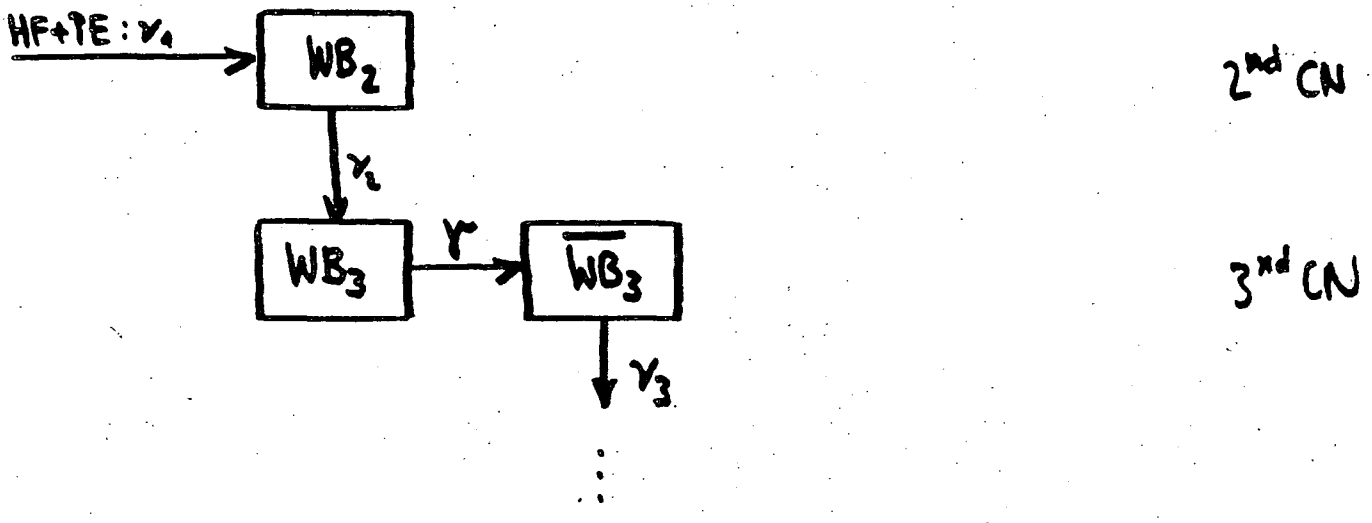


↑

above : consideration of γ decay starts in the first CN

below : ——————— " ——————— 3rd CN

↓



Fission cross sections

1st chance fission:

$$q^{fus}\,\frac{\pi}{k^2}\sum_{J\Pi} g_J \sum_{l\,s\,o} \sum_{c'} \underbrace{\frac{1}{D^{J\Pi}}\int_{\bar{E}-\frac{D^{J\Pi}}{2}}^{\bar{E}+\frac{D^{J\Pi}}{2}} dE\,\frac{T_{\gamma_0 l_0 T_{fc'}}}{N(E,J,\Pi)}}_{\text{average with respect to intermediate class II structures}}\; W_{\gamma_0 s_0 l_0,\,fc'}$$

higher chance fission (contr. of ith CN):

$$\sum_{J\Pi}\int_0^{E_{max}} dE\;\overline{WB}_i(E,J,\Pi)\,R_{fi}(E,J,\Pi)$$

where R_{fi} ... fission probability of ith CN
= sum of transm. coeff.s for direct & indirect fission, divided by $N(E,J,\Pi)$

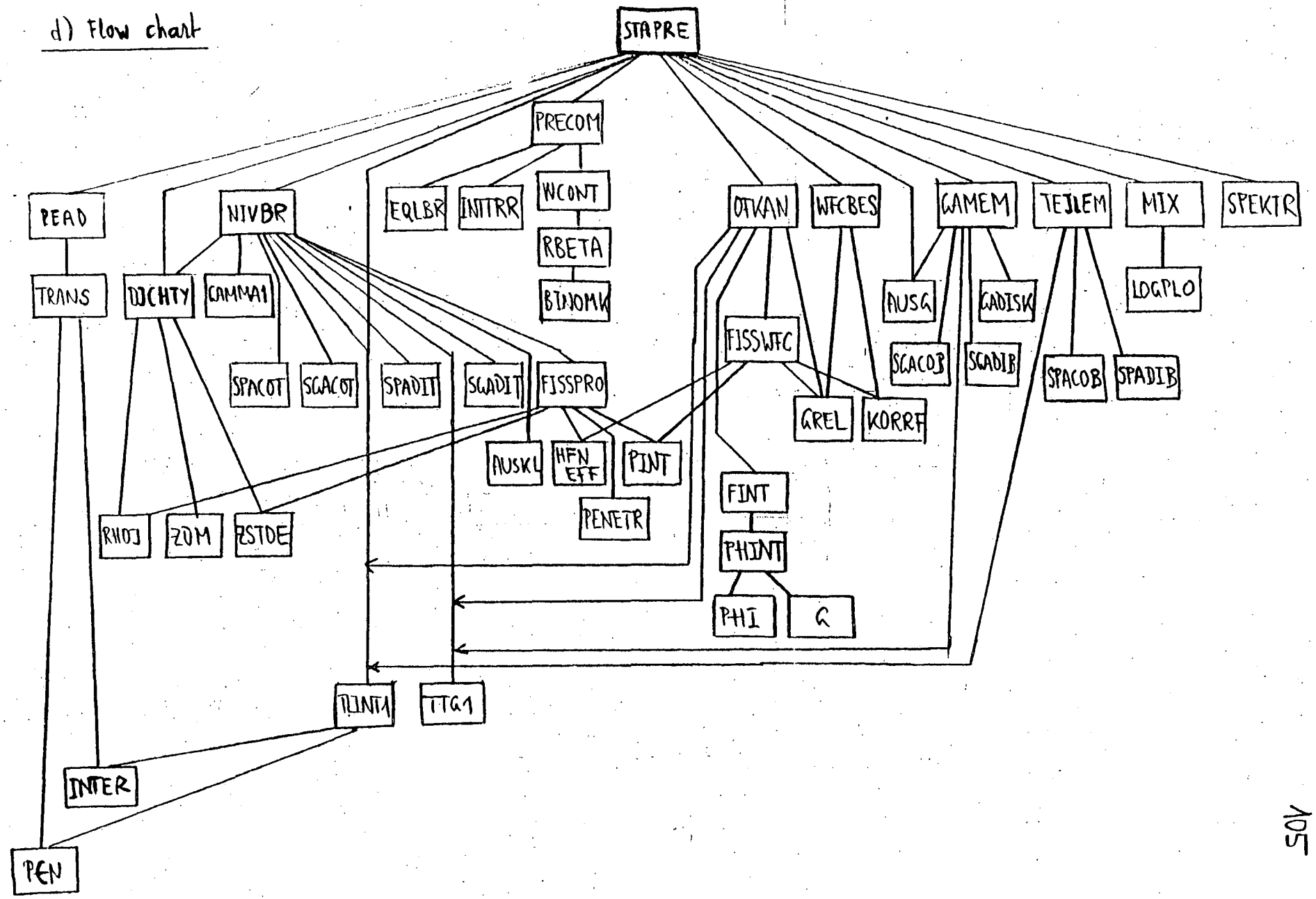
c) list of routines

Main STAPRE control of stat. model calc., loop for emission steps
Sr. READ input
Sr. GAMMA1 calc. of γ ray transmission coefficients
Sr. TRANS preparation of particle transm. —"— (from files supplied as input)
Sr. TLINT1 interpolation of particle transmission coefficients
Sr. INTER interpolation polynomial
Fct. PEN penetration factors

Sr. NIUBR calc. of total level width
Sr. DICHTY level density as fct. of exc. en. and angular momentum
Fct. RHOJ — " — dependence on ang. mom.
Fct. ZDM density of states with given magnetic quantum number
Sr. ZSTDE state density (Fermi gas and/or const. temperature formula)
Sr. SPACOT contribution of particle emission to continuum states to total width
Sr. SGACOT — " — γ ray ——— " ———
Sr. SPADIT — " — particle emission to discrete states to total width
Sr. SGADIT — " — γ ray ——— " ———
Sr. TTG1 interpolation of γ ray transmission coefficients
Sr. FISSPRO fission probability and fission contribution to total width
Sr. AUSKL edit of 2 dim. array
Fct. HFNEFF HF denominator and fission prob. (average over class II states
Fct. PINT interpolation of penetrabilities
Sr. PENETR penetrabilities through fission barrier
Sr. PRECOM calc. of PE contribution
Sr. EQLBR equilibration of population of exciton states
Sr. INTTRR internal transition rates
Sr. WCONT continuum emission rates
Fct. RBETA factor R_ν (cf. p. 53)
Fct. BINOMK binomial coefficients
Sr. OFKAN preparation of WFC factor
Sr. FISSWFC fission contribution to HF denominator and 1st chance fission XS
Sr. WFCBES population resulting from 1st chance part. or γ ray emission (HF)
Sr. GREL limits of orb. ang. momentum in WFC factor
Sr. KORRF numerical integration of WFC

Fct. FINT part of integrand of WFC factor
Fct. PHINT averaging over class II structure
Fct. PHI integrand for averaging over class II structure
Fct. G part of -"- ——— " ———
Sr. AUSG edit of 3 dim. arrays
Sr. GAMEM calc. of population by γ ray emission
Sr. SGACOB population of continuum states by γ ray emission
Sr. SGADIB —"— discrete ——— " ———
Sr. GADISK γ rays between discrete levels
Sr. TEILEM calc. of population by particle emission
Sr. SPACOB population of continuum states by particle emission
Sr. SPADIB —"— discrete ——— " ———
Sr. MIX combination of HF & PE contribution
Sr. LOGPLO logarithmic plot of HF & PE spectrum
Sr. SPEKTR summing of contributions of all emission steps to part. and γ ray prod. sp.

d) Flow chart


STAPRE
PRECOM
WCONT
RBETA
BINOMK
EQLBR
INITRR
READ
TRANS
NIVBR
DJCHTY
GAMMA1
SPACOT
SCACOT
SPADIT
SCADIT
FISSPRO
AUSKL
HFN EFF
PINT
PENETR
RHOJ
ZOM
ZSTDE
OTKAN
FISSWFC
FINT
PHINT
PHI
Q
WFCBES
GREL
KORRF
GAMEM
AUSG
SCACOB
GADISK
SCADIB
TEJLEM
SPACOB
SPADIB
MIX
LOGPLO
SPEKTR
TLINT1
TTG1
INTER
PEN

2) Input

TITEL, in 1st col. : *

NLAUF(I), I=1,7 control # for the reaction

NLAUF(1) ... code number of projectile

NLAUF(I), I≥2 ... code # for particle emitted from (I-1)th CN

Codes : 1 ... neutron

2 ... proton

3 ... α

4 ... deuteron

99 ... non-standard part. (only for NLAUF(1))

N number of CN, 1 ≤ N ≤ 6

NGACOM number of that CN from which the coincidation of γ rays starts, ≤ N

NPAR type of particles whose emission is considered in the HF denominator

1 .. neutrons

2 .. neutrons, protons

3 ... —"— , —"— , α

4 ... —"— , —"— , α, deuterons

NPAR ≥ NLAUF(I) except for NLAUF(1) = 99

LLMAX maximum multipolarity of γ rays

1 ... E1, M1

2 ... E1, M1, E2, M2

3 ... E1, M1, E2, M2, E3, M3

1 ≤ LLMAX ≤ 3

DU binsize (keV) of energy grid

NFISS control number for calc. of fission XS's

0 ... no fission

1 ... explicit consideration of fission channels

2 ... all continuum fission channels are treated as 1 channel

NPHI control # for averaging of WF corrected 1st chance fission XS over intermediate class II structure
0.... by means of use of "effective fission transm. coefficients"
>0... by means of integration

NNWFC control # for WFC
0...on
1...off

GRE limit of HF denominator above which WFC is put =1
default : 50.

NNFREI number of degrees of freedom of level width distr.
default : 1

DDEL desired relative accuracy for integration of WFC
default : .01

NNINT max. # of meshpoints for calc. of integral in WFC
must be a power of 2
default : 64
if >64 => NNINT=64 internally

(PARC(I,1),PARC(I,2)),I=1,N characteristics of CN
PARC(I,1)..chem. symbol } of Ith CN
PARC(I,2)...charge number }

ATAR mass # of target

STAR spin } of target
KPTAR parity (+1 or -1) }

Q binding energy of projectile to target (required only if NLAUF(1)=99)

AGESCH mass # } of projectile; required only if NLAUF(1) = 99
SGESCH spin

EEINL incident energy in lab. system
will be adjusted according to energy grid

KDE control number for variation of inc. energy

KRZZMM total number of inc. energies for which calcs. are to be performed

FM constant (MeV^3) determining the internal transition matrix element for PE model
= 0. .. no PE considered

NPI initial particle number, default : 2

NHI initial hole number, —"— : 1

IPAULI control # for consideration of Pauli principle in internal trans. rates
0 .. off
1 .... on

KTESTP control # for single particle state density g and energy shift $D\Delta$ used in p-h-state density formula

0 or 1 ..... $g = \frac{6}{\pi^2} \cdot \frac{A}{8}$, $D\Delta = 0$

2 or 3 ..... $g = \frac{6}{\pi^2} \frac{A}{8}$, $D\Delta = \frac{12}{\sqrt{A}} * \begin{cases} 0 & \text{odd} \\ 1 & \text{odd mass} \\ 2 & \text{even} \end{cases}$ } nuclei

4 or 5 ..... $g = \frac{6}{\pi^2} \cdot \frac{A}{8}$, $D\Delta = \Delta$

6 or 7 ..... $g = \frac{6}{\pi^2} a$, $D\Delta = 0$

8 or 9 ..... $g = \frac{6}{\pi^2} a$, $D\Delta = \Delta$

↑

odd values : extended protocol

MILANO control # for calc. of emission rates (in PE step) for nuclear induced reactions

0 ... general expressions are used } cf. p. 53

1 ... expressions of Milano group are used

PHIMIL α cluster preformation probability in Milano expression for α part. emission rate

KTEST1 output control # for printing level densities, contributions of particle and photon contr. to HF denominator, fission prob. and total decay widths

0 ... off

1 .. on

KTEST2 output control # for printing WB and $\overline{WB}$

0 ... off

1 ... on

KTEST3 output control # for printing particle and, if calcd., γ ray spectra from decay of each CN

0 .. off

1 ... on

KTESTW control number for WFC protocol

0 .. short

1 .. extended

KGAPR output control number for printing production XS's of γ rays between discrete levels

0 or 1 ... none

≥ 2 .... for levels 2, ..., J where J = min (# of disc. levels, KGAPR)

((PARR(I,K), K=1, NPAR), I=1,N) separation energies (MeV)

PARR(I,K).. sep. energy of particle with code # K from I^{th} CN

LMAX max. orb. ang. mom
Transmission coeffs. } for inc. channel, required only if NLAUF(1) = 99

NTRAN ctrl. # for transm. coeffs.

1 .... one set of — " — for all CN

N .... each CN has its own set of transm. coeffs.

LO(K), K=1, NPAR number of partial waves for all particles
Transmission coeffs. for all particles } NTRAN sets

(DC(L), L=1, 13), ISYMC level density parameters for 1st CN

DC(1).. "a-parameter"
DC(2).. $\eta = I_{eff}/I_{rigid}$ } in Fermi gas formula
DC(3).. Δ

DC(4).. shell correction

DC(5)-DC(12).. parameters regarding const. temperature formula

DC(13)... $I_\perp/I_{rigid}$ for rot. nuclei

ISYMC... control # for ang. mom. dependence of level density

0 ... spherical nuclei

1-5.. deformed —"— with various symmetry properties

-1 ... usual Fermi gas formula (cf. p. 4.)

NDISK number of discrete levels of 1st CN
ED(J), SD(J), KPD(J), J=1, NDISK levels of 1st CN } required only if NCACOM = 1

ED(J).. exc. en.
SD(J) ... spin
KPD(J).. parity (+1 or -1) } of Jth level

Following data are required for each CN ($I = 1, \dots N$):

UB neutron separation energy (MeV)

S1, S2 } spins of s wave neutron resonances

KP parity

GR average total radiation width (meV) at neutron binding energy

NF number of subsequent cards for specifying γ ray str. fcts.
for the present, $NF \leq 1$ (← E1 only)
$NF = \phi$ ... Weisskopf model for all multipolarities

PG(J), J = 1,..6 normalization factors for γ ray str. fcts.

PG(1) ... normalization factor for $f_{\gamma E1}(\varepsilon_\gamma)$
default: by fitting total radiation width to GR

PG(2) ... $f_{\gamma M1}(\varepsilon_\gamma = UB) / f_{\gamma E1}(\varepsilon_\gamma = UB)$

PG(3) ... $f_{\gamma E2}(\varepsilon_\gamma = UB) / f_{\gamma E1}(\varepsilon_\gamma = UB)$

⋮

PG(6) ... $f_{\gamma M3}(\varepsilon_\gamma = UB) / f_{\gamma E1}(\varepsilon_\gamma = UB)$

for J = 2,..6 : default : ratios of Weisskopf units

ERR(L), GRR(L), SRR(L), L = 1,3 parameters of giant resonances of photo absorption cross section

ERR(L) ... position (MeV)
GRR(L) ... width (MeV)
SRR(L) ... peak XS (mb)
} for L^{th} giant resonance

for ERR(L) = Φ. with L ≥ 2 : L^{th} giant res. not considered
for ERR(1) = Φ. : one E1 giant res. with global parameters (Brink Axel)

only for I ≥ NGACOM

ES1 lower limit
ES2 upper limit
FRS reduction factor applied for $\varepsilon_\gamma < ES1$

} describing step in E1 str. fct.
default : no step

fraction of Weisskopf contribution to $f_{\gamma E1}^{\text{photo abs.}}$:

$$\underbrace{f_{\gamma E1}^{\text{weisskopf}}} = FSP * f_{\gamma E1}^{\text{photo abs.}} (\varepsilon_\gamma = UB)$$

this energy independent fraction is added to energy dep. one

(VZD(L,M), M=1,L), L=1,NDISKC γray branching ratios

VZD (L,M) .. branching ratio for γ transition from the Lth to the Mth level of the Ith CN

where NDISKC ... number of discrete levels of Ith CN (in order of ascending energy

VZD (L,M) need not be normalized

VZD(L,M) = 0., M = 1,... L : L^{th} level stable or isomeric

only for I ≥ NGACOM

(DR(L), L=1,13), ISYM level density parameters for residual nuclei after particle emission from I^{th} CN (NPAR cards for each CN)

DR(L), ISYM have the same meaning as DC(L), ISYMC for 1st CN

NAN1, NAME number of levels ($1 \le NAN1 \le 50$), symbol

EDR(J), SDR(J), KPDR(J), J=1,..,NAN1 discrete levels

EDR(J) ... excitation energy
SDR(J) .. spin
KPDR(J) .. parity (+1 or −1)

} of Jth level

} of residual nuclei after part. emission from I^{th} CN (NPAR sets required)

BARR(L), L=1,...12 fission barrier parameters

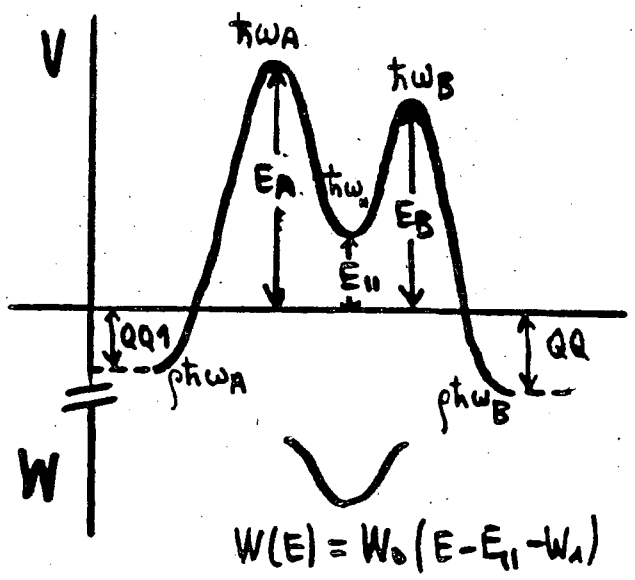
BARR(1) ... E_A
BARR(2) ... $\hbar\omega_A$
BARR(3) ... E_B
BARR(4) ... $\hbar\omega_B$
BARR(5) ... E_{II}
BARR(6) ... $\hbar\omega_{II}$
} in MeV

BARR(7) ... W_0

BARR(8) ... W_1
BARR(9) ... QQ1
BARR(10) ... QQ
} in MeV

BARR(11) ... p , default : p = 2.

BARR(12) .. unassigned



From the quantities BARR(L) a contrl. # NBARR is derived:

NBARR = 1 if BARR(L) ≠ ϕ. for L ≥ 3 single humped barrier
= 2 — " — for L ≥ 5 double humped barrier, complete damping
= 3 if BARR(5) > ϕ. and BARR(6) > ϕ. double humped barrier, partial damping

NSTEP number of meshpoints for integration for averaging over intermediate class II structure ; default value from internal crit.,
NSTEP ≤ INDE * INBJ

only for NFISS ≠ 0

(DR(L), L=1..13), ISYM(NB) level density of continuum transition states

DR(L), ISYM same meaning as above

NFISSD(NB), (DFISS(L,NB), L=1,4) discrete transition states

NFISSD(NB).. number of bandheads (≤ 10)

DFISS (1,NB).. rotational constant (keV)

DFISS (2,NB).. decoupling parameter

DFISS (3,NB).. unassigned

DFISS (4,NB).. energy determining continuum edge of transition states

EB(L,NB), KB(L,NB), PB(L,NB), L=1, NFISSD(NB) heads of rot. bands

EB(L,NB).. exc. en. (MeV)
KB(L,NB)... K quantum #
PB(L,NB)... parity (+1 or -1)
} of Lth band head

} for NB=1,NBARR *)

only if NFISS ≠ 0

*) NBARR = 1 for the only barrier
= 2 for barrier A and barrier B
= 3 for barrier A, barrier B and combined barrier AB

3) Output

a) General part:

Sequence of compound nuclei, for each of them level density parameters and discrete levels of the nuclei resulting from emission of the various particle types are printed, if emission is energetically possible

b) For each incident energy:

- protocol of PE calc.
- -"- of WFC
- then for the sequence of compound nuclei the most important results are printed, optionally extended to include
  - level density
  - contr.s to HF denominator
  - population before and after γ-ray cascades
  - spectra from each CN
- particle & γ ray production spectra summed over emission steps

c) Final part

table of excitation functions

IX) EVALUATION PROCEDURE

Motivation for nuclear model calcs.:

a) to supplement experimental cross sections to supply cross section data for applications in science and technology ("applied science aspect")

— to fill gaps in excitation functions ("interpolation")
Many excitation functions of threshold reaction of importance for reactor neutron dosimetry are based on calculations in some energy regions

— to extend excitation functions to higher energy regions where scarce or no data exist ("extrapolation")
The development of d+Li neutron sources for fusion materials irradiation test facilities requires the knowledge of neutron XS's for energies up to 40–50 MeV. These requirements have to be met by calculations which reproduce data at lower energies. Similar for biomedical applications.

— to produce XS's of interest for which no experimental data at all exist, e.g. for instable target nuclei ("prediction")
Such XS's are of interest for astrophysical applications and also for energy related technology as e.g. for the assessment of the buildup of fission products and actinides.

b) to analyze experimental data in order to check the applicability of the models, eventually refine them, and learn about reaction mechanisms and nuclear structure ("pure science aspect")

1) Retrieval of experimental data

Types of exp. data:

a) cross sections for the reaction(s) of interest, if available

b) all experimental data which may serve for determination or adjustment of the model parameters entering to the calcs.:

- total, total elastic, diff. elastic, diff. inelastic XSs } for choice of opt. model parameters
- strength functions
- resonance densities } for determination of level density parameter
- discrete levels
- cross sections for competing reactions : to confirm whole parameter set and possibly determine level density parameters of nuclei with no resonance data
- cross sections for reactions induced by particles which in the reactions of interest are the outgoing particles or compete with these } to check transm. coeffs. for these particles
- particle production spectra : to check PE model parameters
- photon production spectra, radiation width, parameters of γ abs. XS, γ ray strength fcts. } for determination of γ ray transm. coeffs

activation data — emission data

production XS of specified nucleus by various reaction paths, e.g. (n,pn), (n,np), (n,d)

production XS of specified particle by various reaction paths, e.g. (n,α), (n,nα), (n,pα)

Sources of exp. data:

- EXFOR
- CINDA
- Pertinent papers in journals
- Proceedings of pertinent conferences & symposia
- Compilations (e.g. BNL-325 (1979), vol. 1, INDC compilations, IAEA, Vienna)
- "Table of Isotopes"
- Underlying data bases of previous evaluations
- Internal laboratory reports

2) First choice of model parameters

A) References

a) spherical optical model

— global potentials:

neutrons: F.G. Perey, B. Buck, Nucl. Phys. 32 (1962) 353
D. Wilmore, P.E. Hodgson, Nucl. Phys. 55 (1964) 673
F.D. Becchetti, G.W. Greenlees, Phys. Rev. 182 (1969) 1190

C.A. Engelbrecht, H. Fiedeldey, Ann. Phys. 42 (1967) 642
B. Holmqvist, T. Wiedling, J. Nucl. Energy 27 (1973) 543
L. Rosen et al., Ann. Phys. 34 (1965) 96
protons: G.S. Mani, M.A. Melkanoff, I. Iori, Rept. C.E.A. 2379 (1963)
F.G. Perey, Phys. Rev. 131 (1962) 745
C.A. Johnson, Phys. Rev. Lett. 39 (1977) 1604
α particles: J.R. Huizenga, G. Igo, Rept. ANL-6373 (1961) and Nucl. Phys. 29 (1962) 462
L. McFadden, G.R. Satchler, Nucl. Phys. 84 (1966) 177
O.F. Lemos, Oslo Rept., Series A, № 136 (1972)
Y.S. Park, H.D. Jones, D.E. Bainum, Phys. Rev. C4 (1971) 788

— potentials determined by other authors for specified nuclei or for limited mass region:

neutrons: S. Igarasi, Proc. Conf. Nuclear Cross Sections and Technology, Washington (1975), vol. 1, p. 320
J.P. Delaroche, Ch. Lagrange, J. Salvy, IAEA Consultants Meeting Trieste (1975), IAEA-190, vol. 1, p. 251
Ch. Lagrange, Proc. 3rd Nat. Soviet Conf. Neutron Physics, Kiev (1975), CONF-75061154, ATOMIZDAT (1976)
E.D. Arthur, P.G. Young, Rept. LA-8626-MS (ENDF-304) and Proc. Int. Symp. Neutron XSs 10-50 MeV, Brookhaven (1980), p. 731
E.D. Arthur, P.G. Young, W.K. Matthes, Proc. Int. Symp. Neutron XSs 10-50 MeV, Brookhaven (1980), p. 751

J. Rapaport, V. Kulkarni, R. W. Finlay, Nucl. Phys. A330 (1979) 15
J. Rapaport et al., Phys. Repts. 87 (1982) 25

A. Prince, Proc. Int. Conf. Nucl. Data for Science and Technology, Antwerp (1982), in press

— opt. pot. obtained by means of search on appropriate data, starting from a potential of one of the groups mentioned above

b) Deformed optical model

— pot. determined by other authors for specified nucleus or limited mass region:

neutrons: J. P. Delaroche et al. } see above
Ch. Lagrange }

D. G. Madland, P. G. Young, Proc. Int. Conf. Neutron Physics & Nucl. Data, Harwell (1978), p. 349

— opt. pot. obtained by means of search on appropriate data, starting from sphen. opt. pot. or deformed opt. pot. determined by other authors

(see "step by step fitting procedure for vibr. nuclei," p. 82)

— deformation parameters: from electromagnetic transitions, and analyses of inelastic scatt., also of other particles, on same nucleus

Nuclear Data Sheets, Academic Press, N.Y. and London
and Recent References therein

P. H. Stelson et al., Nucl. Phys. 68 (1965) 97

Y. Yamamouti, Proc. Int. Conf. Nucl. Cross Sections for Technology. Knoxville (1979), NBS Spec. Publ., p. 146

M. Hyukataka et al., J. Phys. Soc. Japan 38 (1975) 606

c) Pre-equilibrium & compound nucleus model:

— level density parameters

W. Dilg, W. Schantl, H. Vonach, M. Uhl, Nucl. Phys. A 217 (1973) 269

A. Gilbert, A.G.W. Cameron, Can. J. Phys. 43 (1965) 1446

J.L. Cook et al., Austral. J. Phys. 20 (1967) 477

— separation energies

A.H. Wapstra, N.B. Gove, Nucl. Data Tables 9 (1971) No 4-5

N.B. Gove, A.H. Wapstra, Nucl. Data Tables 11 (1972) No 2-3

A.H. Wapstra, K. Bos, Atomic Data & Nucl. Data Tables 19 (1977), No 3, p. 215

V.E. Viola et al., Atomic Data & Nucl. Data Tables 13 (1974) No 1

— discrete levels & branching ratios

Nucl. Data Sheets, Acad. Press, N.Y., London

P.M. Endt, C. van der Leun, Nucl. Phys. A 105 (1967) 1
A 115 (1968) 697
A 214 (1973) 1

Table of Isotopes, Lederer & Shirley (eds.), J. Wiley, N.Y., 1978

F. Ajzenberg-Selove, Nucl. Phys. A 281 (1977) 1

- radiation widths

BNL-325, vol. 1

S. M. Zakharova et al., INDC(CCP)-27/L (1972)

M.S. Moore, Proc. Int. Conf. Neutron Phys. and Nucl. Data, Harwell (1978), p. 313

H. Weigmann, G. Rohr, Proc. Symp. Neutron Phys. with Thermal and Resonance Energy Neutrons, Petten (1973), p. 194

- resonance spacings

G. Rohr, Proc. Specialists Meeting on Neutron Data of Structural Materials for Fast Reactors, Geel (1977) p. 614

F. H. Fröhner, Proc. Int. Conf. Neutron Phys. and Nuclear Data, Harwell (1978) p. 268

- fission parameters

J. E. Lynn, Harwell Rept. AERE-R7468 (1974) 324

J. E. Lynn, Proc. Consultants Meeting, Trieste (1975), IAEA-190, vol. 1, p.

B) Recommendations and Remarks:

a) spherical optical model (ABACUS)

- KCL $\left\{ \begin{matrix} 0 \\ 1 \end{matrix} \right\}$ same form for Ch pot. (uniform charge distr. within R_c)
- if imag. pot. comprises volume part only, it must be input as VIM (not VIVOL)
- ——— " ——— & surface part: see p. 70 for ways of specifying

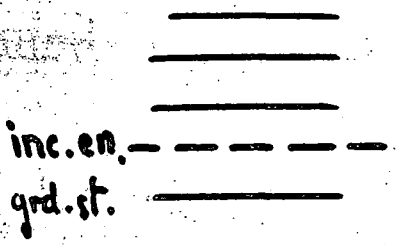
- "parameter scan" comprises not only possibility of varying potential depths and geometrical parameters, but also target nucleus, projectile and incident energy (see manual)
- JUMP=2 at end of input deck is condition for transm. coeffs. to be written to file 7 ("ABACUSTL")
- Hauser Feshbach mode of ABACUS (Class 3) must not be used for incident energies higher than highest considered level, or, more generally speaking: for incident energies for which decay modes other than elastic & inel. scatt. to discrete levels have to be considered (inel. scatt. to continuum states, emission of competing particles)

2) <u>Informed optical model</u> (JUPITOR)

- KTRL(4)=1 consideration of contribution of coupling terms quadr. in α to diag. pot. (vibrational nuclei) } NO
- KTRL(9)= $\left\{\begin{matrix}1\\2\end{matrix}\right\}$ restrictions of range of J ($\bar{m}_J$, resp.) and π loops } test runs only
- KTRL(11)=1 Legendre expansion of pot. (rotational nuclei) YES
- KTRL(12)=1 CFF { YES if you search on potential of your own; NO if you use pot. which was determined with RFF
- KTRL(25)=1 creation of transm. coeffs. (Vienna), not compatible with KTRL(7)=1 (ACC)

program calculates non-vanishing cross sections even for states whose population is not allowed from energy conservation, if they are coupled ("virtual coupling")

e.g.



IICPLE = 4 virtual coupling (negative energy channels)

IIKCAL > 1 physically not meaningful

c) <u>Pre-equilibrium and compound nucleus model</u> (STAPRE)

— consideration of γ competition is necessary

- near thresholds, e.g. : $E_{in} \gtrsim 0$ ... NGACOM = 1
  $E_{in} \gtrsim E_{thr}^{(n,2n)}$ ... NGACOM = 2
  ⋮
- for calc. of γ ray production spectrum ... NGACOM = 1
- for calc of population XS of isomeric state in K^{th} compound nucl. } ... NGACOM ≤ K

— determination of quantity FM:

$$\lambda_+(n=3, \underbrace{E \approx 21\ \text{MeV}}_{}) \approx 5 \times 10^{21}\ s^{-1}$$

found by extensive data analyses by
G.M. Braga-Marcazzan et al., Phys. Rev. C6 (1972) 1398
E. Gadioli, E. Gadioli-Erba, Acta Phys. Slovaca 25 (1975) 126

Since $\lambda_+(n=3, E) = \frac{2\pi}{\hbar} |M|^2 \frac{g[g(E-\Delta_{ph}) - C_{3,2}]^2}{4}$,

where $|M|^2 = FM * A^{-3} * E^{-1}$

$C_{3,2} = 6.5$ } see STAPRE manual

g and Δ_{ph} determined by KTESTP

▷ $$FM = 0.5 * 10^{22} * \frac{6.58 * 10^{-22} * A^3 * 21 * 4}{2\pi\, g\,[g(E-\Delta_{ph})-6.5]^2}$$

slight variation may be necessary to fit exp. data

– importance of level scheme for isomeric state cross sections:

- completeness of level scheme: compare high resolution $(n,n'\gamma)$ data with charged particle measurements; corresponding γ transitions found?
- spin & parity assignment: what multipole types? (E1, M1, E2) spin differences and parities compatible with $\left\{ \begin{array}{l} (-)^L \text{ el.} \\ (-)^{L+1} \text{ magn.} \end{array} \right\}$?

  if decay to several levels observed: spin assignment consistent?

– importance of spin cutoff parameter for calc. of isomeric state XS's

sensitivity to I_{eff}/I_{rigid}

– in PE model: $\Delta_{ph} = \Delta_{pair} = \frac{12}{\sqrt{A}} * \left\{ \begin{array}{ll} 0 & \text{odd-odd} \\ 1 & \text{odd mass} \\ 2 & \text{even-even} \end{array} \right\}$ nuclei, since it

represents at least a simple account for pairing

— for combined Fermi gas and constant temperature level density:

$$\rho(U,J,\pi) = \tfrac{1}{2}\rho(U,J) = \frac{1}{2\sqrt{8}}\frac{1}{\sigma^3(U)}\,\omega(U)\,(2J+1)\exp\left[(J+\tfrac{1}{2})^2/2\sigma^2(U)\right]$$

level density assumed to be parity independent

$\omega(U)$ ... state density
$\sigma(U)$ ... spin cut off parameter

e.g. 3 regions:

$0 \le U < U_1^t$ $\quad \omega(U) = C_1 \exp\left(\frac{U}{T_1}\right)$
$\sigma(U) = \sigma_1$

$U_1^t \le U < U_2^t$ $\quad \omega(U) = C_2 \exp\left(\frac{U}{T_2}\right)$
$\sigma(U) = \sigma_2$

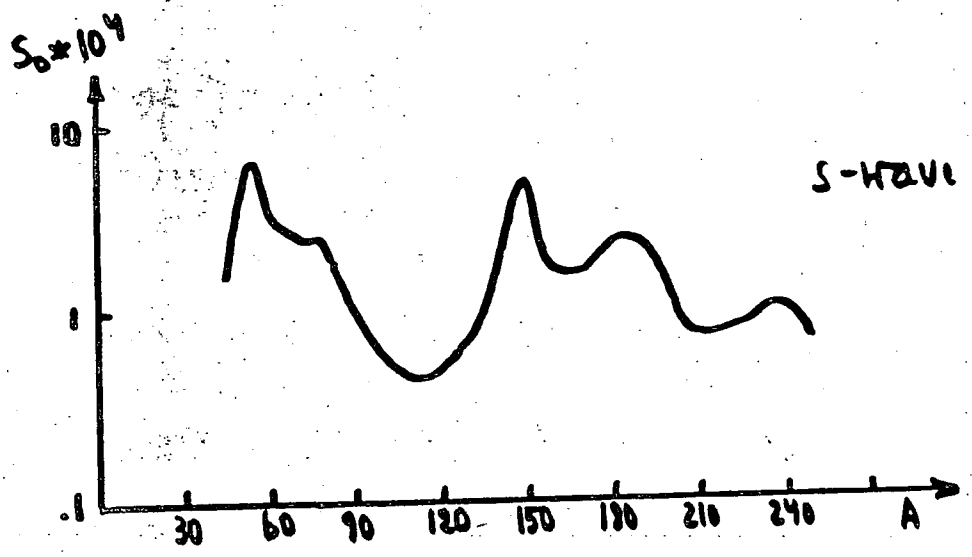
$U_2^t \le U$ $\quad \omega(U) = \frac{\sqrt{\pi}}{12}\,\frac{\exp\left(2\sqrt{a(U-\Delta)}\right)}{a^{1/4}\,(U-\Delta)^{5/4}}$

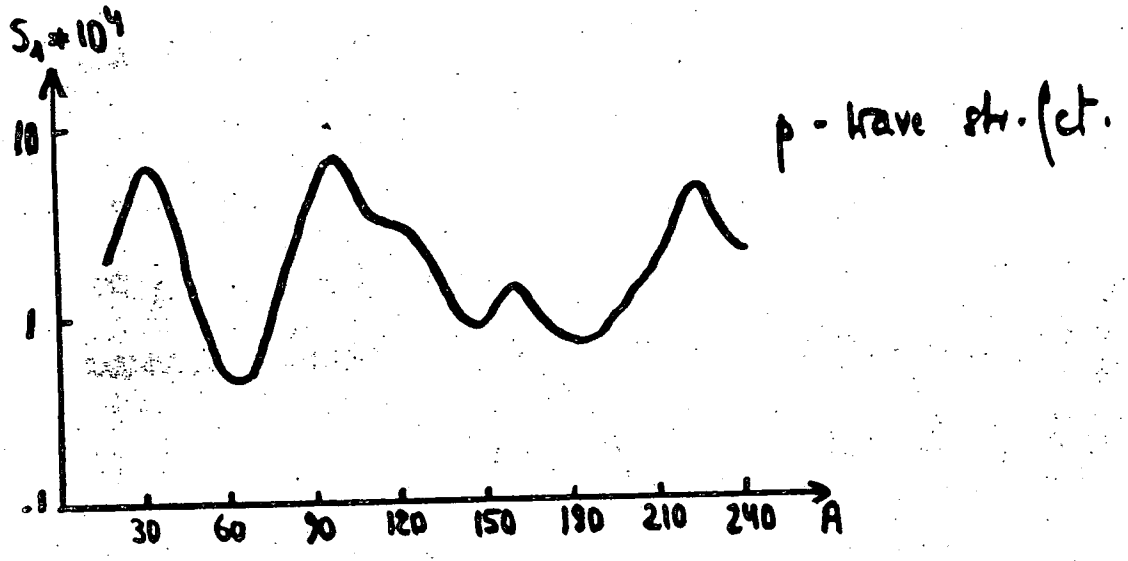
$\sigma^2(U) = \frac{1}{\hbar^2} I_{\parallel} \sqrt{\frac{U-\Delta}{a}}$

at transition energies U_1^t, U_2^t: smooth joining of different forms; if σ are different $\Rightarrow$ ω and ρ cannot be joined smoothly at the same time; usually one joins $\rho(U,J)$ (by appropriate choice of C_i or U_i^t)

parameter variation requires adjustment of parameters in other regions or of transition energies

— choice of energy points for generation of T_i:
in mass regions where str. fcts. have extremum as fct. of A
$\Rightarrow$ for given A strong dependence on energy, even for low energies





T_L must be generated
- to very low energies to avoid extrapolation which relies on constancy of str. fcts.
- with small increments to avoid uncertainties in interpolation

3) Input preparation

manual – automatic

↓

using auxiliary programs which construct input for nuclear model codes from simple input (+ appropriate compiled information)

automatic input construction desirable for

- spherical OM if radial dependence (well form) or energy dependence cannot be handled by SCOM code (ABACUS)
- statistical model, if several reactions involving the same nuclei shall be calculated with a consistent parameter set.

Automatic input construction requires libraries containing transmission coefficients, separation energies (or nuclear masses) and nuclear data as level information, level density parameters, γ decay data, PE model parameters.

Advantage of automatic input preparation:

- ▲ parameters of certain nucleus need not be given repeatedly for each occurrence of this nucleus in different reactions, but only once (to the library)
- ▲ choice and variations of parameters consistent for all considered reactions
- ▲ error probability reduced
- ▲ parameters adjusted to exp. data in previous work can easily be utilized for further evaluations in this mass region

4) Output evaluation

— Check of input parameters

- well depths
- geometr. parameters
- deformation — " —
- inc. energy
- level density parameters
- discrete levels
- PE model parameters
- γ decay — " —

— Comparison of results to exp. data

- total XS, total elastic, abs. XS
- diff. el., diff. inel. XS
- activation cross sections (for single reaction paths)
- isomeric state production XS's (——— " ———)

— Comparison of quantities deduced from results to exp. data

- strength functions, see p. 74
- potential scatt. radius, — " — [$E_0 = 1\,eV$, consider: $1\,fm = 10^{-13}\,cm$ $\sqrt{\hbar/\sigma} = 10^{-12}\,cm$]
- particle production spectra (summed over various reaction paths)

transformation to lab. system may be necessary

$\varepsilon_{rel}^{C.M.}$ ... "channel energy" = energy of rel. motion, C.M. (STAPRE!)

$\varepsilon_{part}^{C.M.}$ ... particle energy, C.M. = channel energy $* \frac{M_{RN}}{M_{CN}}$

RN ... residual } nucleus
CN ... compound }

$\varepsilon_{part}^{lab.}$ ... particle energy, lab.

$$\varepsilon_{part}^{lab} = \varepsilon_{part}^{C.M.} + E_{in}\,\frac{M_{part} * M_{proj}}{M_{RN}^2} = \frac{M_{RN}}{M_{CN}} * \varepsilon_{rel}^{C.M.} + \text{terms } (2^{nd}\text{ order})$$

$$\approx \frac{M_{RN}}{M_{CN}} * \varepsilon_{rel}^{C.M.}$$

$$\frac{\partial\sigma}{\partial\varepsilon_{rel}^{C.M.}} = \frac{\partial\sigma}{\partial\varepsilon_{part}^{lab}} * \frac{\partial\varepsilon_{part}^{lab}}{\partial\varepsilon_{rel}^{C.M.}}$$

$$\Rightarrow \frac{\partial\sigma}{\partial\varepsilon_{part}^{lab}} \approx \frac{M_{CN}}{M_{RN}} * \frac{\partial\sigma}{\partial\varepsilon_{rel}^{C.M.}}$$

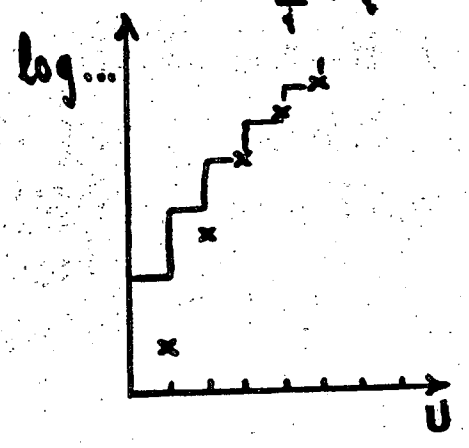
problem of later chance emission : for given particle energy energies of compound and residual nucleus not uniquely determined
=> no exact kinematical treatment possible

for nucleons transformation negligible, for α's necessary

- γ ray production spectra (summed over various reaction paths)
- residual nucleus part. XS (———— " ————)
- "cumulative level densities"

comparison of $\sum_J \int_0^{K*DU} \rho(U,J)\,dU \approx \sum_J \sum_i^K \rho(U_i,J) * DU$ $\quad U_i$...middle of ith bin

with experimental $\sum_i^K N_i$ $\quad K=1,2,\ldots$ $\quad N_i$..# of exp. levels in i^{th} bin



⌐ exp.
× calc.

— cross sections for which compound nucleus model and direct contributions have to be combined :

- o inelastic scattering (also to isomeric states)
- o charged particle emission from heavy nuclei

if no consideration of direct contributions possible => deficiencies of fit should be qualitatively compatible with missing direct interaction contribution (underestimation rather than overestimation, underestimation at the high energy end rather than at low energies ...)

5) Parameter variation (STAPRE)

— increase of level density (by means of increase in "a" or decrease in Δ in case of back shifted Fermi gas) of residual nucleus after emission of specified particle or of transition states at fission barriers enhances emission of this particle or fission and reduces branching ratios for other decay modes

— decrease of FM increases pre-equilibrium fraction and makes 1st chance particle emission spectrum harder ; <u>in general</u> (but not necessarily) this reduces later chance particle emission

e.g.: reaction path (n, 2n) : reduction of FM in general increases (n, n') at the cost of (n, 2n)

reaction path (n, pn) : reduction of FM in general increases (n, p) at the cost of (n, pn)

exception : if a certain decay mode computes more favourably in equilibrium stage (e.g. $\Delta_{pk} = 0$, $\Delta < 0$) => reduction of

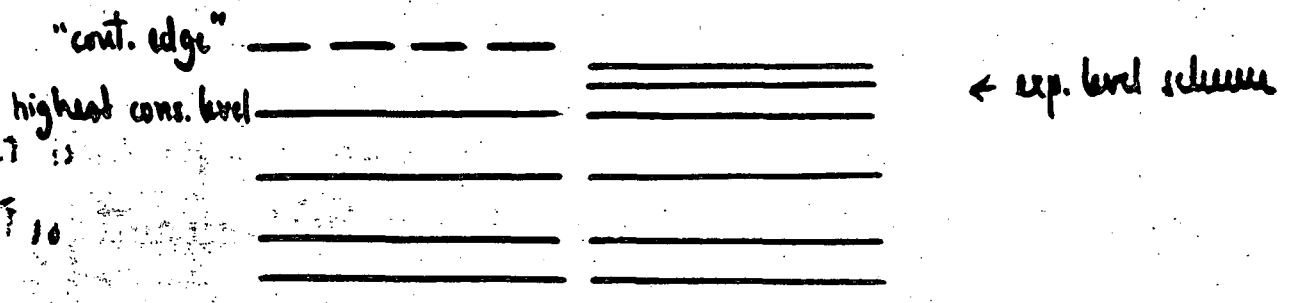
FM may cause decrease in activation XS of res. nucleus of this decay mode, since reduction of equ. portion q_λ^{pre} (cf. p.50, 100) is more effective than making the spectrum harder

- increase in $\overline{\Gamma}_\gamma$ of certain CN increases activation cross section of this CN; effect is appreciable only if essential fraction of this activation XS comes from population of states where γ competition is effective. Important for isomeric state XS^s.

- branching ratios of discrete levels influence γ ray production spectrum and isomeric XS ratio (if corresponding decays belong to cascades which populate different states (ground or isomeric). If branching ratios uncertain => try out other values in order to check effect

- spin and parity assignment of discrete levels: in the case of uncertain spin parity assignment try alternative J^π in order to check influence on results, especially in case of isomeric state cross section calc.

- variation of number of discrete levels:
since the lower limit of the lowest "continuum bin" (← where level density formula is applied) is smallest integer multiple of DU larger than exc. energy of highest considered discrete level (relative to zero-point of energy grid), there may be a region without levels, in contradiction to exp. level scheme:



This deficiency may be overcome by adding or leaving out discrete levels; optimization must for all states simultaneously

e.g.: for ^{50}Cr:

in $^{51}Fe(n,\alpha n)^{50}Cr$: cont. edge is smallest integer multiple of

$$S_\alpha(^{55}Fe) + S_n(^{51}Cr) + E_{(exc)\ level}$$

in $^{50}Cr(n,n')^{50}Cr$: cont. edge is smallest integer multiple of

$$S_n(^{51}Cr) + E_{(exc)\ level}$$

$\Rightarrow$ different positions of cont. edges if $S_\alpha(^{55}Fe) \neq k * DU$ (k integer)

6) Consideration of special features

<u>Problems related to the use of transm. coeffs. created under consideration of direct inelastic scattering</u>

A) <u>Coexistence of direct contributions and PE</u>

If during the OM fitting procedure to exp. diff. inel. XS^s no PE is considered, the PE decay populating the states that had been coupled in the OM fit should not be considered in the statist. model calcs., either, because the direct contribution then fully accounts for the population of these states. Considering direct

reaction contr. and PE would be a double counting; the same is true with respect to the reduction of σ_{abs}:

σ_{abs} in CCOM reduced with respect to SCOM to account for direct r.,

$\sigma_{abs} \rightarrow \sigma_{abs} \cdot q^{pre}$ in Hauser Feshbach part (cf. p. 55, 100) to account for PE.

=> effects all statist. model cross sections

Since direct reactions and PE are considered to describe different reaction mechanisms, both should be considered during the OM fitting procedure. This would require the calc. of angular distributions in PE => in STAPRE not possible

[(Poor) approx.: assumption of isotropy $\frac{\partial^2 \sigma^{pre}}{\partial \Omega \partial \varepsilon} \approx \frac{1}{4\pi} \frac{\partial \sigma^{pre}}{\partial \varepsilon}$]

B) <u>Use of coupled channels transm. coeffs. for outgoing channels</u>

Since for statist. model usually the same T_ℓ are used for formation and decay, the T_ℓ of projectile relative to ground state of target are used also for the system of this particle relative to excited states in outgoing channels (also for the states not considered explicitly in CCC, and for the coupled states ($T^J_{1\ell j}$ instead of $T^J_{n\ell j}$, cf. p. 35, 77)). Therefore the effects of absorption of flux to the coupled channels which is related to the collective nature of ground st. and coupled states are considered also where no such effects occur, in particular also for other nuclei if NTRAN = 1. It would be preferable not to use CC T_ℓ for outgoing channels. This is at present not possible in STAPRE.

Isospin correction for p induced reactions

Isospin of target T_t

in p induced reactions : 2 isospins of CN can be formed $T_< = T_t - \frac{1}{2}$

$T_> = T_t + \frac{1}{2}$

isospin mixing : population can be transferred between $T_<$ and $T_>$ states

Calc. without isospin corresponds to consideration of $T_<$ states only

Formulation : S. Grimes et al., Phys. Rev. C5 (1972) 85

Assumptions :
- isospin mixing consists in transfer of fraction μ of the population of $T_>$ states to $T_<$ states (μ.. mixing parameter
- for considered energies the density of $T_>$ states of residual nuclei negligible

in particular for (p,n) reactions:

$$\sigma_{pn}(\mu) = \left(\frac{2T_0}{2T_0+1} + \mu\frac{1}{2T_0+1}\right)\sigma_{abs}\frac{\Gamma_n}{\Gamma_n+\Gamma_\alpha+\Gamma_p*\left(\frac{2T_0}{2T_0+1}+\mu\frac{1}{2T_0+1}\right)}$$

where $\Gamma_n, \Gamma_p, \Gamma_\alpha$ are the widths obtained without cons. of isospin ($\mu=1$)

$$\triangleright \quad \frac{\Gamma_p}{\Gamma_n} = \frac{\sigma_{pp}(\mu=1)}{\sigma_{pn}(\mu=1)} \qquad \frac{\Gamma_\alpha}{\Gamma_n} = \frac{\sigma_{abs}-\sigma_{pn}(\mu=1)-\sigma_{pp}(\mu=1)}{\sigma_{pn}(\mu=1)}$$

Define $f(\mu) = \frac{2T_0}{2T_0+1} + \mu\frac{1}{2T_0+1}$

$$\triangleright \quad \sigma_{pn}(\mu) = f(\mu)\,\sigma_{abs}\frac{1}{1+\frac{\sigma_{abs}-\sigma_{pn}(\mu=1)-\sigma_{pp}(\mu=1)}{\sigma_{pn}(\mu=1)}+f(\mu)\frac{\sigma_{pp}(\mu=1)}{\sigma_{pn}(\mu=1)}}$$

$$\boxed{\sigma_{pn}(\mu) = f(\mu)\,\sigma_{pn}(\mu=1)\frac{1}{1-\frac{\sigma_{pp}(\mu=1)}{\sigma_{abs}}(1-f(\mu))}}$$

Correction of OM results due to non-consideration of capture

Usually, in OM codes no competing reactions other than el. + inel. scatt. are considered (cf. p. 123). Capture computes with these decay modes even at lowest energies:

$$\sigma_{abs} = \sigma_{capt} + \sigma_{c.el.} \text{ instead of } \sigma_{abs} = \sigma_{c.el.} \; !$$

Calculate σ_{capt} from statist. model and correct $\sigma_{c.el.}$ for non-consideration of capture in the OM:

$$\boxed{\sigma_{c.el.} = \sigma_{c.el}\big|_{OM} * \frac{\sigma_{abs} - \sigma_{capt}}{\sigma_{abs}}}$$

Necessary to satisfy ENDF/B consistency checks.

7) Accuracy

A) Rough estimate of uncertainties of calculated cross sections from comparison to exp. data

- if exp. XS's are reproduced reasonably => uncertainties of calcd. XS's comparable to experimental uncertainties
- if exp. XS's are reproduced badly => uncertainties of calcd. XS's difficult to estimate, even if one doubts the experiment
- if no exp. XS's for considered reaction exist => estimated uncertainty depends on how well the chosen parameter set is confirmed by reproduction of cross sections of competing XS's, level data, resonance data, XS's of "inverse reactions"... (cf. p. 117)

B) Estimate of uncertainties of calculated cross sections from uncertainties of the parameters

cross section values are assumed to be functions of n parameters $p_1 \ldots p_n$ which are known with uncertainties $\Delta p_1, \ldots \Delta p_n$

$\Longrightarrow$ uncertainty of cross section :

$$\Delta\sigma_{calc}(E_i) = \left[\left(\frac{\partial\sigma_{calc}(E_i)}{\partial p_1}\Delta p_1\right)^2 + \left(\frac{\partial\sigma_{calc}(E_i)}{\partial p_2}\Delta p_2\right)^2 + \ldots + \left(\frac{\partial\sigma_{calc}(E_i)}{\partial p_n}\Delta p_n\right)^2\right]$$

whereby the quantities $\frac{\partial\sigma_{calc}(E_i)}{\partial p_k}\Delta p_k$ will in general be derived from the changes in cross sections if all parameters except p_k are kept fixed and only the parameter p_k in question is changed by the estimated amount Δp_k from its most probable value

uncertainties of the calculated cross section values for different energies are correlated to a high degree due to the fact that most parameter changes result in an increase or decrease of the whole excitation function

from the above formula rather large $\Delta\sigma_{calc}$ result, if one uses for Δp_m the uncertainties of the parameters without considering that there is the additional constraint of reproducing exp. cross sections

if at least in a small energy region (usually 14-15 MeV) very accurate experimental data exist, from the condition that the changes in the calcd. XS at this energy due to variations of the parameters shall be at most equal to $\Delta\sigma_{exp}$

smaller values for the Δp_m can be determined, from which smaller uncertainties of the whole calcd. excitation function result.

Description of correlations by means of covariance matrices, see:

F. Perey, Proc. Int. Conf. Nuclear Data for Reactors and Other Applied Purposes, Harwell (1978)

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Practical part: Description of the problems treated in the workshops

1) Optical model calculations for ^{48}Ti+n

Spherical optical model calculations by means of the code ABACUS were performed using the potentials by

J. Rapaport, Phys. Repts. 87 (1982) 25 and

E.D. Arthur, P.G. Young, Rept. LA-8626-MS.

As both these potentials differ from what is provided for in ABACUS with respect to energy or radial dependence, an existing computer program for ABACUS input construction was modified so as to handle these potentials. The resulting s-wave strength function, total cross section and differential elastic cross section at 2.9 MeV were compared to experimental data by the following authors:

Quantity	Energy	Reference
S_o	2.7 - 300 keV	Allen et al., Exfor 30359.017
S_o,R'	17.6 - 270 keV	BNL-325
σ_{total}	.389 MeV	Bowman et al., Exfor 11600.012
σ_{total}	14.2 MeV	Djumin et al., Exfor 40149.004
$\frac{\partial\sigma_{el}}{\partial\Omega}$	2.9 MeV	Pasechnik et al., Exfor 40045.002

The sensitivity of the results to variations in the depths of real and imaginary potential was studied by means of the parameter scan option of ABACUS. As both potentials were found to reproduce the experimental data reasonably although they had been determined for slightly heavier nuclei and, in the case of the Rapaport potential, for energies above 7 MeV only, they were also used to prepare neutron transmission coefficients for the statistical model calculations.

2) Calculation of transmission coefficients for ^{48}Sc+p and ^{45}Ca+α .

For the ^{48}Ti+n statistical model calculations, charged particle transmission coefficients were generated using the code ABACUS. For each particle type, two different potentials were used, namely

for protons:

G.S. Mani et al., Rept. C.E.A.-2379 (1963)

F.G. Perey, Phys. Rev. 131 (1962) 745

for α-particles:

J.R. Huizenga et al., Rept. ANL-6373 (1961)

O.F. Lemos, Orsay Rept., Series A, No. 136 (1972)

Also for these calculations, some programming work regarding input construction was necessary.

3) Statistical model calculations for ^{48}Ti+n

Input data for the code STAPRE were prepared for the reactions (n,2n), (n,p), (n,α), (n,np), (n,nα) on ^{48}Ti. During the input preparation the use of various compilations of parameters necessary for STAPRE calculations was demonstrated and the models into which these parameters enter were repeated. The above reactions were chosen in order to be able to study the effect of parameter variations on all competing decay modes of the intermediate nuclei ^{49}Ti, ^{48}Ti simultaneously and to compare the calculations with the following experimental data:

Quantity	Energy	Reference
(n,α)XS	14.1 MeV	Yu Wen Yu et al., Exfor 11583.003
(n,p)XS	14.5 MeV	E.B. Paul et al., Exfor 11274.026
- " -	12.7-17 MeV	F. Gabbard et al., Exfor 11494.006
- " -	14.5 MeV	M. Hillman, Exfor 11610.004
- " -	14.7 MeV	D. Crumpton, Exfor 20931.005
- " -	5.8-14.1 MeV	M.T. Swinhoe et al., Exfor 20986.005
- " -	14.8 MeV	R. Prasad et al., Exfor 30336.011
- " -	14.7 MeV	V.K. Tikku et al., Exfor 30394.003
(n,np)XS	14.7 MeV	S. Qaim et al., CINDA Suppl. 78
α production spectrum, p production spectrum	15 MeV	S. Grimes et al., Nucl. Sci. Eng. 62 (1977) 187

The calculations were performed with the various sets of transmission coefficients described in 1) and 2). During the level density parameter variations which were necessary for improving the agreement of the calculations with the (n,α) and (n,p) cross sections, a method for checking the compatibility of the varied

parameters with experimental level information was practiced. The 2nd chance charged particle emission cross sections could not be calculated during the course time, and therefore the comparison of the production spectra could not be performed but advice was given for this kind of investigation.

4) Optical model calculations for $^{238}U+n$

Coupled channels optical model calculations were performed with the code IUPITOR, using potentials determined by:

V.A. Konshin, Proc. Winter Course Nucl. Theory for Applications, Trieste, 1980, IAEA-SMR-68/I(1981) 139

A. Prince, International Nucl. Model Codes Comparison Study, NEANDC 128 "U"

The results were compared to the experimental total and elastic cross sections given in "Compilation of Actinide Neutron Nuclear Data", NEANDC(OR) 153/L and the experimental strength functions mentioned in J.P. Delaroche et al., Proc. Consultants Meeting on Nucl. Theory for Neutron Nuclear Data Evaluation, Trieste, 1975, IAEA-190 (1976) 251. Special investigation was devoted to the dependence of the strength functions on the number of states coupled virtually to the ground state. As the reproduction of the available experimental data by the calculations with the Konshin potential was satisfactory, neutron transmission coefficients were created with this potential and processed for use in the code STAPRE.

5) Statistical model calculations for $^{238}U+n$

As time was not sufficient for the statistical model part of the ^{238}U sample evaluation, recommendations regarding options and parameter values for the STAPRE input to be prepared were left to the participants in written form, together with a graphic representation of experimental excitation functions for (n,γ) and (n,f) on ^{238}U and their reproduction by STAPRE calculations performed by M. Uhl at the IRK (unpublished).