COULOMB EXCITATION DATA ANALYSIS CODE

GOSIA

T. CZOSNYKA*, D. CLINE and C.Y. WU

Nuclear Structure Research Laboratory, University of Rochester

Rochester, NY 14627, USA

* Permanent address: Heavy Ion Laboratory, Warsaw University

Banacha 4, 02-097 Warszawa, Poland

CONTENTS

INTRODUCTION

Coulomb excitation, understood as the nuclear excitation caused solely by the electromagnetic field acting between the colliding nuclei, is a powerful probe of collective nuclear structure. The main advantage of Coulomb excitation lies in the fact that, unlike the nuclear reactions, the interaction can be described by the known, well-established theory of electromagnetic processes, thus the internal structure can be studied in a model-independent way. Well below the Coulomb bareer short-ranged nuclear forces are negligible, while the long-ranged electromagnetic interaction still gives rise to a considerable excitation of the nuclear structure, notably to the excitation of nuclear levels resulting from the collective degrees of freedom. The recognition of Coulomb excitation as a method of studying collective (preeminently, but not only, quadrupole) motion in nuclei dates back to the early 1950's. The review paper by Cline [CLI86] contains a short summary of the early Coulomb excitation work, complete with the extensive list of references. Since then, Coulomb excitation with light-ion beams has been extensively exploited to measure the reduced excitation probabilities and quadrupole moments of the lowest excited states. The experiments performed using the light-ion beams can be easily interpreted because of the applicablity of first- and second order perturbation theory due to the fact that only one and two step excitation processes need to be taken into account (see e.g. the extensive discussion of the perturbation approach in [ALD75]). The situation changes dramatically when the heavy-ion beams, available from the newest generation of accelerators, are employed. Multiple Coulomb excitation, observed with such beams, populates many excited states (up to spin ≈ 30h in strongly deformed nuclei) producing an enormous amount of information concerning the electromagnetic structure of the nuclei. An adequate semiclassical theory of multiple Coulomb excitation has been developed in 1956 [ALD56], followed by the first multiple Coulomb excitation computer program COULEX (Winther, deBoer in [ALD66]). COULEX has provided the first opportunity to treat the

multiple Coulomb excitation quantatively, converting the assumed set of the reduced matrix elements of electromagnetic operators to the excitation amplitudes; thus making possible to test the model predictions. However, the ultimate goal of model-independent extraction of the electromagnetic structure parameters (reduced matrix elements) from the heavy-ion experiments could not be achieved until recently. The main difficulty lies in a number of reduced matrix elements influencing the heavy-ion excitation, more than a hundred when the heaviest beams are used on sufficiently deformed targets. In such a case one must first overdetermine the problem by collecting enough experimental data, what requires efficient data acquisition apparatus, then be able to reproduce the large set of data by fitting the matrix elements. An attempt to fully exploit the potential advantages of multiple Coulomb excitation has resulted in considerable development of both experimental methods and analysis software. The efficiency of data collection has been very much enhanced by the development of position sensitive, parallel plate avalanche counters (PPAC's). PPAC type counters make possible to reconstruct the kinematics of each scattering event at rates up to 10 MHz, thus, since Coulomb excitation is for a given beam/target combination a function of scattering angle, allow to conduct several "logical" experiments during a single accelerator run. Moreover, event-by-event kinematic reconstruction is used to correct for considerable Doppler shifts of observed γ energies, dramatically improving the quality of the γ-ray spectra. Ref. [VAR86] gives an example and some technical details of a PPAC system designed for the Coulomb excitation work. Further clarification of the complicated γ-ray spectra has been achieved by employing Compton-suppressed γ-ray germanium detectors.

Initially multiple Coulomb excitation data have been analysed by comparing these data with the results obtained with COULEX coupled to a γ-deexcitation program. The sets of matrix elements required as input data to COULEX were taken from model predictions and the conclusions were drawn based on better or worse agreement obtained. However, the results of such a model-dependent analyses were not conclusive, primarily due to the unknown sensitivity of the experimental data to assumed matrix elements and in some cases have proven to be incorrect. A model-independent analysis of multiple

Coulomb excitation data, using the formalism employed by COULEX, is not practical taken into consideration the numerical effort necessary for such a task, by far exceeding even the capability of the newest generation computers. To overcome this problem it is necessary to construct simple approximation to the Coulomb excitation formalism, accurate enough to determine a search strategy in a multidimensional space of the matrix elements parametrizing both excitation and decay processes. The development of such an approximation become the basis of the Rochester Coulomb excitation data analysis program, GOSIA, presented in this report.

GOSIA was originally developed at Nuclear Structure Research Laboratory of The University of Rochester in 1980 [CZ083] and has been, over next years, expanded and improved on a basis of the experience gained by the Rochester-Uppsala-Warsaw-Liverpool Coulomb excitation collaboration. A few revisions of the code have been done at NSRL to improve its efficiency and reliability and to accomodate the new technical developments. The latest version of GOSIA and the associated quadrupole sum rules program SIGMA are dated April 1991.

GOSIA is an experiment-oriented program. Although providing the possibility of running theoretical calculations (i.e. evaluation of excitation amplitudes and γ-decay yields for a given set of the matrix elements) it is primarily designed to perform a fit of the matrix elements to reproduce the large amount of experimental data. These data not only include the γ-yields observed in a number of independent experiments, but also available spectroscopic information, such as branching ratios, E2/M1 mixing ratios, nuclear level lifetimes and previously measured E2 matrix elements. All this information combined allow to uniquely determine the full set of matrix elements for an investigated nucleus together with the realistic estimate of the errors of the fitted matrix elements. Finally, using the associated quadrupole sum rules code, SIGMA, it is possible, on a basis of the results obtained with GOSIA, to evaluate, in a model-independent way, the expectaction values and the statistical distribution of the E2 moments, providing a clear insight into the collective properties of the nuclear states.

For a comprehensive summary of the Coulomb excitation analysis

methods it is necessary to provide some information about the algorithms used for this purpose. The effectiveness of data analysis is still very much dependent on the ability to choose the best ways of using the computer codes, such as GOSIA. Therefore we have decided to extend this report beyond the typical program write-up to make possible the most efficient utilization of the code. A short overview of the semiclassical Coulomb excitation formalism and the theory of subsequent decay of the excited nucleus is presented in Chapter I. The fast Coulomb excitation approximation, which is a basis of GOSIA, is described in Chapter II. Chapter III is a presentation of the numerical methods used, while Chapter IV contains the input instructions. The quadrupole sum rules and the description of the associated code SIGMA are contained in Chapter V. The details of the operations on the permanent files, created and used by GOSIA and SIGMA, are given in Chapter VI.

I. COULOMB EXCITATION AND GAMMA DECAY OF EXCITED NUCLEUS

The semiclassical theory of Coulomb excitation is exhaustively discussed in the Alder/Winther monograph of the subject [ALD75]. This fundamental work presents some alternative approaches to the formal description of electromagnetic excitation. Most of them, being valuable for better understanding the nature of the processes in question, are nevertheless not viable practically. Therefore, the following outline of Coulomb excitation theory is limited to the formalism being actually used in the code. Particularly, the differences between semiclassical and fully quantal descriptions will not be discussed. Concentrating on multiple excitation we will also pay less attention to widely used and known perturbation theories. Also, the presentation of deexcitation theory will strictly follow the formalism used in GOSIA.

I.1. SEMICLASSICAL THEORY OF COULOMB EXCITATION AND ITS APPLICABILITY

Pure Coulomb excitation, understood as exclusively electromagnetic interaction, occurs when the ranges of nuclear forces of both interacting nuclei are completely separated in space. Usually the condition is expressed as:

$$\eta = \frac{a}{2\lambda\!\!\!^{-}} = \frac{Z_1 Z_2 e^2}{\hbar v_I} \gg 1 \qquad 1.1$$

where a denotes the classical distance of closest approach, $\lambda\!\!\!^{-}$ is the reduced wavelength of incoming projectile with initial velocity v_I, $Z_1 e$ and $Z_2 e$ are charges of projectile and target. A convenient formula for maximum safe bombarding energy in head-on collisions was given by Cline [CLI69]

$$E_{max}\ (MeV) = 1.44\ \frac{A_1 + A_2}{A_2} \cdot \frac{Z_1\ Z_2}{1.25(A_1^{1/3}+A_2^{1/3})+5} \qquad 1.2$$

where index "1" denotes projectile, "2" is used for target (this convention will be used consequently). Criterion 1.2 corresponds to a separation of nuclear surfaces of about 5 fm.

Considerable simplification is achieved assuming classical treatment of two-body kinematics. A classical description of kinematics is justified if the size of the incoming projectile wavepacket is small compared to the dimensions of its trajectory, which is once more assured by the validity of 1.1. It is easily checked using 1.1 and 1.2, that heavy-ion induced Coulomb excitation yields values of η ranging from 10^2 to 10^3. Therefore, the validity of a classical description of the scattering kinematics is closely connected to the assumption of non-intervention of the nuclear forces; thus the semiclassical approach is applicable par excellence for all processes of pure electromagnetic nature.

The semiclassical approach is not able to take into account the modification of the trajectory due to the energy transfer. To the first order, an effect of energy transfer can be described by symmetrization of relevant excitation parameters, i.e. taking an average of these parameters corresponding to perturbed and unperturbed orbits (see below). More accurate determination of energy transfer effects is not possible, since in the classical kinematics picture it is not known at which point of the trajectory this transfer actually took place. Fortunately, in most cases the excitation energy in pure electromagnetic processes does not exceed a small fraction of total bombarding energy, so the first-order correction, introduced by a symmetrization procedure, is quite adequate. Further assumptions made concern the time separation of excitation and decay processes. The effective collision time is of order $10^{-19} \div 10^{-20}$ sec, being thus orders of magnitude shorter than mean lifetimes of nuclear states. This allows the excitation and γ decay to be treated sequentially. Finally, using the expansion of the electromagnetic interaction potential in a multipole series [BOH69] one can represent this potential as a sum of

three factors: monopole-monopole interaction, defining the kinematics only; mutual monopole-multipole interaction and mutual multipole-multipole interaction. The third term is weak compared to the monopole-multipole term and within desired accuracy can be neglected. This treatment yields a convenient separation of the Schrodinger equation, i.e., the excitation of both projectile and target can be independently expressed as:

$$ih\frac{\delta}{\delta t}|\psi_{1,2}\rangle = (H^{o}_{1,2} + V_{1,2}(\bar{r}(t)))\ |\psi_{1,2}\rangle \qquad 1.3$$

where $V_{1,2}(\bar{r}(t))$ stands for monopole-multipole interaction between projectile (multipole) and target (monopole) - indexed by 1 - or vice versa, indexed by 2. The monopole-monopole interaction determines the time-dependence of the potential by the classical trajectory $\bar{r}(t)$. As can be seen, target and projectile nuclei can be interchanged, therefore we will use indices 1 and 2 only where the distinction is necessary. To solve the time-dependent Schrodinger equation 1.3 we represent $|\psi(\bar{r},t)\rangle$ as a linear combinaton of free-nucleus wave functions $\phi(\bar{r})$, taken with time-dependent coefficients of the form:

$$|\psi(\bar{r},t)\rangle = \sum_n a_n(t)|\phi_n(\bar{r}\rangle \exp(-iE_n t/h) \qquad 1.4$$

with $$H^{o}|\phi_n\rangle = E_n|\phi_n\rangle$$

Substituting 1.4 to 1.3 one gets:

$$ih\sum_n \frac{da_n(t)}{dt}|\phi_n(\bar{r})\rangle\exp(-iE_n t/h) = \sum_n a_n(t)V(t)|\phi_n(\bar{r})\rangle\exp(-iE_n t/h) \qquad 1.5$$

Taking into account orthonormality of the free nucleus wavefunctions $|\phi_n\rangle$ ($\langle\phi_k|\phi_n\rangle = \delta_{kn}$) we finally obtain:

$$\frac{da_k(t)}{dt} = -\frac{i}{h}\sum_n a_n(t)\ \langle\phi_k|V(t)|\phi_n\rangle \exp\frac{it}{h}(E_k - E_n) \qquad 1.6$$

The system of differential equations 1.6 defines the complex expansion coefficients $a_k(t)$. Before collision, the nucleus is assumed to be in the ground state, thus the initial condition (corresponding to $t = -\infty$) can be expressed as $a_k = \delta_{k0}$, where index 0 stands for ground state. The nucleus after collision is then described by the set of excitation amplitudes $a_k(t = \infty)$, defining excitation probabilities. ($P_k = a_k a_k^*$, as follows from 1.4). As mentioned above, the interaction potential V(t) can be expanded into a multipole series:

$$V_{1,2}(t) = \sum_{i=1}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \frac{4\pi\, Z_{2,1} e}{2\lambda+1} (-1)^{\mu} S_{\lambda\mu}(t)\, M_{1,2}\,(\lambda,-\mu) \qquad 1.7$$

where $$S_{\lambda\mu}(t) = \frac{Y_{\lambda\mu}(\theta(t),\Phi(t))}{[r(t)]^{\lambda+1}} \qquad 1.8a.$$

for electric and

$$S_{\lambda\mu}(t) = \frac{1}{c\cdot\lambda} \frac{\frac{d\bar{r}}{dt} \cdot (\bar{r} \times \nabla)}{[r(t)]^{\lambda+1}} Y_{\lambda\mu}(\theta(t),\Phi(t)) \qquad 1.8b.$$

for magnetic excitation ($Y_{\lambda\mu}$ denotes standard normalized spherical harmonics). The symbol $M(\lambda,\mu)$ stands for electric and magnetic multipole moments, as defined e.g. in [BOH69] :

$$M(E\lambda,\mu) = \int \rho(\bar{r})\, r^{\lambda}\, Y_{\lambda\mu}(\theta,\Phi) d^3\bar{r} \qquad 1.9a$$

$$M(M\lambda,\mu) = \frac{1}{c(\lambda+1)} \int r^{\lambda}\, \bar{j}\,(\bar{r})\, (\bar{r} \times \nabla) Y_{\lambda\mu}(\theta,\Phi)\, d^3\bar{r} \qquad 1.9b$$

$\rho(\bar{r})$ and $\bar{j}(\bar{r})$ being spatial charge and current distributions of a free nucleus, respectively. Inserting 1.7 to 1.6 one obtains the parametrization of electromagnetic excitation by the matrix elements of multipole moment operators:

$$\frac{da_k(t)}{dt} = -i \frac{4\pi Z_{1,2} e}{h} \sum_n a_n(t) \exp \frac{it}{h} (E_k - E_n) \sum_{\lambda\mu} (-1)^{\mu} \qquad 1.10$$

$$\cdot S_{\lambda\mu}(t) \langle \Phi_k | M(\lambda, -\mu) | \Phi_n \rangle$$

To express the time-dependent functions $S_{\lambda\mu}(t)$ it is convenient to introduce a frame of coordinates with the z-axis along the symmetry axis of the incoming particle trajectory and y-axis in the trajectory plane defined in such a way that the incoming particle velocity component v_y is positive. The x-axis then is defined to form a right-handed cartesian system of coordinates (Fig. I.1).

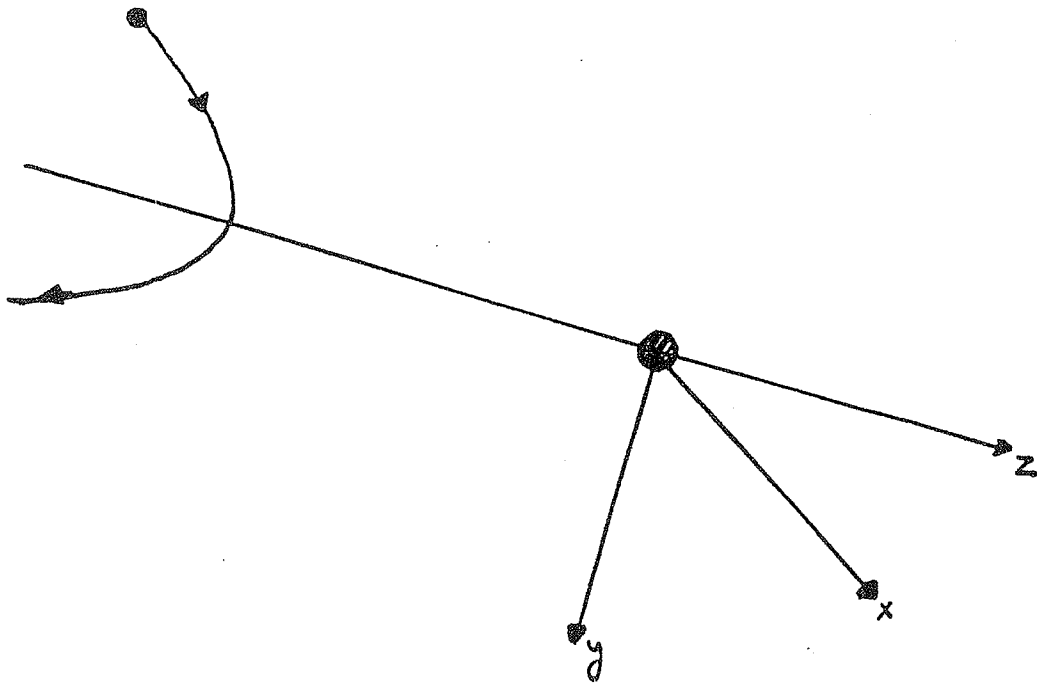


Fig. I.1 Coordinate system used to evaluate the Coulomb excitation amplitudes.

In this system of coordinates, one can describe relative two-body motion, treated as a classical Kepler problem, introducing two parameters ϵ and ω. The parameter ϵ, called the orbit eccentricity, is expressed by the center-of-mass scattering angle θ_{cm}:

$$\epsilon = \frac{1}{\sin\frac{\theta_{cm}}{2}} \qquad 1.11$$

The parameter ω, which replaces time, is given by:

$$t = \frac{a}{v}\,(\epsilon\sinh\omega + \omega) \qquad 1.12$$

where a is the distance of closest approach in a head-on collision. This parametrization yields the following expression for the length of the radius-vector $\bar{r}$:

$$r = a(\epsilon\cosh\omega + 1) \qquad 1.13$$

Explicitly, cartesian coordinates are expressed by ϵ and ω as:

$$\begin{aligned} x &= 0 \\ y &= a(\epsilon^2-1)^{1/2}\sinh\omega \\ z &= a(\cosh\omega + \epsilon) \end{aligned} \qquad 1.14$$

It is easily seen that the closest approach corresponds to $\omega=0$. The functions $S(t)$ are replaced by dimensionless "collision functions" $Q(\epsilon,\omega)$:

$$Q^E_{\lambda\mu}(\epsilon,\omega) = a^\lambda \frac{(2\lambda-1)!!}{(\lambda-1)!}\left(\frac{\pi}{2\lambda+1}\right)^{1/2} r(\omega) S^E_{\lambda\mu}(t(\omega)) \qquad 1.15a$$

for electric excitations, and

$$Q^{M}_{\lambda\mu}(\epsilon,\omega) = \frac{c}{v}\, a^{\lambda}\, \frac{(2\lambda-1)!!}{(\lambda-1)!}\, \left(\frac{\pi}{2\lambda+1}\right)^{1/2} r(\omega) S^{M}_{\lambda\mu}(t(\omega)) \qquad 1.15b$$

for magnetic excitations. In addition, it is convenient to replace the multipole operator matrix elements $\langle I_s M_s | M(\lambda,\mu) | I_f M_f \rangle$ by reduced matrix elements $\langle I_s || M(\lambda) || I_f \rangle$ using the Wigner-Eckart theorem:

$$\langle I_s M_s | M(\lambda,\mu) | I_f M_f \rangle = (-1)^{I_s - M_s} \begin{pmatrix} I_s & \lambda & I_f \\ -M_s & \mu & M_f \end{pmatrix} \langle I_s || M(\lambda) || I_f \rangle \qquad 1.16$$

It is also presumed that the phase convention for the wavefunctions $|I\rangle$ is such, that the reduced matrix elements are real. We also symmetrize the parameters a and v_I, averaging between elastic scattering values and the values resulting from decreasing the bombarding energy by the excitation energy. Insertion of 1.11 through 1.16 into 1.10, taking into account symmetrization, yields the final system of differential equations for the excitation amplitudes a_k (the following formulas are given already with numerical representation of physical constants, corresponding to energies in MeV, reduced electric multipole matrix elements in $eb^{1/2}$ and reduced magnetic multipole matrix elements in $\mu_n . b^{(1-1)/2}$, μ_n being the nuclear magneton):

$$\frac{da_k}{d\omega} = -i \sum_{\lambda\mu n} Q_{\lambda\mu}(\epsilon,\omega) \varsigma^{(\lambda\mu)}_{kn} \cdot \langle I_k || M(\lambda) || I_n \rangle \cdot \exp(i\xi_{kn}(\epsilon \sinh\omega + \omega)) \cdot a_n(\omega) \qquad 1.17a$$

The one-dimensional indexing of excitation amplitudes a_k involves all magnetic substates of states $|I\rangle$, which from a point of view of a theory of electromagnetic excitation are treated as independent states. The parameters ξ_{kn}, so called adiabaticity parameters, reflecting time fluctuations of nuclear wavefunctions are given by:

$$\xi_{kn} = \frac{Z_1 Z_2 \sqrt{A_1}}{6.34977} \{(E_p - sE_k)^{-1/2} - (E_p - sE_n)^{-1/2}\} \qquad 1.17b$$

$$s = (1 + A_1/A_2)$$

E_p being the bombarding energy. The above is valid for target excitation, while for projectile excitation indices 1 and 2 are to be interchanged. The same convention is valid for coupling parameters $\zeta_{kn}^{(\lambda\mu)}$ given by:

$$\zeta_{kn}^{(\lambda\mu)} = (2\lambda+1)^{1/2}(-1)^{I_n - M_n} \begin{pmatrix} I_n & \lambda & I_k \\ -M_n & \mu & M_k \end{pmatrix} \psi_{kn} \qquad 1.17c$$

$$\text{with} \quad \psi_{kn} = C_\lambda^{E(M)} \frac{Z_1 \sqrt{A_1}}{(sZ_1 Z_2)^\lambda} \{(E_p - sEk)(E_p - sEn)\}^{(2\lambda-1)/4} \qquad 1.17d$$

where the numerical coefficients $C_\lambda^{E(M)}$ are different for electric and magnetic excitation and are given explicitly as:

$$C_\lambda^E = 1.116547 . (13.889122)^\lambda \cdot \frac{(\lambda-1)!}{(2\lambda+1)!!}$$

$$C_\lambda^M = (v/c)\ C_\lambda^E/95.0981942 \qquad 1.17e$$

The explicit expressions for the collision functions $Q(\epsilon,\omega)$ for E1 to E6 and M1,M2 are compiled in Table I.1. As pointed out in Ref. [ALD75], Appendix J, one can account for the dipole polarization effect by modifying the collision functions corresponding to E2 type of excitation:

$$Q_{2\mu}(\epsilon,\omega) \rightarrow Q_{2\mu}(\epsilon,\omega) \cdot (1 - z\,\frac{a}{r}) \qquad 1.18a$$

where:

$$z = d \cdot \frac{E_p A_2}{Z_2^2\ (1 + A_1/A_2)} \qquad 1.18b$$

d being an adjustable empirical E1 polarization strength. A widely accepted value of d is .005 if the bombarding energy E_p is in MeV. From 1.13 follows:

$$\frac{a}{r} = \frac{1}{\epsilon \cosh\omega + 1} \qquad 1.18c$$

The useful symmetry properties of the Q's are the following:

$$Q_{\lambda\mu}(\epsilon,-\omega) = Q^{*}_{\lambda\mu}(\epsilon,\omega) \qquad 1.19$$

and, for electric excitation:

$$\begin{aligned} Q_{\lambda\mu}(\epsilon,\omega) &= Q_{\lambda-\mu}(\epsilon,\omega) \\ Q_{\lambda\mu}(\epsilon,-\omega) &= (-1)^{\mu} Q_{\lambda\mu}(\epsilon,\omega) \end{aligned} \qquad 1.20$$

while for magnetic excitation:

$$\begin{aligned} Q_{\lambda\mu}(\epsilon,\omega) &= -Q_{\lambda-\mu}(\epsilon,\omega) \\ Q_{\lambda\mu}(\epsilon,-\omega) &= (-1)^{\mu+1} Q_{\lambda\mu}(\epsilon,\omega) \end{aligned} \qquad 1.21$$

It should be noted, that for backscattering ($\theta_{cm} = 180°$; $\epsilon=1$) all electric Q's with $\mu\neq 0$ vanish, as well as all magnetic Q's; therefore the magnetic quantum number is conserved. This is physically understandable, since the process along the z-axis cannot change the magnetic quantum number. The conservation of magnetic quantum number, exactly true for backscattering, is approximately valid for an arbitrary scattering angle due to the dominance of electric collision functions with $\mu=0$. The backscattering is extremely important experimentally, providing the closest possible approach of the nuclei taking part in the excitation process and therefore providing the maximum information available from Coulomb excitation.

The coefficients ζ, which define coupling of the nuclear states, are dependent on Z,A and energy of the projectile. It is interesting to see the effect of using various beams on a given target, assuming the maximum safe bombarding energy of the projectile given by 1.2. Neglecting symmetrization, one gets from 1.2 and 1.17c:

$$\zeta \sim \left(\frac{Z_1 A_1 d}{s Z_2}\right)^{1/2} \left(\frac{1.44}{d}\right)^{\lambda} \qquad 1.22$$

$$d = 1.25\ (A_1^{1/3} + A_2^{1/3}) + 5$$

It can easily be seen, taking into account correlation of A_1 and Z_1, that the coupling coefficients ζ are almost directly proportional to the charge number of a projectile. Consequently, coming from lighter to heavier beams, one observes excitation of a growing number of levels, the number of matrix elements influencing the process increasing ever faster.

The parameter ξ, usually called the adiabaticity parameter, results from time oscillations of the nuclear eigenfunctions. The appreciable mutual excitation of nuclear levels is possible only when the relative oscillation of their eigenfunctions is slow on the scale of the effective collision time. This implies that the Coulomb excitation cross sections generally increase with decreasing ξ. Taking into account that the excitation energy is small compared to the bombarding energy, we can expand 1.17b in a series. This yields:

$$\xi_{kn} \sim \frac{E_n - E_k}{E_p \sqrt{E_p}} \qquad 1.23$$

It is easily seen that small level energy differences are preferable for Coulomb excitation. (Note the completely opposite behavior of deexcitation process). 1.23 also shows that increasing energy of the projectile enhances the Coulomb excitation not only because of increased coupling parameters ζ but also because of decreased values of ξ.

A convenient way to visualize the excitation process is to introduce so-called orbital integrals $R(\epsilon,\zeta)$, defined as:

$$R_{\lambda\mu}(\epsilon,\xi) = \int_{-\infty}^{\infty} Q_{\lambda\mu}(\epsilon,\omega)\ \exp\left(i\xi(\epsilon\sinh\omega+\omega)\right)\ d\omega \qquad 1.24$$

The quantities R directly determine the excitation amplitudes, provided the

applicability of the first-order perturbation approach. Generally, the formal solution of 1.17a can be expressed by an infinite integral series as:

$$\bar{a}\ (\omega=\infty) = \bar{a}_o + \{\int_{-\infty}^{\infty} A\ (\omega_o)d\omega_o\}\bar{a}_o + \{\int_{-\infty}^{\infty} A\ (\omega_1)d\omega_1 \int_{-\infty}^{\omega_1} A\ (\omega_o)d\omega_o\}\ \bar{a}_o +$$

$$\ldots + \{\int_{-\infty}^{\infty} A\ (\omega_n)d\omega_n \int_{-\infty}^{\omega_n} A\ (\omega_{n-1})d\omega_{n-1}\cdots\int_{-\infty}^{\omega_1} A\ (\omega_o)d\omega_o)\}\ \bar{a}_o + \ldots \qquad 1.25$$

where $\bar{a}$ stands for the vector of the amplitudes and $A(\omega)$ is the right-hand side matrix operator of 1.17a. The initial vector $\bar{a}_o$ has the ground state amplitude equal to 1, all other components vanish. Each term of 1.25 corresponds to given order excitation, i.e., connects a number of matrix elements equal to the number of integrations. Assuming weak interaction, the first-order perturbation theory expresses the excitation amplitudes of the states k directly coupled to the ground state as the linear term of 1.25:

$$a_k = \sum_{\lambda} \zeta_{ko}^{(\lambda\mu)} \cdot R_{\lambda\mu}\ (\epsilon, \xi_{ko})\ \langle I_k||M(\lambda)||I_o\rangle \qquad 1.26$$

$$\mu = M_o - M_k$$

index "0" denoting the ground state. Note that 1.26 (and more general 1.17) Ais valid for a fixed polarization of a ground state, thus for non-zero ground state spin one must average the excitation amplitudes over all possible magnetic substates of the ground state. This explicitly means:

$$a_k = \frac{1}{(2I_o+1)^{1/2}} \sum_{m_o} a_k\ (m_o) \qquad 1.27$$

$$P_k = a_k a^*_k \qquad 1.28$$

where $a_k(m_o)$ denotes the excitation probability of state k with ground state polarization m_o. The formula 1.26 has been extensively used to determine reduced excitation probabilities:

$$B(\lambda, I_k \} \; I_f) = \frac{1}{2I_k+1} \langle I_k || M(\lambda) || I_f \rangle^2 \qquad 1.29$$

in all cases the one-step excitation assumption can apply. In addition to their direct applicability to weak Coulomb excitation processes, the orbital integrals R give some general idea about the relationships between different modes of excitation. As an example, Fig. I.2 shows the quadrupole orbital integrals R_{20} and $R_{2\pm1}$ as functions of ξ for θ_{cm}=180° (R_{20} reaches maximum, $R_{2\pm1}$ vanishes) and θ_{cm}=120° (optimum scattering angle for $\Delta m = \pm 1$ excitation).

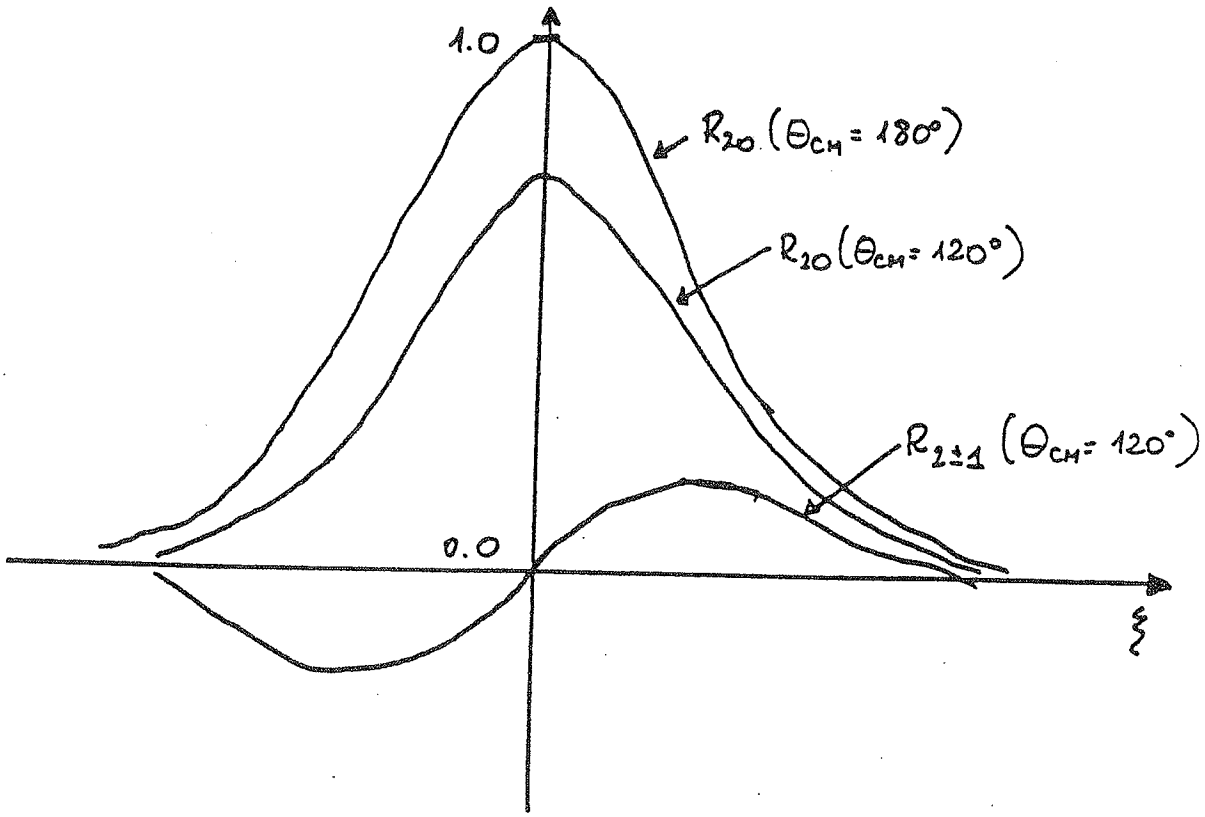


Fig. I.2 The orbital integrals R_{20} and $R_{2\pm1}$

The applicability of first and second order perturbation theories is limited to the light-ion induced Coulomb excitation, or, for heavy-ion beams, to beam

energies far below the safe bombarding energy. In case of a typical multiple Coulomb excitation experiment the system of differential equations 1.17 must be solved numerically. It is, for example, estimated that the excitation probability of the first excited 2^+ of ^{248}Cm bombarded with a 641 MeV ^{136}Xe beam is still sensitive to the excitation modes involving 30-th order products of the reduced matrix elements. This proves that the perturbation-type simplifications are generally not feasible. An efficient fast approximation to the Coulomb excitation problem is presented in Chapter II.

Table I.1

Electric and Magnetic Collision Functions $Q_{\lambda\mu}(\epsilon,\omega)$

$a=\cosh\omega+\epsilon \qquad b=\epsilon\cosh\omega+1 \qquad c=(\epsilon^2-1)^{1/2}\sinh\omega$

λ	μ	$Q^E_{\lambda\mu}(\epsilon,\omega)$
1	0	$\frac{1}{2}\cdot\frac{a}{b^2}$
1	±1	$-i\cdot\frac{1}{2\sqrt{2}}\frac{c}{b^2}$
2	0	$\frac{3}{4}\cdot\frac{2a^2-c^2}{b^4}$
2	±1	$-i\frac{3\sqrt{3}}{2\sqrt{2}}\cdot\frac{ac}{b^4}$
2	±2	$-\frac{3\sqrt{3}}{4\sqrt{2}}\frac{c^2}{b^4}$
3	0	$\frac{15}{8}\cdot\frac{a(2a^2-3c^2)}{b^6}$
3	±1	$-i\frac{15\sqrt{3}}{16}\cdot\frac{c(4a^2-c^2)}{B^6}$
3	±2	$-\frac{15\sqrt{15}}{8\sqrt{2}}\frac{ac^2}{b^6}$
3	±3	$i\frac{15\sqrt{5}}{16}\frac{c^3}{b^6}$
4	0	$\frac{35}{32}\frac{3a^4-24a^2c^2+3c^4}{b^8}$
4	±1	$-i\frac{35\sqrt{5}}{16}\frac{ac(4a^2-3c^2)}{b^8}$
4	±2	$-\frac{35\sqrt{5}}{16\sqrt{2}}\frac{c^2(6a^2-c^2)}{b^8}$
4	±3	$i\frac{35\sqrt{35}}{16}\frac{ac^3}{b^8}$
4	±4	$\frac{35\sqrt{35}}{32\sqrt{2}}\frac{c^4}{b^8}$

λ	μ	$Q^{E}_{\lambda\mu}(\epsilon,\omega)$
5	0	$\frac{3\sqrt{5}}{256}\,\frac{a[-14a^2(a^2+9c^2)+30a^4]}{b^{10}}$
5	±1	$-i\,\frac{315}{256}\sqrt{30}\cdot ca^2\,\frac{(-21c^2+8a^2)}{b^{10}}$
5	±2	$-\frac{315\sqrt{210}}{128}\,c^2a\,\frac{-3c^2+2a^2}{b^{10}}$
5	±3	$i\,\frac{315\sqrt{35}}{256}\,\frac{c^3(9a^2-b^2)}{b^{10}}$
5	±4	$\frac{945\sqrt{70}}{256}\,\frac{c^4a}{b^{10}}$
5	±5	$-i\,\frac{945\sqrt{7}}{256}\,\frac{c^5}{b^{10}}$
6	0	$\frac{963}{256}\cdot\frac{2\Delta a\,[-a^2(11c^2+46^2)+5b^4]-5b^6}{b^{12}}$
6	±1	$\frac{693\sqrt{42}}{512}\,\frac{ac[3a^2(-11c^2+b^2)+5b^4]}{b^{12}}$
6	±2	$-\frac{693\sqrt{105}}{512}\,\frac{c^2[3a^2(-11c^2+5b^2)+b^4]}{b^{12}}$
6	±3	$-i\,\frac{693\sqrt{105}}{256}\,\frac{ac^3(-11c^2+8b^2)}{b^{12}}$
6	±4	$\frac{2679\sqrt{14}}{512}\,\frac{c^4(11a^2-6^2)}{b^{12}}$
6	±5	$-i\,\frac{2079\sqrt{77}}{256}\,\frac{ac^5}{b^{12}}$
6	±6	$-\frac{693\sqrt{231}}{512}\,\frac{c^6}{b^{12}}$

λ	μ	$Q^{M}_{\lambda\mu}(\epsilon,\omega)$
1	0	0
1	± 1	$\mp \frac{\sqrt{2}}{4} (\epsilon^2-1)^{1/2} \frac{1}{b^2}$
2	0	0
2	± 1	$\mp \frac{3\sqrt{6}}{16} (\epsilon^2-1)^{1/2} \frac{a}{b^4}$
2	± 2	$-i \frac{3\sqrt{6}}{16} (\epsilon^2-1)^{1/2} \frac{c}{b^4}$

I.2 GAMMA DECAY FOLLOWING ELECTROMAGNETIC EXCITATION

The decay of a Coulomb-excited nucleus can be treated as completely separated in time from the excitation process. The initial condition for the decay can be described by a statistical tensor, expressing the state of polarization of the decaying level:

$$\rho_{k-\chi'}(I) = (2I+1)^{1/2} \sum_{MM'} (-1)^{I-m'} \begin{pmatrix} I & k & I \\ -M' & \chi & M \end{pmatrix} a^{*}_{IM'} a_{IM} \qquad 1.30$$

where we explicitly denote excitation amplitude of a substate $|\ IM\ >$ with two-dimensional indexing. Averaging 1.30 over all possible polarizations of a ground state we get:

$$\rho_{k\chi}(I) = \frac{(2I+1)^{1/2}}{2I_o+1} \sum_{M_o MM'} (-1)^{I-M'} \begin{pmatrix} I & k & I \\ -M' & \chi & M \end{pmatrix} a^{*}_{IM'}(M_o) a_{IM}(M_o) \qquad 1.31$$

It is easily seen that:

$$\rho_{oo}(I) = P_I \qquad 1.32$$

The angular distribution of gamma radiation can be expressed as (this is valid in an arbitrary coordinate frame with the origin at the decaying nucleus):

$$\frac{d^2\sigma}{d\Omega_p d\Omega_g} = \sigma_R(\theta_p) \frac{1}{2\gamma(I_1)\sqrt{\pi}} \sum_{\substack{k \text{ even} \\ \chi}} \rho^{*}_{k\chi}(I_1) \sum_{\lambda\lambda'} \delta_\lambda \delta^{*}_{\lambda'} F_k(\lambda\lambda' I_2 I_1) Y_{k\chi}(\theta_\gamma, \phi_\gamma) \qquad 1.33$$

Here $\sigma_R(\theta_p)$ denotes the scattering angle dependent Rutherford cross-section, $F_k(\lambda\lambda' I_2 I_1)$ are γ-γ correlation coefficients (as defined, e.g., in FRA65), $Y_{\kappa\chi}(\theta_\gamma, \phi_\gamma)$ are normalized spherical harmonics. The quantities δ_1 are the

$I_1 \to I_2$ transition amplitudes for multipolarity λ, related to the emission probability $\gamma(I_1)$ by:

$$\gamma(I_1) = \sum_{\lambda n} |\delta_\lambda(I_1 \to I_n)|^2 \qquad 1.34$$

An explicit form of $F_k(\lambda\lambda' I_2 I_1)$ can be expressed in terms of Wigner's 3-j and 6-j symbols

$$F_k(\lambda\lambda' I_2 I_1) = (-1)^{I_1+I_2-1} [(2k+1)(2I_1+1)(2\lambda+1)(2\lambda'+1)]^{1/2} \cdot \begin{pmatrix} \lambda & \lambda' & k \\ 1 & -1 & 0 \end{pmatrix} \begin{Bmatrix} \lambda & \lambda' & k \\ I_1 & I_1 & I_2 \end{Bmatrix} \qquad 1.35$$

while δ_1 is given by:

$$\delta_\lambda = i^{n(\lambda)} \frac{1}{(2\lambda+1)!!\, h^{\lambda+1}} \left(\frac{8\pi(\lambda+1)}{\lambda}\right)^{1/2} \left(\frac{E_\gamma}{c}\right)^{\lambda+1/2} \frac{\langle I_2 || E(M)\lambda || I \rangle}{(2I_1+1)^{1/2}} \qquad 1.36$$

$$n(\lambda) = \begin{cases} \lambda & \text{for } E\lambda \text{ transitions} \\ \lambda+1 & \text{for } M\lambda \text{ transitions} \end{cases}$$

The coordinate system used for evaluation of excitation probabilities is no longer convenient to determine angular distributions of gamma radiation, as it is not fixed with respect to the laboratory frame. Therefore, it is useful to define the z-axis along the beam direction with the x-axis in the plane of orbit in such a way, that the x-component of the impact parameter is positive. The y-axis is then defined to form a right-handed system (Fig. I.3)

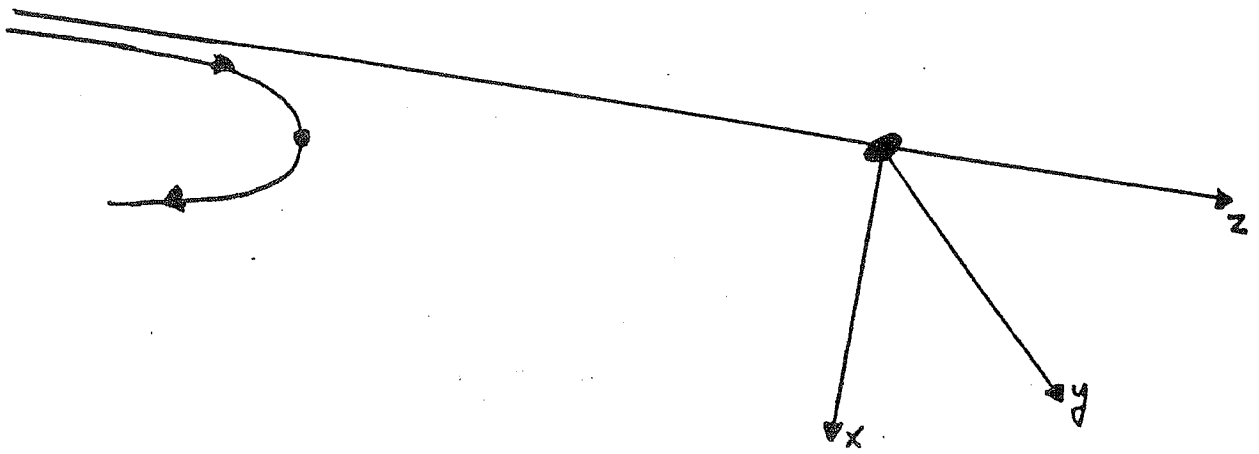


Fig. I.3 The coordinate system used to describe the γ-decay of a Coulomb-excited nucleus.

The statistical tensors ρ_{kx} in the new coordinate frame are obtained by rotation with Euler angles $(\pi/2,(\pi+\theta)/2,\pi)$:

$$\rho_{k\chi} \rightarrow \sum_{\chi'} \rho_{k\chi'} D^{k}_{\chi'\chi} \left(\frac{\pi}{2}, \frac{\pi+\theta}{2}, \pi\right) \qquad 1.37$$

the rotation functions $D^{k}_{xx'}(\alpha,\beta,\gamma)$ being defined according to [BOH69]:

$$D^{k}_{\chi\chi'}(\alpha,\beta,\gamma) = e^{i\chi\alpha}\, d^{k}_{\chi\chi'}(\beta)\, e^{i\chi'\gamma} \qquad 1.38$$

with:

$$d^{k}_{\chi\chi'}(\beta) = \left[\frac{(k+\chi')!\,(k-\chi')!}{(k+\chi)!\,(k-\chi)!}\right]^{1/2} \cdot \qquad 1.39$$

$$\sum_{m} \binom{k+\chi}{k-\chi'-m} \binom{k-\chi}{m} (-1)^{k-\chi'-m} \left[\cos\frac{\beta}{2}\right]^{2m+\chi+\chi'} \left[\sin\frac{\beta}{2}\right]^{2k-2m-\chi-\chi'}$$

Inserting 1.38 and 1.39 to 1.37 one obtains:

$$\rho_{k\chi} \rightarrow (-1)^{\chi} \cdot \sum_{\chi'} i^{\chi'} \, d^{k}_{\chi',\chi}\left(\frac{\pi+\theta}{2}\right) \rho_{k\chi'} \qquad 1.40$$

A complete description of the γ-decay should also involve the depolarization of the excited levels due to the hyperfine interaction, i.e. the interaction between the stripped electron shells and the nucleus. This effect can be taken into account by introducing the k-dependent attenuation coefficients, G_k, multiplying the statistical tensors (this approach is described in Section I.2.1). The attenuation of the angular distribution due to the hyperfine interactions is usually significant in case of thin-target experiments, while all the G_k's equal unity if the decaying nucleus has been stopped in the target prior to the γ decay. Introducing the decay statistical tensors, $R_{k\chi}$, one can shortly represent the basic formula 1.33, including the hyperfine interaction effect, as:

$$\frac{d^2\sigma}{d\Omega_p d\Omega_\gamma} = \sigma_R(\theta_p) \sum_{k\chi} R_{k\chi}(I,I_f) \, Y_{k\chi}(\theta_\gamma , \phi_\gamma) \qquad 1.41$$

where:

$$R_{k\chi}(I,I_f) = \frac{1}{2\gamma(I)\sqrt{\pi}} G_k \rho_{k\chi} \sum_{\lambda\lambda'} \delta_\lambda \delta^{*}_{\lambda'} F_k(\lambda\lambda' I_f I) \qquad 1.42$$

is the decay statistical tensor describing the mixed electric and magnetic transition from a state I to a state I_f. The Coulomb excitation statistical tensors are purely real for even values of k in the frame of coordinates introduced above, thus $\rho_{k\chi} = \rho^{*}_{k\chi}$. Moreover, taken into account the selection rules for electromagnetic transitions, it is easily seen that the products $\delta_\lambda \delta^{*}_{\lambda'}$ are also real. Consequently, the decay statistical tensors are purely real

The above formulas can directly be used to describe γ-decay of a level fed exclusively by Coulomb excitation. With multiple excitation, however, significant feeding from decay of higher-lying levels must be taken into account. The related modification of the statistical tensors can be

expressed as:

$$R_{k\chi}(I,I_f) \rightarrow R_{k\chi}(I,I_f) + \sum_n R_{k\chi}(I_n,I)\ H_k(I,I_n) \qquad 1.43$$

where the summation extends over all levels I_n directly feeding level I. The explicit formula for the H_k coefficients is:

$$H_k(I,I_n) = \frac{[(2I+1)(2I_n+1)]^{1/2}}{\gamma(I)} \sum_\lambda (-1)^{I+I_n+\lambda+k} |\delta_\lambda|^2 (1+c(\lambda)) \begin{Bmatrix} I & I & k \\ I_n & I_n & \lambda \end{Bmatrix} \qquad 1.44$$

where $c(\lambda)$ is the internal conversion coefficient of the $I_n \rightarrow I$ transition. Formula 1.44 is used to sequentially modify the deexcitation statistical tensors, starting from the highest non-negligible levels. This operation transforms the deexcitation statistical tensors, which, inserted into 1.41, define the unperturbed angular distributions following Coulomb excitation. One must however take into account experiment-related perturbations, namely the effects of the detection methods and relativistic corrections due to in-flight decay. These effects can be significant when using thin targets and heavy ion beams. An overview of the methods used in GOSIA to account for experimental perturbations is presented in the following subsections.

I.2.1 NUCLEAR DEORIENTATION EFFECT

In typical Coulomb excitation experiments, both projectile and target particles recoil into vacuum in highly excited ionic states which subsequently decay to a ground state. The fluctuating hyperfine fields cause the depolarization of the nuclear states, the effect known as nuclear deorientation effect. This in turn causes the attenuation of the angular distribution of the γ-rays which can be accounted for by introducing the spin and lifetime dependent attenuation coefficients G_k, multiplying the decay statistical tensors. The widely known Abragam and Pound theory [ABR53] has been extensively used to describe nuclear deorientation and is proven to work well in cases where the particles recoil into high-pressure gas. However, significant discrepancies from the Abragam and Pound model were detected for recoil into vacuum. We therefore use (with some modifications introduced) the two-state deorientation model ([BOS77], [BRE77]), which seem to correlate well existing data despite the far-reaching simplification enforced by the complexity of the problem.

Within the framework of the two-state model, the electrons may either belong to a "fluctuating" state while the excited electronic structure decays to the ground state or to a "static" state, corresponding to the equilibrium configuration. Since the excitation and decay of the stripped electron shells cannot be described exactly it is assumed that all the processes taking place in the fluctuating state are purely random. The rate of transition from fluctating to static state, Λ^*, is an adjustable parameter of the model. The time-dependent deorientation coefficients $G_k(t)$ are then given by :

$$G_k(t) = e^{-\Lambda^* t} G_k^{(\text{fluct.})}(t) + \int_0^t \Lambda^* G_k^{(\text{fluct.})}(t') \cdot e^{-\Lambda^* t'} G_k^{(\text{stat.})}(t-t')\,dt' \qquad 1.45$$

where (see [BOS77], [BRE77] and references therein for the details of the derivation):

$$G_k^{(stat.)}(t) = \langle a_k \rangle + (1-\langle a_k \rangle)e^{-\Gamma t} \qquad 1.46$$

with $\langle a_k \rangle$ given by:

$$\langle a_k \rangle = \sum_1 p(J_1) \cdot \sum_F \frac{(2F+1)^2}{2J_1+1} \begin{Bmatrix} F & F & k \\ I & I & J_1 \end{Bmatrix}^2 \qquad 1.47$$

F being the vector sum of the nuclear spin I and the electronic spin J_1. J_1 is the ground state spin of the deexcited atom, i.e. the ground state spin of an atom with the charge number equal to the charge number of the investigated nucleus less the number of stripped electrons. To determine the atomic ground state spins J_1 and their probabilities $p(J_1)$ we use the standard Nikolayev-Dmitriev stripping formula [NIK68]:

$$\begin{aligned} h &= \frac{1}{1+\left(\frac{.012008c}{v} Z^{.45}\right)^{5/3}} \\ Q_0 &= Zh^{0.6} \\ \sigma_Q &= (Q_0(1-h))^{1/2} \end{aligned} \qquad 1.48$$

where a Gaussian charge state distribution centered around Q_0 with the width σ_Q is assumed. Γ has the meaning of the width of the Larmor frequency distribution resulting from the assumption of many ionic ground states, as well as many long-lived excited atomic states, involved in the static part of the interaction. This distribution is assumed to be Lorentzian, with Γ treated as an adjustable parameter of the model. Fluctuating state attenuation factor $G^{(fluct.)}(t)$ is given by:

$$G_k^{(fluct.)} = (1-\lambda_k \tau_c)\exp(-\lambda_k t) \qquad 1.49$$

where τ_c is the mean time between random reorientations of the fluctuating hyperfine field and :

$$\lambda_k = \frac{1-\langle a_k \rangle}{\tau_c} \left(1-\exp\left(\frac{-\langle \omega^2 \rangle \tau_c^2}{1-\langle a_k \rangle}\right)\right) \qquad 1.50$$

with $\langle \omega^2 \rangle$ being an average Larmor frequency in the fluctuating state:

$$\langle \omega^2 \rangle = \frac{1}{3}k(k+1)\sum_{J_i} p(J_i)\frac{a^2(J_i)}{h^2}J_i(J_i+1) \qquad 1.51$$

Practically, the averaging over fluctuacting state atomic spins J_i in 1.51 is not possible since the spin distribution is not known. One must therefore use the single mean value of J_i, treated as one more model parameter. The parameter $a(J_i)$ is defined as:

$$a(J_i) = \mu_n g \frac{\bar{H}}{J_i} \qquad 1.52$$

where μ_n is the nuclear magneton and g stands for the gyromagnetic factor. The mean magnetic field $\bar{H}$ in fluctuating state is approximated as:

$$\bar{H} = KZ\left(\frac{v}{c}\right)^x \qquad 1.53$$

with both K and x being adjustable parameters.

The formula 1.49 is only valid, however, for t much larger than τ_c. Taking into account that τ_c is of the order of a few picoseconds, which is about a typical lifetime of the collective nuclear levels, and that we are interested in time-integral attenuation coefficients, we have to introduce a correction to 1.49 in the time range of τ_c. Since $G^{(fluct.)}(t)$ can also be easily derived for t→0, it is practical to introduce an interpolating function between time ranges t→0 and t much greater than τ_c, being chosen as a linear combination of two exponential time-decay functions which allow to keep the mathematics at the minimum. This procedure yields for the time-integral coefficients G_k:

$$G_k = \lambda_I \int_0^\infty G_k(t)\exp(-\lambda_I t)dt = G_k^{BS}[1+\frac{\lambda_k\tau_I(r-2p^2\tau_I\tau_c)}{(r+p\tau_I)(r+2p\tau_I)}] \qquad 1.54$$

where:

$$G_k^{BS} = \frac{1+\Lambda^*\tau_I(\frac{1+<a_k>\Gamma\tau_I}{1+\Gamma\tau_I})}{r} \qquad 1.55$$

is an original formula from [BOS77], $\tau_I = 1/\lambda_I$ is the mean lifetime of a nuclear state, while r and p are given by:

$$r = (\Lambda^*+\lambda_k)\tau_I+1 \qquad 1.56$$

$$p = \frac{(9\lambda_k^2+8\lambda_k\tau_c(<\omega^2>-\lambda_k^2))^{1/2}-3\lambda_k}{4\lambda_k\tau_c} \qquad 1.57$$

The correction to the original model in most cases does not exceed 10% and is easily evaluated since no additional parameters have been introduced. The recommended parameters of the nuclear deorientation model are listed in section IV.3, included in the description of the VAC switch of the CONT suboption.

I.2.2 RELATIVISTIC ANGULAR DISTRIBUTION CORRECTION

The coordinate system used to evaluate the angular distribution of the decay γ-rays, having the z-axis coincident with the laboratory-fixed beam direction, can easily be translated to the fixed laboratory system just by proper definition of the ϕ angle, taking care of the rotation of the x-y plane, dependent on the recoil velocity direction. This is true as long as the relativistic effects can be neglected and the tranformation from the decaying-nucleus-centered system to the laboratory system can be treated as Galilean. However, this assumption may not hold for heavy-beam, thin-target experiments. In this case the recoil velocity can reach up to 10% of the velocity of light, so that the transformation from the decaying nucleus centered system of coordinates to the laboratory system should be Lorentzian. The first order description of this effect is given in [ALD75] while an alternate approach, based on second-order Lorentz transformation of decay statistical tensors is presented in [LES71] and is actually used in GOSIA, fitting well the deexcitation formalism employed by the code. Denoting v_{recoil}/c as β and using RN for recoiling nucleus centered system with the z-axis defined by the recoil direction and LAB for the laboratory-fixed system we obtain, to second order in β:

$$\frac{dW^{LAB}(\theta,\phi)}{d\Omega_\gamma} = \{ (1-\beta^2)+\beta U+\frac{1}{2}\beta^2 V \} \frac{dW^{RN}(\theta,\phi)}{d\Omega_\gamma} \qquad 1.58$$

where the angular distribution W can shortly be written as:

$$\frac{dW^{RN}(\theta,\phi)}{d\Omega_\gamma} = \sum_{k_\chi \text{even}} a_{k\chi} Y_{k\chi}(\theta,\phi) \qquad 1.59$$

which is basically a short form of 1.33. It is assumed that the statistical tensors ρ_{kx} of 1.33 have been modified to account for the feeding from above

and the deorientation effect. Transformation of the a_{kx} tensor to the RN system is easily done using the rotation matrices $D^k_{xx'}$ (1.38). Operators U and V are defined as:

$$U = T + 2\cos(\theta) \qquad 1.60$$

$$V = T^2 + 4\cos(\theta)\cdot T + 6\cos^2(\theta) \qquad 1.61$$

where:

$$T = \frac{1}{2}\left[\sin(\theta)\ e^{-i\phi}\ L_+ - \sin(\theta)\ e^{i\phi}\ L_-\right] \qquad 1.62$$

L_+ and L_- being the raising and lowering operators for spherical harmonics:

$$L_+ Y_{k\chi} = \left[(k-\chi)(k+\chi+1)\right]^{1/2} Y_{k+1\ \chi} \qquad 1.63$$

$$L_- Y_{k\chi} = \left[(k+\chi)(k-\chi+1)\right]^{1/2} Y_{k-1\ \chi} \qquad 1.64$$

The transformation 1.58 changes the even-order spherical harmonics to the linear combinations of spherical harmonics. Therefore, the effect of the modification 1.58 on the angular distribution of γ-rays can be represented as a modification of ρ_{kx} tensors. Ordering the relativistic correction by the powers of β we can finally write:

$$\frac{dW^{LAB}(\theta,\phi)}{d\Omega_\gamma} = \frac{dW^{RN}(\theta,\phi)}{d\Omega_\gamma} + \beta \sum_{k\ odd} b_{k\chi} Y_{k\chi}(\theta,\phi) + \beta^2 \sum_{k\ even} b_{k\chi} Y_{k\chi}(\theta,\phi) \qquad 1.65$$

where the b_{kx} tensors result from 1.58 and are given by linear combinations of a_{kx} components. The result of 1.65 can be represented as modified statistical tensor and rotated back to the laboratory frame of coordinates. It should be noted that due to relativistic correction, terms involving odd-k spherical harmonics appear. The maximum k value is increased by 2. The relativistic correction formalism presented above results in an elegant modification of the decay statistical tensors and is used to the full extent in GOSIA despite the minor importance of some of the correction terms involved.

I.2.3. GAMMA DETECTOR SOLID ANGLE ATTENUATION FACTORS

Discussing the angular distribution of the γ-rays we have been so far concerned only with a well-defined direction of observation, given by the pair of angles (θ_g,ϕ_g). To reproduce an experiment one must, however, take into account the finite size of the γ detectors as well as the γ-ray absorption mechanism. A practical method to account for these effects has been suggested by Krane ([KRA72] and references therein). This method is applicable for the coaxial germanium detectors, almost exclusively used in the type of the experiments we are concerned with. The method of Krane introduces γ energy dependent attenuation factors, $Q_k(E_g)$, multiplying the final decay statistical tensors, defined as:

$$Q_k(E_g) = \frac{J_k(E_g)}{J_0(E_g)} \qquad 1.66$$

where:

$$J_k(E_g) = \int_0^{\alpha_{max}} P_k(\cos\alpha)K(\alpha)(1-\exp(-\tau(E_g)x(\alpha))\sin(\alpha)d\alpha \qquad 1.67$$

and α is the angle between the detector symmetry axis and the γ-ray direction, τ is an energy-dependent absorption coefficient of the active germanium layer and x stands for the angle-dependent path length in the detector. P_k are standard Legendre polynomials, while the function $K(\alpha)$ can be introduced to account for the effect of the γ-ray passing through the inactive, p-type core of the detector as well as the absorbers in front of a detector, commonly used to attenuate X-rays. $K(\alpha)$ can be written as:

$$K(\alpha) = \exp-(\sum_i \tau_i(E_g) x_i(\alpha)) \qquad 1.68$$

where the summation extends over various absorbers and the p-core. The Q_k factors, resulting from 1.66, have to be evaluated numerically. In order not to repeat this procedure for every γ energy of interest, it is practical to fit a simple analytic function describing the energy dependence, as discussed in section III.

To reprodce the experiment one should, in addition to the effects discussed in previous sections, include the integration of 1.33 over the particle detection range and, at least for the long-lived states include the correction due to in-flight decay, i.e. the time-dependent change in the angular position and the solid angle of a detector as seen by the decaying nucleus. These effects are treated numerically in GOSIA, the algorithms used being presented in Chapter III.

II. APPROXIMATE EVALUATION OF EXCITATION AMPLITUDES

Numerical integration of the system of differential equations 1.17, defining the excitation process, requires most of the computational effort needed to reproduce the experiment. Usually this takes 90-95% of the total computer time for each evaluation of the γ-yields following Coulomb excitation. Therefore, it is essential to replace the exact Coulomb excitation formalism by a fast and sufficiently accurate approximation in order to enable iterative fitting of matrix elements. To construct such an approximation, we first limit ourselves to the couplings $\Delta m=0$ and $\Delta m=\pm 1$ only (as pointed out in Chapter I, the strength of the interaction rapidly decreases with Δm) and we neglect the magnetic excitation. Denoting the ω-dependence of the right-hand side operator of 1.17a by $f_{lm}(\omega)$ we can rewrite the system of differential equations 1.17a as:

$$\frac{da_k}{d\omega} = \sum_{lmn} \zeta_{kn}^{(lm)} \cdot M_{kn}^{(l)} \cdot f_{lm}(\omega) a_n(\omega) \qquad 2.1$$

where $f_{lm}(\omega)$ is explicitly given as:

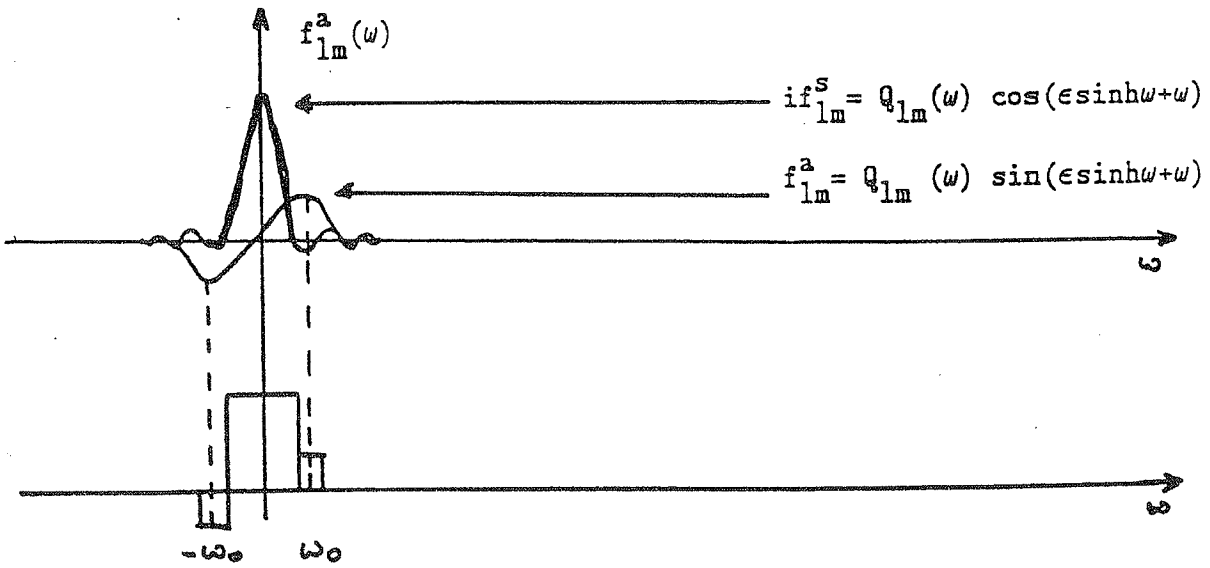
$$f_{lm}(\omega) = -iQ_{lm}(\omega)\exp[i(\epsilon\sinh\omega+\omega)] \qquad 2.2$$

where $M_{kn}^{(l)} = \langle k||E(M)\lambda||n\rangle$.

For both $m=0$ and $m=\pm 1$ the function $f_{lm}(\omega)$ can be expressed as a sum of two components, one antisymmetric in ω and real, the other symmetric in ω and imaginary:

$$f_{lm}(\omega) = f_{lm}^{a}(\omega) + if_{lm}^{s}(\omega) \qquad 2.3$$

These properties of the $f(\omega)$ function assure the unitarity of the right hand side operator of 2.1. Significant simplifications of the Coulomb excitation formalism can be achieved by replacing the ω-dependent functions by the constant effective interaction strengths extended only over finite ranges of ω. For most important $\Delta m=0$ couplings $f^{s}_{1m}(\omega)$ is localized around $\omega=0$, while $f^{a}_{1m}(\omega)$ is negligible anywhere except the vicinity of $\pm\omega_0$, ω_0 being case-dependent. Following this observation, one can approximate the total interaction by assuming the effective, constant interaction strengths covering three regions completely separated in ω - an antisymmetric part, extended over a finite ω range around some value of $\omega=-\omega_0$, a symmetric part around $\omega=0$, and the reflection of the antisymmetric part around $\omega=\omega_0$, as schematically presented below:



$\Delta m=\pm 1$ couplings can be treated in a similar way, although the separation of symmetric and antisymmetric components in ω is not as pronounced in this case. Nevertheless, taken into account the weakness of these couplings and their second-order importance, it is not worthwhile to construct more accurate approximation.

According to the above model, the system of differential equations describing the Coulomb excitation can be represented as three independent equations of the form:

$$\frac{d\bar{a}}{d\omega} = A_1^* \bar{a}(\omega) \; ; \quad \bar{a}_0 = a(\bar{-\omega}); \quad -\omega_1 \leq \omega \leq -2\omega_0+\omega_1$$

$$\frac{d\bar{a}}{d\omega} = i\, A_2^* \bar{a}(\omega); \; \bar{a}_0 = \bar{a}(-2\omega_0 + \omega_1); \quad -2\omega_0+\omega_1 < \omega \leq 2\omega_0-\omega_1 \qquad 2.4$$

$$\frac{d\bar{a}}{d\omega} = -A_1^* \bar{a}(\omega) \; ; \; \bar{a}_0 = \bar{a}(2\omega_0 - \omega_1); \quad 2\omega_0-\omega_1 < \omega \leq \omega_1$$

where the matrix operators A^* result from replacing the functions f_{lm} of 2.2 with effective constants over specified ranges. The sequential set of equations 2.4 has an obvious solution:

$$\bar{a}(\infty) = \exp(-A_1) \exp(-iA_2) \exp(A_1) \bar{a}(-\infty) \qquad 2.5$$

where the matrix operators A correspond to A^* in 2.4, differing only by appropriate scaling to eliminate the independent variable ranges from the final formula. The A matrices are purely real and fulfill the symmetry conditions:

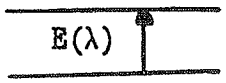
$$\begin{aligned} A_{1ki} &= -A_{1ik} \\ A_{2ki} &= A_{2ik} \end{aligned} \qquad 2.6$$

The relations 2.6, resulting from the symmetry properties of the reduced matrix elements and coupling coefficients ζ, assure the conservation of total excitation probability. The matrix elements of A can be explicitly written as:

$$\begin{aligned} A_{1ik} &= M_{ik}^{(l)} \cdot \zeta_{ik}^{(lm)} \cdot q_a^{(lm)} \\ A_{2ik} &= M_{ik}^{(l)} \cdot \zeta_{ik}^{(lm)} \cdot q_s^{(lm)} \end{aligned} \qquad 2.7$$

where $q_{alm}^{(\;)}$ and $q_{slm}^{(\;)}$ are effective strength parameters, replacing $f_{lm}^{(a)}(\omega)$

and $f_{lm}^{(s)}(\omega)$, respectively. These parameters are functions of ϵ and ξ, thus for a given experiment one needs to determine them as functions of ξ only, the excentricity ϵ assumed constant. The most flexible way of obtaining the q parameters is to extract them from the exact excitation calculation for a two-level system. Let us consider the simple case:



$$I^{\pi} = \lambda^{(-1)^{\lambda}}; \quad m=0$$
$$I^{\pi} = 0^{+}$$

with the reduced matrix element M connecting both levels. For this case, the A matrices are explicitly given as:

$$A_1 = \begin{pmatrix} 0 & -q_a^{(10)} M\zeta \\ q_a^{(10)} M\zeta & 0 \end{pmatrix}$$
$$A_2 = \begin{pmatrix} 0 & q_s^{(10)} M\zeta \\ q_s^{(10)} & 0 \end{pmatrix} \qquad 2.8$$

and, according to 2.5:

$$a(0^+) = \cos(q_s^{(\lambda 0)} M\zeta) + i\sin(q_s^{(\lambda 0)} M\zeta) \cdot \sin(2q_a^{(\lambda 0)} M\zeta)$$
$$a(I^{\pi}) = -i\sin(q_s^{(\lambda 0)} M\zeta) \cdot \cos(2q_a^{(\lambda 0)} M\zeta) \qquad 2.9$$

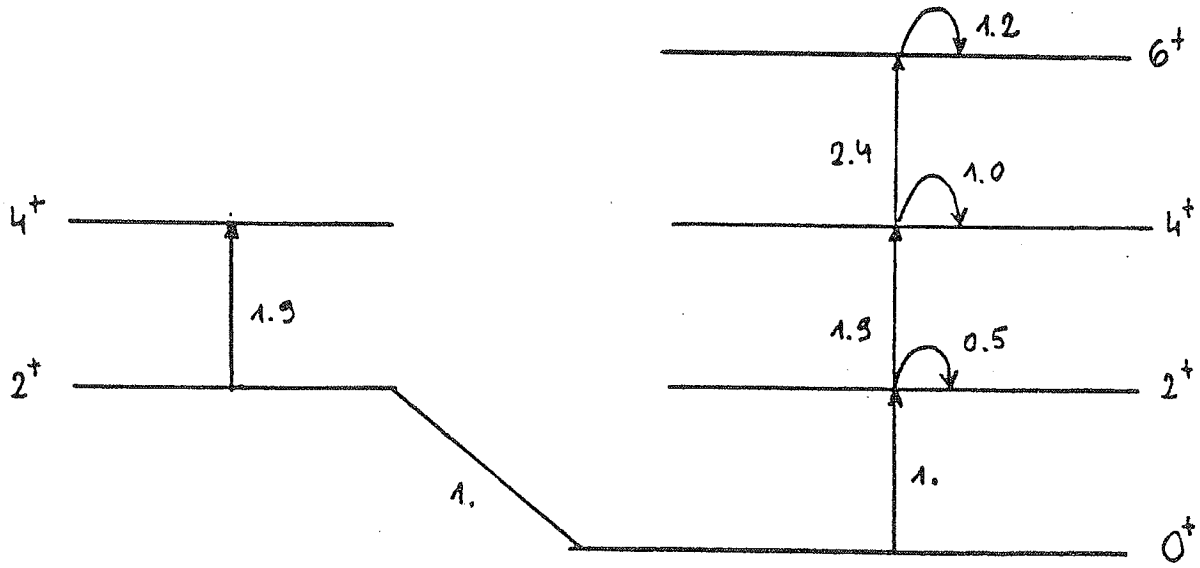
The above yields:

$$q_s^{(\lambda 0)} = \frac{\mathrm{Arccos}(\mathrm{Re}\ a(0^+))}{M\zeta}$$
$$q_a^{(\lambda 0)} = -\mathrm{arctg}\left(\frac{\mathrm{Im}\ a(0^+)}{\mathrm{Im}\ a(I^{\pi})}\right)/2M\zeta \qquad 2.10$$

Using 2.10 it is possible to extract q parameters substituting the excitation amplitudes resulting from the exact calculation, i.e. the solution of 1.17. A similar procedure can be applied to find the q

parameters corresponding to $\Delta m = \pm 1$ coupling.

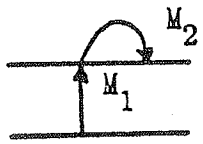
The approximate formula 2.5 works best in cases where the ξ-parameters range is not excessively wide. This practically assures good performance in all cases of multiple Coulomb excitation, since, as discussed in Chapter I, small values of ξ are required to enable multiple excitation. To demonstrate the reliability of the semianalytic approximation, let us consider the test case in which we simulate the Coulomb excitation of a Z=46, A=110 nucleus by a 200 MeV ^{58}Ni beam. The target nucleus is described by the level and coupling scheme (of course having nothing to do with the real ^{110}Pd):



level energy differences all equal to 0.5 MeV. All reduced E2 matrix elements are given in units of e.b. Comparison between the exact solution of Eq. 1.17 and the approximate solution using 2.5 is as follows:

Level	Excitation amplitude (Population)	
	1.17	2.5
0_1^+	.494 + .018i (.244)	.499 - .145i (.265)
2_1^+	.134 + .139i (.032)	.161 + .096i (.035)
4_1^+	-.205 + .391i (.194)	-.186 + .407i (.200)
6_1^+	-.176 + .388i (.145)	-.192 + .312i (.134)
2_2^+	.276 + .266i (.119)	.284 + .157i (.105)
4_2^+	-.482 - .165i (.260)	-.445 - .236i (.254)

The A matrix approximation is generally more than adequate to calculate derivatives of level populations with respect to the matrix elements, using internal correction factors (see chapter III) to account for differences between the approximate and the exact approach. It also provides a useful tool to investigate (at least qualitatively) the Coulomb excitation process. As an example, let us consider the influence of the quadrupole moment in the two-level system:



extensively discussed in the Alder-Winther monograph [ALD75]. To simplify the notation, let us denote:

$$q_s^{(20)}(0^+\to 2^+) \cdot M_1 \zeta^{(20)}_{0^+2^+} = q$$

$$q_a^{(20)}(0^+\to 2^+) \cdot M_1 \zeta^{(20)}_{0^+2^+} = q_1 \qquad 2.11$$

$$q_s^{(20)}(2^+\to 2^+) \cdot M_2 \zeta^{(20)}_{2^+2^+} = Q$$

Note that there is no antisymmetric component of the interaction for the quadrupole moment, since $\xi=0$.

The A matrices can then be written as:

$$A_1 = \begin{pmatrix} 0 & -q_1 \\ q_1 & 0 \end{pmatrix}$$

$$A_2 = \begin{pmatrix} 0 & q \\ q & Q \end{pmatrix} \qquad 2.12$$

yielding:

$$\exp(\pm A_1) = \begin{pmatrix} \cos q_1 & \mp \sin q_1 \\ \pm \sin q_1 & \cos q_1 \end{pmatrix} \qquad 2.13$$

$$\exp(-iA_2) = e^{iQ/2} \begin{pmatrix} \cos p - \frac{1}{2} i \frac{Q}{p} \sin p & -\frac{iq}{p} \sin p \\ -\frac{iq}{p} \sin p & \cos p + \frac{1}{2} i \frac{Q}{p} \sin p \end{pmatrix}$$

where $p = \frac{1}{2} (Q^2 + 4q^2)^{1/2}$

Using 2.5 one gets:

$$a_{2^+} = \frac{1}{2} i e^{iQ/2} \frac{\sin p}{p} (Q \sin 2q_1 - 2q \cos 2q_1) \qquad 2.14$$

which results in an excitation probability:

$$P_{2+} = \frac{1}{4} \frac{\sin^2 p}{p^2} (Q \sin 2q_1 - 2q \cos 2q_1) \qquad 2.15$$

The formula 2.15 is a generalization of the second-order perturbation theory result. Taking into account only the lowest order terms in q, q_1 and Q one gets:

$$P_{2+} \approx q^2 \left(1 - 2Q \cdot \frac{q_1}{q}\right) \qquad 2.16$$

as predicted by second-order perturbation theory. It should be observed, that the influence of the quadrupole moment is significant only if the ratio of antisymmetric to symmetric q parameters is high, which physically corresponds to a large value of ξ. As can be seen from 2.14, the primary effect of the static moment is rotation of the complex excitation amplitude, due to the exp(iQ/2) factor. This allows rather accurate measurements of static moments in cases of interferring paths of excitation, i.e., when a state is excited in a comparable way via two or more sequences of couplings. In the situation like that the phases the partial excitation amplitudes are summed with are of primary importance.

In general, 2.10 is only a semianalytical formula, since for complex cases exponents of A matrices must be evaluated numerically. Nevertheless, numerical determination of exp(A) operators is much faster than the integration of a system of differential equations. Application of the A matrix approximation for fitting of matrix elements to reproduce experimental data will be discussed in some more detail in Chapter III. It is also worth observing that the truncation of Taylor series approximating the exp(A) operators provides a way to generate perturbation theory of a given order, thus being useful to investigate weak excitation processes.

III. NUMERICAL METHODS

GOSIA is designed to perform various functions defined by the user-specified sequence of options. In a simplest mode GOSIA can be used to calculate the excitation probabilities, population of the levels and γ-decay statistical tensors 1.30, thus providing an equivalent of COULEX. Activating the γ-decay module of the code, one can extend this type of calculation to obtain the γ yields for a single value of bombarding energy and scattering angle, as well as perform the integration over the specified ranges of the bombarding energy (due to the projectile energy loss in a target) and of the projectile scattering angle to reproduce real experimental conditions. These calculations require an input set of matrix elements treated as fixed data. The main purpose of GOSIA is, however, to fit the matrix elements to reproduce available experimental data. GOSIA can handle simultaneously the experimental γ yields (up to 48000) observed in 50 independent experiments. Additional data, i.e. branching ratios (max. 50), lifetimes of the nuclear levels (max. 10), E2/M1 mixing ratios (max. 20) and previously measured E2 matrix elements (max. 30) may also be used. All these data and their experimental uncertainties are used to construct a least-squares statistic, usually called χ^2 or penalty function. The minimum of this statistic, treated as a function of matrix elements, defines the solution, while its distribution in a vicinity of the minimum determines the errors of fitted matrix elements. In the present version of the code, the investigated nucleus is described by maximum of 75 energy levels, with the number of magnetic substates not exceeding 600. The levels may be coupled with up to 500 matrix elements (E1 through E6 and M1, M2), any number of them allowed to be declared as the variables to be fitted.

As mentioned before, direct use of the full Coulomb excitation formalism to perform the minimization is out of question due to computer time necessary for repeated calculations. The mimimization can be accelerated using the approximation presented in Chapter II. Significant

amount of time can also be saved if the recoil-velocity correction (I.2.2) is neglected. The effect of both replacing the full excitation formalism by the matrix approximation and neglecting the relativistic correction is only weakly dependent on the matrix elements, therefore it is feasible to introduce the "correction factors", accounting for the differences between full and approximate calculations which are assumed to be independent of the fitted matrix elements. The minimization can thus be performed using only the fast, approximate formalism, with correction factors refreshed by running the full calculation only periodically. In addition, the Coulomb excitation approximation is only applied to $\Delta m=0$ and $\Delta m=\pm 1$ couplings, thus an effect of truncation of the number of magnetic substates being taken into account is also included in the correction factors, since it is not strongly dependent on the actual set of matrix elements.

Further acceleration of the fitting procedure is made possible by replacing the integration over experiment-dependent scattering angle and bombarding energy ranges with a single calculation of the Coulomb excitation induced γ yields assuming the mean values of these parameters. This approximation is also not explicitly dependent on the fitted matrix elements, thus the difference between the integration procedure and the result of using the mean values of bombarding energy and scattering angle can be accounted for by introducing another set of correction factors, treated as constants. Actually, it is convenient to apply this correction to the experimental yields, i.e. to rescale the experimental data according to the comparison of integrated and "mean" yields. This is initially done using a starting set of matrix elements and the resulting "corrected experimental yields" are subsequently used as the experimental values for fitting (this procedure is presented in detail in Section III.4). Thus, the fitting of matrix elements is performed using two levels of iteration - first, external, is to replace the experimental ranges of bombarding energy and scattering angle with the average values of these parameters, while second, internal, is the actual minimization of the least-squares statistic. After the convergence at the internal level is achieved, one should recalculate the correction to the experimental yields with the current set of matrix elements and repeat the minimization. Usually, for thin targets and not

excessively wide range of scattering angles, the second repetition of external iteration already yields negligible changes in the matrix elements found by the minimization. It has also been checked, that even if no particle coincidences were required only 2-3 recalculactions on the external level were necessary despite the integration over full solid angle.

Estimation of the errors of fitted matrix elements is a final step for the Coulomb excitation data analysis. This rather complicated procedure is discussed in Section III.6. A separate program, SELECT, has been written to reduce the considerable computational effort required for this task using the information obtained during minimization. This information, preprocessed by SELECT, is fed back to GOSIA. Optionally, the results of minimization and error runs can be used to evaluate quadrupole sum rules by a separate code SIGMA (Chapter V).

The extraction of the matrix elements from experimental data requires many runs of GOSIA. During these runs GOSIA creates and updates a number of disk files, containing the data needed to resume the analysis or to execute SELECT or SIGMA codes. The details of permanent file manipulation are presented in Chapter VI.

Relatively modest central memory requirements of GOSIA (about 1.5MB) are due to the sharing of the same memory locations by different variables when various options are executed and to replacing the straightforward multidimensional arrays (such as e.g. matrix elements) with catalogued vectors and associated logical modules. The description of the code given in this chapter will therefore not attempt to account for its internal organization, which is heavily dependent on the sequence of options executed and, in general, of no interest to the user. Instead, it will concentrate on the algorithms used and the logic employed in GOSIA. The basic knowledge of the algorithms is essential since the best methods of using the code are strongly case-dependent, so much freedom is left to the user to choose the most efficient configurations according to the current needs.

All three codes- GOSIA, SIGMA and SELECT- are written in the standard FORTRAN77 to make their implementation on various machines as easy as possible. The necessary modifications should only involve the output FORMAT statements, which are subject to some restrictions on different systems.

III.1 COULOMB EXCITATION AMPLITUDES AND STATISTICAL TENSORS

The state of a Coulomb excited nucleus is fully described by the set of excitation amplitudes, $a_{IM}(M_o)$, defined by the solution of Eq.1.17a at $\omega=\infty$, or, approximately, by the matrix expansion 2.5., used for minimization and error estimation. To set up the system of coupled-channel differential equations 1.17a one has first to define the level scheme of an excited nucleus. Certainly, from a practical point of view, the level scheme should be truncated according to the experimental conditions in such a way that reasonable accuracy of the excitation amplitudes of the observed states is obtained with a minimum of the levels included in the calculation. As a rule of thumb, two levels above the highest observed state in each collective band should be taken into account to reproduce a given experiment reliably. Truncation of the level scheme at the last observed level leads to an overestimation of the excitation probability of this level due to the structure of the coupled-channels system 1.17a, while by including additional levels above, even if their position is only approximately known, it is possible to eliminate this effect.

The solution to the coupled-channels system 1.17a should, in principle, involve all magnetic substates of a given state $|I\rangle$, treated as independent states within a framework of the Coulomb excitation formalism. However, due to the approximate conservation of the magnetic quantum number in the coordinate system used to evaluate the Coulomb excitation amplitudes (as discussed in Chapter I) it is practical to limit the number of the magnetic substates taken into account for each polarization of the ground state, M_o. In any case the excitation process follows the "main excitation path", defined as a set of magnetic substates having the magnetic quantum number equal to M_o, the remaining magnetic substates being of less and less importance as the difference between their magnetic quantum number and M_o increases. Relative influence of the excitation of magnetic substates outside the main excitation path is experiment-dependent, therefore GOSIA

allows the user to define the number of magnetic substates to be taken into account separately for each experiment. This choice should be based on the requested accuracy related to the quality of the experimental data, keeping in mind that reasonable truncation of the number of the magnetic substates involved in Coulomb excitation calculations directly reduces the size of the coupled channels problem to be solved.

The integration of the coupled differential equations 1.17a should be in theory carried over the infinite range of ω, which, practically, must be replaced with a finite range wide enough to assure the desired accuracy of the numerical solution. To relate the effect of truncating the ω-range to the maximum relative error of the absolute values of the excitation amplitudes, a_c, we use the criterion:

$$\frac{1}{4}\,\frac{\int_{-\infty}^{\infty} Q_{\lambda 0}(\epsilon=1,\omega)\,d\omega - \int_{-\omega_{max}}^{\omega_{max}} Q_{\lambda 0}(\epsilon=1,\omega)\,d\omega}{\int_{-\infty}^{\infty} Q_{\lambda 0}(\epsilon=1,\omega)\,d\omega} \leq a_c \qquad 3.1$$

where, as a worst case, we take into account the backscattering geometry ($\epsilon=1$), thus $\Delta m \neq 0$ couplings vanish for the electric excitations (there is no magnetic excitation for backscattering, as discussed in Chapter I, moreover, the magnetic excitation is weak enough to be neglected at the excitation stage for any scattering angle, therefore we will limit ourselves to the electric excitation only). Factor 1/4 is introduced in 3.1 to account for the further decrease of the importance of the excitation taking place at large $|\omega|$ due to the high-frequency oscillation introduced by the exponential term of 1.17a. Using the normalization property of the collision functions:

$$\int_{-\infty}^{\infty} Q_{\lambda\mu}(\epsilon=1,\omega)\,d\omega = 1 \qquad 3.2$$

and the asymptotic, pure exponential form of collision functions for large $|\nu|$ one finally gets:

$$\omega^{max} \geq \alpha_\lambda - \frac{1}{\lambda} \ln a_c \qquad 3.3$$

where the values of α_1 can easily be found from the asymptotic form of the collision functions and are given in a table below, together with the resulting ω^{max} assuming $a_c=10^{-5}$ which is the default value in GOSIA.

Table III.1

Multipolarity	α_1	ω^{max} for $a_c=10^{-5}$
E1	-.693	10.82
E2	.203	5.96
E3	.536	4.37
E4	.716	3.59
E5	.829	3.13
E6	.962	2.88

The range of integration over ω corresponding to a given accuracy level decrease, as can be seen in Table III.1, with multipolarity. Following this observation, the coupling between energy levels corresponding to a given multipolarity is being included in GOSIA only within the integration range

assigned to this multipolarity, which is a time-saving feature in cases many multipolarities have to be included. For Mλ couplings, neglected so far, the integration ranges have been set according to :

$$\omega^{max}(M\lambda) = \omega^{max}(E(\lambda+1)) \qquad 3.4$$

The actual integration of the coupled-channel system of differential equations 1.17a is performed in GOSIA using the Adams-Moulton predictor-corrector method. According to this algorithm, first the predicted solution at $\omega+4\Delta\omega$, based on a knowledge of the solution at $\omega+3\Delta\omega$ and the derivatives at four points, ω, $\omega+\Delta\omega$, $\omega+2\Delta\omega$ and $\omega+3\Delta\omega$ is found using:

$$\bar{a}(\omega+4\Delta\omega) = \bar{a}(\omega+3\Delta\omega)+\frac{\Delta\omega}{24}\{55\dot{\bar{a}}(\omega+3\Delta\omega)-59\dot{\bar{a}}(\omega+\Delta\omega)+37\dot{\bar{a}}(\omega+\Delta\omega)-9\dot{\bar{a}}(\omega)\} \qquad 3.5$$

and then corrected by:

$$\bar{a}(\omega+4\Delta\omega) = \bar{a}(\omega+6\Delta\omega)+\frac{\Delta\omega}{24}\{9\dot{\bar{a}}(\omega+4\Delta\omega)+19\dot{\bar{a}}(\omega+3\Delta\omega)-5\dot{\bar{a}}(\omega+2\Delta\omega)+\dot{\bar{a}}(\omega+\Delta\omega)\} \qquad 3.6$$

where the excitation amplitudes are once again treated as a vector and a dot symbolically denotes the differentiation with respect to ω. The predicted solution is used to obtain the derivatives defined by the right-hand side of 1.17a at $\omega+4\Delta\omega$, employed to evaluate the corrector 3.6. Stepsize, $\Delta\omega$, is controlled on a basis of the comparison of the predicted and corrected solutions. The accuracy test parameter, d, is defined as 1/14 of the absolute value of the maximum difference between predicted and corrected excitation amplitudes at a current value of ω. Stepsize is then halved if $d \geq a_c$ or doubled if $d \leq a_c/50$. This procedure assures the adjustment of the stepsize according to the strength of the interaction and is performed every n steps, n being an adjustable parameter defined by the user (n=1 used in GOSIA as a default). The Adams-Moulton integration algorithm with stepsize

control is usually faster than Runge-Kutta type methods, thus it has been employed in GOSIA despite some drawbacks. The most important one is when the interaction, defined by the left-hand side of 1.17a, is weak in most of the integration range, peaking only around some value of the independent variable. In this case the stepsize will be subsequently doubled and can become excessively large when the strong interaction region is reached, consequently, even though the loss of accuracy is detected, the overall accuracy of integration would be already irretrievably lost. This situation actually happens for the light ion excitation or, generally, at small scattering angles and can be detected by checking the sum of excitation probabilities provided in the output of GOSIA. The recommended procedure if the sum of probabilities differs significantly from unity is to switch off the stepsize control for a given experiment using the INT switch of CONT suboption (see IV.3) rather than decrease the accuracy parameter a_c. This is due to the fact that GOSIA uses the table of Q_{lm} functions and hiperbolic functions with a tabulation step $\Delta\omega$=.03 which defines the minimum stepsize of the integration independent of the accuracy requested, allowing to obtain the highest accuracy approximately corresponding to $a_c=10^{-6}$. Moreover, changing the requested accuracy a_c may not solve the stepsize control problem, but result only in extending the integration range, thus rather making this problem more likely to occur.

An another drawback of the Adams-Moulton method compared to the Runge-Kutta algorithms is that Adams-Moulton algorithm is not self-starting, requiring the initial solutions at four points. This problem can be overcame by employing the Runge-Kutta algorithm to provide the starting values, then switching to the more efficient Adams-Moulton method (note that the same procedure is to be applied when the stepsize is changed, since restarting the integration with different stepsize require the knowledge of the solution at new independent parameter intervals). The Runge-Kutta integration algorithm has been actually used in COULEX to provide the starting solution for both the initialization of the integration and the changes of stepsize. In GOSIA the starting solutions are found from a first-order perturbation approach, valid at large values of ω, using the asymptotic form of the collision functions. It is assumed, that the ground

state is connected to at least one excited state with E1,M1 or E2 matrix element. The initial excitation amplitudes can then be found as the combinations of trigonometric and integral-trigonometric functions, the latter being evaluated using rational approximation (given for example in [ABR72]). To fully eliminate switching to the Runge-Kutta algorithm, the new starting values when changing the stepsize are evaluated using backward interpolation. This procedure is reliable enough to assure reasonable accuracy while considerably speeding up the integration.

The integration of the system 1.17a should be in principle repeated for each possible polarization of the ground state, M_o. However, the reflection symmetry in the plane of the orbit yields in the coordinate system used to evaluate the excitation amplitudes:

$$a_{Im}(M_0) = (-1)^{\Delta\pi+I_0-I} a_{I\ -m}(-M_0) \qquad 3.7$$

where $\Delta\pi=0$ if there is no parity change between the ground state and a given excited state $|\ I\rangle$ and $\Delta\pi=1$ otherwise. Using the symmetry relation 3.7 one has only to solve the coupled-channel system 1.17a for the ground state polarizations $M_o \leq 0$, the solution of the coupled-channel system for $M_o \geq 0$ being defined by the relation 3.7. As mentioned before, due to the approximate conservation of the magnetic quantum number in the frame of coordinates used, one practically has to take into account only a limited subset of magnetic substates beyond the main excitation path. This explicitly means that if n magnetic substates have been specified by the user to be included in the Coulomb excitation calculation then for each excited state, I, and ground state polarization, M_o, GOSIA will catalog the magnetic substates according to the inequality:

$$\min(I,-M_0+n) \geq m \geq \max(-I,-M_0-n) \qquad 3.8$$

which, by virtue of 3.7, defines simultaneously a set of excitation amplitudes obtained with the inverse polarization of the ground state in a range given by:

$$\max(-I, M_0-n) \leq m \leq \min(I, M_0+n) \qquad 3.9$$

allowing for the summation of excitation amplitudes to form a statistical tensor defined by 1.31 for $+M_0$ and $-M_0$ at the same time.

A special simplification of the solution of 1.17a occurs for the ground state spin equal to 0 (even-even nuclei). In this case only $m \leq 0$ substates are explicitly included for numerical integration, the values of the excitation amplitudes and their derivatives for $m>0$ substituted during the integration using 3.7. Therefore, a separate setup of the system of coupled-channels equations 1.17a is constructed by GOSIA for even-even nuclei, resulting in the appreciable increase of the speed of the integration if $I_0=0$.

The statistical tensors ρ_{kx} are first evaluated according to 1.31 in the coordinate system used to calculate the excitation amplitudes, then rotated to a new system, more convenient to describe the γ-deexcitation, as discussed in Chapter I. This transformation is done using the rotation matrices according to 1.40. Rotated statistical tensors are treated as an interface between the Coulomb excitation and γ-deexcitation modules of the code, providing the complete information needed to calculate the γ-decay. These tensors can be either calculated using the full Coulomb excitation formalism or using the fast matrix approximation.

III.2 APPROXIMATE EVALUATION OF THE COULOMB EXCITATION AMPLITUDES

The matrix approximation 2.5 is used in GOSIA to evaluate the Coulomb excitation amplitudes within the minimization and error estimation modules. The level and matrix elements scheme used for this procedure is identical to that employed for the full calculation , as presented in III.1, with two exceptions. First, the number of magnetic substates taken into account beyond the main excitation path, n, can only assume values of 0 or 1. Second, only E1 through E4 multipolarities are used to construct the matrix approximation, which practically means that E5 and E6 matrix elements can not be fitted, being only included in full excitation formalism to satisfy the possible theoretical interest (although not foreseeable in a near future). The only additional information needed is the knowledge of the effective strength parameters, q_a and q_s, as introduced in the formula 2.7. The effective strength parameters depend on the experimental conditions as well as on the energy difference of the levels coupled by a given matrix element, thus, in principle, should be assigned to every matrix element independently for each experiment. However, from a point of view of the memory requirements, this approach is not feasible, therefore it has been chosen to create the maps of q parameters at the discrete ξ points for every experiment and to obtain the actual parameters using the linear interpolation. The q parameters should be independent of the coupling strength ζ (1.17c) if the model were perfect, but practically some weak ζ dependence is still present. A significant improvement of the matrix approximation accuracy can thus be obtained by including the first-order ζ-dependence correction for the prevailing $\Delta m=0$ couplings, which is equivalent to define the q-parameters as:

$$q(\Delta m=0;\xi,\zeta) = a(\xi)M\zeta + b(\xi) \qquad 3.10$$

where M symbolically stands for a matrix element associated with a given coupling. The q parameters for $\Delta m=\pm 1$ couplings are still treated as the functions of ξ only, the possible improvement of the approximation introduced by the ζ-dependence correction being negligible because of the weakness of these couplings.

The map of the q parameters is generated and stored when a separate option (IV.12) is executed and read if either the minimization command (IV.15) or the error estimation command (IV.6) is encountered. For each experiment GOSIA establishes the ranges of ξ and ζ according to the level scheme (the maximum decay energy defines the maximum value of ξ) and the specified limits of the matrix elements (IV.14) which determine maximum value of ζ. The q parameters are extracted following the method discussed in Chapter II (2.10) using the two-level system described using preset values of ζ and ξ. For each ξ meshpoint fifty values of ζ, covering the whole range, are used to fit the coefficients a and b (3.10) by the usual linear regression ($\Delta m=0$ only). Ten ξ meshpoints are used for all multipolarities, thus the map consists of ten pairs (a,b) for each multipolarity and experiment for both q_a and q_s corresponding to $\Delta m=0$ couplings while $\Delta m=\pm 1$ are treated as ζ-independent, therefore only coefficients b are computed and stored.

The q parameters map, once generated, should not be recalculated unless the ranges of ξ or ζ were changed by including additional levels or couplings resulting in a higher maximum decay energy or by expanding the limits of the matrix elements. It is always recommended to keep these ranges at a reasonable minimum, most important the range of ξ. This can be achieved by eliminating the couplings between levels having no influence on both excitation and deexcitation, but creating the high-energy decays. As a rule, the matrix approximation reliability improves with decreasing values of ξ, thus by narrowing its range one usually obtains faster convergence of the minimization.

The approximate excitation amplitudes are computed according to the formula 2.5, with A matrices defined by 2.7. An algorithm:

$$\begin{aligned} \bar{a}_p(0) &= \bar{a}(0) \\ \bar{a}_p(n+1) &= \frac{1}{n+1} A\, \bar{a}_p(n) \\ \bar{a}(n+1) &= \bar{a}(n) + \bar{a}_p(n+1) \end{aligned} \qquad 3.11$$

equivalent to the Taylor series expansion is used to iteratively evaluate the product of the matrix exponentials acting on the initial amplitudes vector $a = a(\omega=-\infty)$. The convergence of this procedure is controlled by monitoring the sum of excitation probabilities and the evaluation of matrix exponentials is truncated if this sum differs from unity by less than user-specified accuracy. In some cases, the summation 3.11 may not converge within requested accuracy due to the computer-dependent roundoff error propagation. This usually happens when the matrix elements of A operators are large, so to overcome this problem it may be necessary to logically subdivide the matrix operators using the identity:

$$\exp(A)\bar{a} = \exp(A/2)\exp(A/2)\bar{a} \qquad 3.12$$

which is done by GOSIA automatically, with the message:

EXP(A) EXPANSION FAILURE- EXP. N NEW SUBDIVISION(L,K)

issued, specifying experiment number N and number of times the subdivision of either A_1 or A_2 operator (L=1 or 2) was performed K. Usually a single subdivision is sufficient to assure the default accuracy 10^{-5} for any Coulomb excitation experiment, thus more subdivisions done probably points out to the unreasonable values of the matrix elements.

The matrix operators used for the fast approximation are sparse and are never stored as matrices. Instead, the expansion 3.11 is performed using the fact, that non-zero elements of these operators correspond to the matrix elements, as follows from 2.7, therefore the catalog of the matrix elements is used to avoid dummy multiplications. The resulting excitation amplitudes are then used to calculate the statistical tensors exactly like the solution of the full Coulomb excitation coupled channel calculation.

III.3 CALCULATION OF THE GAMMA YIELDS

The Coulomb excitation statistical tensors evaluated in the coordinate frame, having the z-axis along the incoming beam direction and the x-axis in the scattering plane (Fig. I.3), are the interface between the excitation and deexcitation modules of GOSIA. The deexcitation module, activated automatically if OP,YIEL (IV.29) is encountered in the input stream, first establishes the decay scheme, common for all the experiments defined. The γ-decays are ordered "chronologically", i.e. from the highest to the lowest to take into account the effect of feeding. This has nothing to do with the user-defined sequence of the observed γ yields, which can be defined arbitrarily and will be assigned by the code to the proper decays on a basis of the initial and final state indices provided by the user in an experimental yields file (IV.30). The initialization of the decay module involves the calculation of the $F_k(\lambda\lambda' I_f I)$ coefficients for each decay (see Eq. 1.35) which are not dependent neither on the matrix elements nor on the experimental conditions and can be stored to avoid recalculating them for each experiment and for each set of the matrix elements during the minimization. The same holds for the decay amplitudes, δ_1, divided by the appropriate matrix elements (see Eq. 1.36). The evaluation of the γ yields is then fast compared to the Coulomb excitation calculation, involving, for different experiments and matrix element sets, only the recalculation of the deorientation effect and the transformation of the Coulomb excitation statistical tensors to the decay statistical tensors, R_{kx}, including the feeding from above (1.43). The tensors R_{kx} are calculated in the system of coordinates originating in the decaying nucleus, as defined by Fig. I.3, thus one has to transform them to the laboratory-fixed system. As long as the distance traveled by the decaying nucleus is negligible this tranformation consists of the relativistic velocity correction, outlined in Section I.2.2. It should be noted, that this transformation is time-

consuming and it is not performed when calculating the gradients used during minimization, its effect absorbed into internal correction coefficients (III.5.3). Finally, using the symmetry properties of the decay tensors and the spherical harmonics, the double differential cross sections for the γ decay from a state I to a state I_f can be written in the purely real form as:

$$\frac{d^2\sigma(I\to I_f)}{d\Omega_p\, d\Omega_\gamma} = \sigma_R(\theta_p) \sum_{\substack{k \\ \chi\geq 0}} R_{k\chi}(I,I_f;\theta_p) P_{k\chi}(\theta_\gamma)(2\cos\chi(\phi_p-\phi_\gamma)-\delta_{\chi 0}) \qquad 3.13$$

where P_{kx} stands for the Legendre spherical function. It should be noted that Eq.3.13 is given in the laboratory system of coordinates, differing from the scattering plane oriented system by the definition of the ϕ angle. The ϕ angle in the laboratory-fixed system of coordinates is given by the difference between the particle ϕ angle and the γ ϕ angle, therefore the user-defined frame of coordinates is only restricted to have an origin corresponding to the position of the target and the z-axis along the beam direction, with the x and y axes defined arbitralily. As long as all the angles are consistently given in the same frame of coordinates the definition of the angular distribution is unique.

The double-differential cross section, defined by 3.13, describes the angular distribution of γ rays assuming that the direction of observation is well-defined, i.e. the detector used can be treated as a point detector. The finite size of a γ detector results in the attenuation of the angular distribution, which can be taken into account by introducing the attenuation coefficients, Q_k, transforming the decay statistical tensors, R_{kx}, according to:

$$R_{k\chi} \to R_{k\chi} Q_k \qquad 3.14$$

The attenuation coefficients Q_k are generally dependent on the geometry of the γ detector, the γ-ray energy and the materials used for the γ-ray detection. It is assumed, that the decay γ-rays were detected using the

coaxial Germanium detectors, optionally equipped with a set of absorbers frequently used to attenuate unwanted X- and low energy γ-rays. Such kind of an apparatus is almost exclusively used to study the discrete γ-ray spectroscopy. Assuming that the symmetry axes of the Ge detectors are aligned with the target the procedure outlined in Section I.2.3 is used in GOSIA to evaluate the Q_k factors. The absorption coefficients data for Ge and most commonly used absorber materials - Al, Fe, Cu, Cd/Sn, Ta and Pb - are built in the code. The Q_k attenuation factors are γ-energy dependent, thus, as a compromise between the extensive storage and the necessity of recalculating them during each step of minimization or error calculation, a two-parameter fit of the γ-energy dependence is performed in a separate step and only the fitted parameters are stored on a permanent file read in by GOSIA prior to the first γ decay calculation. The fitted formula, well describing the γ-energy dependence is given by:

$$Q_k(E_\gamma) = \frac{C_2 Q_k(E_0) + C_1 (E_\gamma - E_0)^2}{C_2 + (E_\gamma - E_0)^2} \qquad 3.15$$

where E_0=50 keV with no graded absorbers or only a combination of Al, C, and Fe specified and E_0=80, 100, or 150 keV if the Cd/Sn, Ta or Pb layers were employed as absorbers, respectively. The shift in "zero" energy is intended to provide a smooth dependence above the highest absorption cutoff point. It is assumed, that the γ transitions of energies below the highest cutoff point are of no interest, therefore no attempt is made to fit this region. $Q_k(E_0)$ in 3.15 stands for the attenuation coefficient for the "zero" energy calculated according to the prescription of I.2.3., while C_1 and C_2 are fitted to reproduce the energy dependence obtained using this formalism.

To reproduce the experimentally observed γ intensities for a given beam energy and scattering angle θ_p the double-differential cross sections, as defined by 3.13 including the γ detector solid angle attenuation factors (3.14), should be integrated over the ϕ angle range defining the particle detector shape for this scattering angle (note that from a point of view of the Coulomb excitation an independent experiment is defined only by the scattering angle and the bombarding energy for the same beam). Also, the

solid angle factor, $\sin(\theta)$. where θ is the projectile or target laboratory scattering angle, dependent on which particle has been detected, should be taken into account. The γ-decay intensities, referred to as "yields", are therefore defined in GOSIA as:

$$Y(I \to I_f) = \sin(\theta_p) \int_{\phi_p} \frac{d^2\sigma(I \to I_f)}{d\Omega_\gamma \, d\Omega_p} \, d\phi_p \qquad 3.16$$

where the integrand is given by 3.13. The integration over the ϕ angle is trivial since the ϕ-dependence is analytical, described only by a single cosine function, as seen from 3.13. According to the input units requested by GOSIA (Section IV) the yields will be calculated in units of mb/srad/rad (i.e. milibarns per steradian of the γ solid angle per radian of the particle scattering angle). This holds for the γ yields calculated using OP,POIN (IV.18). The reproduction of the experimentally observed yields should, however, involve the integration over the particle scattering angle including the beam energy loss in the target, thus the fully integrated yields, obtained using OP,INTG, have a different meaning, as described in Section III.4.

So far, we have neglected the effect of the geometric displacement of the origin of the system of coordinates due to in-flight decay, i.e. we have assumed that all observed decays originate at the center of a target, thus the relativistic velocity correction is the only one needed to transform the nucleus-centered system to the laboratory-fixed system. This approximation is adequate as long as the mean lifetimes of the decaying states are in the subnanosecond range. For the cases in which longer-lived states are of interest GOSIA provides an optional first-order treatment to correct for the geometric displacement. To treat this effect rigorously, one has to take into account both the change of the angles of the γ detectors, as seen by the decaying nucleus, and the change of the solid angles subtended by the detectors. For a given direction of the recoil the observed yield of the decay of a state having the decay constant λ can be written as:

$$Y = \lambda \int_0^\infty \exp(-\lambda t) S(t) Y(t) dt \qquad 3.17$$

where S(t) denotes the time dependence of the solid angle factor, while Y(t) stands for the time dependence of the "point" angular distribution. To the lowest order the product S(t)Y(t) is expressed as:

$$S(t)Y(t) \approx Y(0) + pt \qquad 3.18$$

where p stands for the time derivative of this product taken at t=0 (note that S(0)=1, thus S(0)Y(0) = Y(0)). Inserting 3.18 into 3.17 and using the displacement distance, s, as an independent variable instead of time we finally obtain for mean lifetime τ:

$$Y = Y(0) + v\tau p \qquad 3.19$$

where p is calculated numerically using a second set of yields evaluated in a point shifted by s in the recoil direction, i.e. :

$$p = \frac{S(s)Y(s) - Y(0)}{s} \qquad 3.20$$

where S(s), assuming that the the displacement is small compared to the distance to the detector, r_0, is calculated as:

$$S(s) = \frac{r_0^2}{(\bar{r}_0 - \bar{s})^2} \qquad 3.21$$

The displacement correction requires the γ yields to be calculated twice for each evaluation, thus should be requested only when necessary to avoid slowing down the execution.

III.4 INTEGRATION OVER THE PROJECTILE SCATTERING ANGLE AND THE ENERGY LOSS IN A TARGET - CORRECTION OF EXPERIMENTAL γ YIELDS

An exact reproduction of the experimentally observed γ yields requires the integration over a finite scattering angle range and over the range of bombarding energies resulting from the projectile energy loss in a target. The γ-decay formalism presented in Section III.3 has so far assumed that the projectile scattering angle, θ_p, and the bombarding energy, E_b, are constant for a given experiment. Using the definition of the "point" yields (3.16) the integrated yields, $Y_i(I \to I_f)$, are given by:

$$Y_i(I \to I_f) = \int_{E_{min}}^{E_{max}} dE \frac{1}{(\frac{dE}{dx})} \int_{\theta_{p,min}}^{\theta_{p,max}} Y(I \to I_f) d\theta_p \qquad 3.22$$

Note that both the Rutherford cross section and the solid angle factor, $\sin\theta_p$, are already included in the definition of the "point" yields, as well as integration over the detected particle ϕ angle.

The electronic stopping powers, dE/dx, in units of MeV/(mg/cm^2), are defined by an user-specified table assuming the common energy meshpoints for all experiments. The actual values of the stopping powers are obtained using the Lagrange interpolation. The double integral is then evaluated numerically using the discrete Simpson rule. GOSIA performs the integration in two separate steps - first, the full Coulomb excitation coupled-channel calculation is done at each of the user-specified (θ_p,E) meshpoints to evaluate the "point" γ-yields, next, the actual numerical integration is performed according to the user-defined stepsizes in both dimensions. The "point" yields at the (θ_p,E) points as required by the fixed stepsizes are evaluated from the meshpoint values using the logarithmic scale Lagrangian interpolation. The θ_p-E mesh is limited to a maximum of 11x11 points, while

up to 100 steps in each dimension can be defined for the integration. Subdivision of the calculated mesh improves the accuracy of integration, since Lagrangian interpolation provides the information of the order dependent on the number of meshpoints, while Simpson method is a fixed second-order algorithm. In addition, in cases for which the $\phi_p(\theta_p)$ dependence is complicated, as for the large parallel-plate detectors where kinematical and mechanical constraints may create such shapes, the user may optionally choose to input this dependence at the subdivision meshpoints. The interpolation is then performed between the values divided by ϕ_p ranges to assure continuity, then the user-given dependence is used to estimate the yields at the subdivision meshpoints.

The calculation of yields at the meshpoints requires the full coupled-channel Coulomb excitation calculation, thus is time-consuming. Consequently, one should only specify a minimum number of meshpoints needed to achieve a reasonable accuracy.

The integrated yields are calculated in units of mb/srad times the target thickness (mg/cm^2) which for the thick targets should be assumed to be the projectile range in the target.

The integration module of GOSIA is almost exclusively used in conjunction with the correction module, invoked by the OP,CORR command (IV.4), used to transform the actual experimentally observed yields to the ones to which the subsequent fit of the matrix elements will be made. This operation is done to avoid the time-consuming integration while fitting the matrix elements and is treated as an external level of iteration. An effect of the finite scattering angle and bombarding energy ranges as compared to the "point" values of the yields is not explicitly dependent on the matrix elements, thus the fit can be done to the "point" values and then the integration/correction procedure can be repeated and the fit refined until the convergence is achieved. Usually no more than two integration/correction steps are necessary to obtain the final solution, even in case of the experiments performed without the particle-γ coincidences, covering the full particle solid angle. The correction module of GOSIA uses both the integrated yields and the "point" yields calculated at the mean scattering angle and bombarding energy, as defined in the EXPT (IV.8) input, to

transform the actual experimental yields according to:

$$Y^{c}_{exp}(I \to I_f) = Y_{exp}(I \to I_f) \frac{Y(I \to I_f)}{Y_i(I \to I_f)} \qquad 3.23$$

where the supersript "c" stands for the "corrected" value. To offset the numerical factor resulting from the energy-loss integration the lowermost yield observed in a γ-detector labeled as #1 for the first experiment defined in the EXPT input is renormalized in such a way that the corrected and actually observed yield are equal. This can be done because the knowledge of the absolute cross-section is not required by GOSIA, therefore, no matter how the relative cross-sections for the various experiments are defined, there is always at least one arbitrary normalization factor for the whole set of experiments. This normalization factor is being fitted by GOSIA together with the matrix elements, as dicussed in the following section (III.5). The renormalization procedure results in the "corrected" yields being as close as possible to the original values if the same target has been used for the whole set of the experiments analyzed, thus the energy-loss factor in the integration procedure is similar for the whole set of the experiments. One shold be, however, aware of the fact, that the correction factors may differ significantly for different experiments, thus the corrected yields, normalized to a user-specified transition, always given in the GOSIA output, should be used to confirm that the result is reasonable rather than absolute values.

III.5 MINIMIZATION

The minimization, i.e. fitting the matrix elements to the experimental data by finding a minimum of the least-squares statistic is the most time-consuming stage of the Coulomb excitation analysis. A simultaneous fit of a large number of unknown parameters (matrix elements) having in general a very different influence on the data is a complex task, which, to whatever extent algorithmized, still can be slowed down or speeded up dependent on the way it is performed. GOSIA allows much freedom for the user to define a preferred strategy of the minimization. A proper use of the steering parameters of the minimization procedure can significantly improve the efficiency of fitting dependent on the case analyzed - in short, it still takes a physicist to get the results!. The following overview of the fitting methods used by GOSIA is intended to provide some ideas about how to use them in the most efficient way.

III.5.1 DEFINITION OF THE LEAST-SQUARES STATISTIC

A set of the matrix elements best reproducing the experimental data is found by requesting the minimum of the least-squares statistic, $S(\mathbb{M})$. The matrix elements will be treated as a vector ordered according to the user-defined sequence. The statistic S is in fact an usual χ^2-type function, except of the normalization to the number of data points rather than the number of degrees of freedom which cannot be defined due to a very different sensitivity of the excitation/deexcitation process to various matrix elements, as discussed in more detail in Section III.6. The statistic S, called CHISQ in the output from GOSIA, is explicitly given by:

$$S(\bar{M}) = \frac{1}{N} (S_y + S_1 + \sum_i w_i S_i) \qquad 3.24$$

where N is the total number of data points (including experimental yields, branching ratios, lifetimes, mixing ratios and known E2 matrix elements) and S_y, S_1 and S_i are the components resulting from various subsets of the data, as defined below. Symbol w stands for the weight ascribed to a given subset of data.

The contribution to the total S function from the measured γ-yields following the Coulomb excitation, S_y, is defined as:

$$S_y = \sum_{I_e,I_d} w_{I_e I_d} \sum_{k(I_e,I_d)} (C_{I_e I_d} Y_k^c - Y_k^e)^2 / \sigma_k^2 \qquad 3.25$$

where the summations extend over all experiments (I_e), γ-detectors (I_d) and experiment- and detector-dependent observed γ-yields, indexed by k. The weights ascribed to the various subsets of data ($w_{I_e I_d}$) can be choosen independently for each experiment and γ-detector, facilitating the handling of data during the minimization (particurarly, some subsets can be excluded by using a zero weight without modifying the input data). Superscript "c" denotes calculated yields, while superscript "e" stands for experimental data, with σ_k being the experimental errors. Coefficients $C_{I_e I_d}$ are the normalization factors, connecting calculated and experimental yields (see III.5.2). The next term of 3.24, S_1, is an "observation limit" term, intended to prevent the minimization procedure from finding physically unreasonable solutions producing the γ transitions which should be, but have not been observed. We introduce an experiment and detector dependent observation upper limit, $u(I_e,I_d)$, being a ratio of the lowest observable intensity to that of the user-specified normalization transition (see IV.29). S_1 is defined as:

$$S_1 = \sum_j \left(\frac{Y_j^c(I_e,I_d)}{Y_n^c(I_e,I_d)} - u(I_e,I_d) \right)^2 / u^2(I_e,I_d) \qquad 3.26$$

the summation extending over the calculated γ transitions not defined as experimentally observed and covering the whole set of the experiments and γ-detectors defined, provided that the upper limit has been exceeded for a given transition. The terms added to S_1 are not counted as data points, thus the normalization factor N is not increased to avoid the situation in which the fit could be improved by creating the unreasonable transition intensities at the expense of the normalization factor.

The remaining terms of 3.24 account for the spectroscopic data available, namely the branching ratios, the mean lifetimes, the E2/M1 mixing ratios and the known E2 matrix elements. Each S_i term can be written as:

$$S_i = \sum_{n_i} (d^c_{n_i} - d^e_{n_i})^2 / \sigma^2_{n_i} \qquad 3.27$$

where the summation extends over all the spectroscopic data included in the input to GOSIA, d and σ being the data points and their errors, respectively. In case of the known E2 matrix elements the absolute values of the transitional matrix elements are used (since usually only the B(E2) values are known), while the diagonal matrix elements are taken including the sign. The user-defined weigths, w_i, common for a given group of data, once again provide the easy way of manipulating the spectroscopic information according to the current needs without modifying the input.

The least-squares statistic S is used to determine a set of the matrix elements fitted to the experimental data as well as to ascribe the errors of the fitted matrix elements, which are defined by the shape of the S hypersurface in the space of the matrix elements (see Section III.6).

III.5.2. NORMALIZATION CONSTANTS

To relate the calculated and experimental yields it is necessary to introduce the normalization constants, treated as an additional set of parameters (we assume that the experiments are conducted without the total flux measurement, which would provide the required normalization). An alternate approach would be to fit the yields normalized to the intensity of a specified transition. Such an approach, however, has severe drawbacks, namely the increased uncertainties to be ascribed to the data, elimination of one data point for each γ detector and, last but not least, a danger of obtaining a wrong result if, for some reason, the transition choosen for the normalization was incorrect (being, for example, an uresolved doublet with an unknown component). A number of the unknown normalization constants can be considerably reduced by using the fixed relative γ detector efficiencies, known, after being corrected for the γ-energy dependence, from the intensity calibration. This reduces the number of fitted normalization constants to one per experiment, instead of one per γ detector. A further reduction is possible if a set of experiments resulted from dividing the data acquired during a single physical run into the scattering angle slices, as in case of the experiments conducted using the position-sensitive particle detectors. By monitoring the singles (i.e. the events for which the detection of the γ-ray is not required) one obtains the relative normalization for various scattering angle slices, which includes the Rutherford cross section, the solid angle factor and the particle detector efficiency. GOSIA provides an option to "couple" such sets of experiments by including the relative normalization of various experiments in the relative normalization of the γ detectors. The relative normalization between the experiments should be given as the ratio of singles divided by the mean particle ϕ and θ ranges for an appropriate slice. As an example, let us consider a "physical" experiment, conducted using the position-sensitive particle detector and three γ detectors. The full range of the scattering angle was logically

divided into two slices, subtending the mean ranges $(\Delta\theta_1,\Delta\phi_1)$ and $(\Delta\theta_2,\Delta\phi_2)$, respectively. Assuming that monitoring the singles yielded N_1 events for "logical" experiment 1 and N_2 events for "logical" experiment 2 one can find the relative normalization of experiment 2 with respect to experiment 1 as:

$$C(2:1) = \frac{N_2\ \Delta\phi_1\Delta\theta_1}{N_1\ \Delta\phi_2\Delta\theta_2} \qquad 3.28$$

Assuming the intensities of a calibration peak in three γ detectors used were I_1, I_2 and I_3, respectively, one can finally specify the relative normalization of these detectors for both coupled experiments as:

$$\begin{array}{ll} I_1, I_2, I_3 & \text{exp. 1} \\ C(2:1)I_1, C(2:1)I_2, C(2:1)I_3 & \text{exp. 2} \end{array}$$

Note that all six values can be arbitrarily rescaled, because of the remaining single absolute normalization factor to be fitted by the code. For example all six can be divided by I_1 to have unity for the first γ detector in experiment 1, the remaining values being then relative to this detector. Finally, GOSIA provides also a possibility of treating all the γ detectors as independent, in which case the user-specified normalization constants become redundant, since the fit is done to each γ detector independently.

The fitted absolute normalization constanst are found by requesting that:

$$\sum_k (CC_k Y_k^c - Y_k^e)^2/\sigma_k^2 = \min \qquad 3.29$$

where the summation extends over all yields belonging to the subsets of data coupled by the relative normalization constants, C_k. From 3.29 results:

$$C = \frac{\sum_k C_k Y_k^c Y_k^e/\sigma_k^2}{\sum_k C_k^2 (Y_k^c)^2/\sigma_k^2} \qquad 3.30$$

The procedure of finding the normalization constants for all the coupled subsets of data is repeated in GOSIA each time the S function is evaluated, which means that the changes in normalization constants are included on the same basis as the changes of the matrix elements while searching for the minimum of S and the errors of resulting matrix elements.

III.5.3. INTERNAL CORRECTION COEFFICIENTS

Replacing the coupled-channel Coulomb excitation calculation by the semianalytic approximation (see Chapter II and Section III.2) makes possible to speed up the calculations so that the fitting of the matrix elements becomes feasible. Both the minimization procedure and the error evaluation procedure use the approximate excitation calculation mode. To improve the accuracy of this approximation (involving on the excitation side the replacement of the coupled-channel calculation by the fast approximation as well as simultaneous truncation of the number of magnetic substates taken into account and, on the deexcitation side, neglect of the time-consuming relativistic coordinate system transformation) the internal correction factors, correcting the effect of the approximations made, are introduced according to:

$$c_k = \frac{Y_k^c(\text{full})}{Y_k^c(\text{appr.})} \qquad 3.31$$

The correction factors c_k, calculated and stored for all experimentally observed γ transitions, multiply the approximate values of the γ yields. A multiplicative correction has been chosen to assure that the correction factors remain relatively constant (i.e. independent of the matrix elements) in the vicinity of a set of matrix elements used to evaluate them. As could be expected, the discrepancy between full and aproximate calculations is most prominent for the uppermost levels, due to the error propagation. The excitation probability of the uppermost levels, however, depends mostly on a single product of the squares of matrix elements connecting these levels to the ground state. It is easily seen that in such a case the correction factors will not depend on the actual values of the matrix elements, no matter how much they differ from unity.

The internal correction factors translate the γ yields resulting from the approximate calculation to the ones resulting from the full

calculation for a fixed set of the matrix elements. However, since the dependence of the correction factors on matrix elements is weak, it can be assumed that the correction is valid locally in the neighbourhood of the point of origin, understood as a set of matrix elements used to evaluate the correction factors. The correction factors should be refreshed in course of minimization dependent of how much the current set of matrix elements has changed compared to the point of origin. To decide when to recalculate the internal correction factors GOSIA uses a S-function decrease criterion, i.e. the correction factors are refreshed every time the value of S drops by an user-specified factor compared to its value at which the last recalculation took place. This allows to spare the time-consuming recalculations of the correction factors while still far from minimum (by requesting the recalculation only when the value of S dropped significantly) and to gradually increase the accuracy by changing the S-drop criterion while approaching the final solution.

The internal correction factors are not evaluated for the unobserved γ transitions, thus it it possible that, if the cumulative error due to the approximations used is significant, some of the calculated unobserved transitions may exceed the upper limits given by the user, contributing to the least-squares statistic S. GOSIA issues a warning pointing out to all the γ transitions (resulting from the approximate calculation) exceeding upper limits. Comparing the listed transitions with the comparison of the calculated and experimental yields, by default following the completion of the minimization and obtained using the full calculation, one can detect the transitions being significantly too strong due to the deficiency of the approximation used. It is then recommended to include such transitions as experimentally observed, with the large errors ascribed, to force the code to include them in the correction factors table.

III.5.4. STEEPEST DESCENT MINIMIZATION

A choice of the minimization strategy is always dependent on a specific characteristic of a function to be minimized. While it is generally possible to tailor the strategy in a case the function to be minimized can be expressed analytically, the multidimensional search for a minimum of a function which can only be evaluated numerically - which is a case of the multiple Coulomb excitation analysis - cannot be fully algorithmized to provide an universal optimum strategy, thT¼326minimization procedure should leave much room for the user intervention, based on both intuition and understanding of the processes being analyzed. The most commonly used minimization strategies - simplex, variable metric and gradient algorithms- perform better or worse dependent on the case. In our case the simplex-type methods are not useable, because the exact calculation is replaced by the fast approximation. The correction factors, valid only locally, are introduced, thus the construction of a simplex involving the points far from the matrix elements set used for evaluating the correction factors is not reliable. In turn, the variable metric method, based on an exact solution of the second-order approximation to the S function is efficient only if the second-order approximation is justified within a wide range of the parameters, which is usually not true for the Coulomb excitation analysis (in addition, the variable metric method requires that a second derivative matrix is calculated and stored, thus extending both the computing time and the central memory requirements to perform a single step of minimization without much improvement compared to the steepest descent method, dicussed below if the function is far from quadratic). Considering the above, the gradient methods are the only ones suitable for fitting the large sets of matrix elements to the Coulomb excitation data. GOSIA offers two gradient-type methods which can be choosen by the user dependent on the case analyzed - a simple steepest descent minimization, outlined below, and a gradient+derivative method, described in Section III.5.5.

The steepest descent method is one of the most commonly used methods of minimization based on the local behaviour of the function to be minimized. Assuming local validity of a first-order Taylor expansion around the central set of arguments, $\bar{x}_o$, any function can be approximated as:

$$f(\bar{x}) = f(\bar{x}_0) + \nabla_0 \Delta\bar{x} + \ldots \qquad 3.32$$

with ∇_o being a gradient, i.e. a vector of derivatives calculated at point $\bar{x}_o$, explictly defined as:

$$\nabla_{0,i} = \frac{\partial f}{\partial x_i} \qquad 3.33$$

The steepest descent method is based on a simple observation that the local decrease of the function to be minimized, f, is maximized if the change of the vector of the parameters, $\Delta\bar{x}$, is antiparallel to the gradient. As long as a minimized function is not multivalued and does not have saddle points a simple iteration scheme:

$$\bar{x} \rightarrow \bar{x} - h\nabla \qquad 3.34$$

provides a safe and efficient way to minimize it using the gradient evaluated at each succesive point $\bar{x}$. The stepsize, h, must be found by performing one-dimensional minimization along the direction antiparallel to the gradient. Assuming the locally quadratic behaviour of the function f, the value of h is expressed by:

$$h = \frac{\nabla^2}{\nabla J \nabla} \qquad 3.35$$

where J is the matrix of second derivatives of f with respect to $\bar{x}$, i.e.:

$$J_{ik} = \frac{\partial^2 f}{\partial x_i \partial x_k} \qquad 3.36$$

The estimation of the stepsize according to 3.36 is, however, out of

question, since the second-derivative matrix is never calculated in GOSIA and, moreover, the assumption of local quadraticity is in general not valid. Instead, an iterative procedure is used to find a minimum along the direction defined by the gradient, based on a well known Newton-Raphson algorithm of finding the zeros of the arbitrary functions. A search for a minimum of a function is equivalent to finding a zero of its first derivative with respect to the stepsize h, according to the second-order iterative scheme:

$$h \rightarrow h - \frac{\frac{\partial f}{\partial h}}{\frac{\partial^2 f}{\partial h^2}} \qquad 3.37$$

which can be repeated until the requested convergence is achieved, unless the second derivative of f with respect to h is negative, which implies that the quadratic approximation cannot be applied even locally. In such a case, the minimized function is sampled stepwise until the Newton-Raphon method becomes applicable when close enough to the minimum along the direction of the gradient. One-dimensional minimization is stopped when the absolute value of the difference between two subsequent vectors of parameters is less than the user-specified convergence criterion.

The gradients in GOSIA are evaluated numerically, using the forward-difference formula or, optionally, the forward-backward approximation. While the forward difference formula

$$\frac{\partial f}{\partial x_i} = \frac{f(x_1,x_2,\ldots x_i+h,\ldots) - f(x_1,x_2,\ldots x_i,\ldots)}{h} \qquad 3.38$$

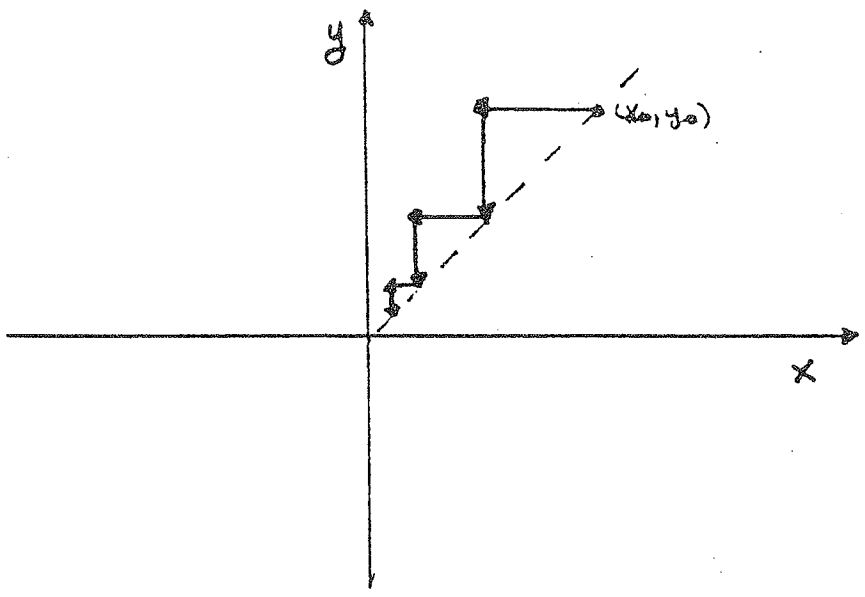
requires only one calculation of the minimized function per parameter in addition to the evaluation of the central value $f(x_1,x_2,\ldots x_n)$, the forward-backward formula

$$\frac{\partial f}{\partial x_i} = \frac{f(x_1,x_2,\ldots x_i+h,\ldots) - f(x_1,x_2,\ldots x_i-h,\ldots)}{2h} \qquad 3.39$$

requires two calculations of the minimized function per parameter. The forward-backward formula should then only be requested in the vicinity of the minimum, where the accuracy of the numerical calculations start to play an important role.

III.5.5. GRADIENT+DERIVATIVE MINIMIZATION

The steepest descent minimization, efficient if a minimized function is smooth in the space of parameters, shows considerable drawbacks when dealing with fuctions having sharp "valleys" superimposed on the smooth surfaces. Such valleys are created by the strong correlation of two or more parameters. In case of the Coulomb excitation analysis, the valleys are introduced mainly by including the accurate spectroscopic data, specially the braching ratios, which fix the ratio of two transitional matrix elements. Note, that even if the branching ratio is not introduced as an additional data point, the valley will still be present in the yield component of the least-squares statistic S if both transitions depopulating a given state were observed. To demonstrate this deficiency of the simple steepest descent method, let us consider a model situation in which a two-parameter function $f(x,y)=x^2+(x-y)^2$ is minimized, starting from a point x=y. The term $(x-y)^2$ creates a diagonal valley leading to the minimum point (0,0). Using the analytic gradient and the stepsize given by 3.35, it is easily seen that the minimization using the steepest descent method will follow a path shown below:



instead of following the diagonal. To facilitate handling of the two-dimensional valleys, introduced by the spectroscopic data, GOSIA offers a gradient+derivative method, designed to force the minimization procedure to follow the two-dimensional valleys, at the same time introducing the second-order information without calculating the second order matrix (3.36), thus speeding up the minimization even if the surface of minimized function is smooth. Generally, to minimize a locally parabolic function:

$$f(\bar{x}) = f(\bar{x}_0) + \nabla_0 \Delta\bar{x} + \frac{1}{2}\Delta\bar{x}\ J\ \Delta\bar{x} \qquad 3.40$$

one can look for a best direction of a search expressed as a linear combination of an arbitrary number of vectors, $\bar{P}_i$, not necessarily orthogonal, but only linearly independent. This is equivalent to requesting that:

$$f(\bar{x}_0 - \sum_i \alpha_i \bar{P}_i) = \min \qquad 3.41$$

with respect to the coefficients α_i. Merging 3.40 and 3.41 we get:

$$f(\bar{x}_0) - \sum_i \alpha_i (\nabla_0 \bar{P}_i) + \frac{1}{2} \sum_{ij} \alpha_i \alpha_j \bar{P}_i J\ \bar{P}_j = \min \qquad 3.42$$

which can be written in the vector form as:

$$f(\bar{x}_0) - \bar{\alpha}\ \bar{\beta} + \frac{1}{2}\ \bar{\alpha}\ R\ \bar{\alpha} = \min \qquad 3.43$$

with a set of coefficients α_i treated as a vector $\bar{\alpha}$ and:

$$\beta_i = \nabla_0 \bar{P}_i$$
$$R_{ij} = \bar{P}_i\ J\ \bar{P}_j \qquad 3.44$$

The matrix R is symmetric following the symmetry of J, thus the solution for the vector $\bar{\alpha}$ is given by:

$$\bar{\alpha} = R^{-1} \bar{\beta} \qquad 3.45$$

To construct the gradient+derivative minimization algorithm we use two directions - the gradient, defining a direction of steepest descent, and a derivative of the gradient with respect to the displacement along its direction:

$$\bar{D} = \lim_{h \to 0} \frac{\bar{\nabla}(\bar{x}_0 + h\bar{\nabla}_0) - \bar{\nabla}_0}{h} \qquad 3.46$$

It is easily checked that as long as the quadratic approximation 3.40 is valid:

$$\bar{D} = J\bar{\nabla}_0 \qquad 3.47$$

Using the identity resulting from the symmetry of J:

$$\bar{\nabla}_0 J^2 \bar{\nabla}_0 = (J\bar{\nabla}_0)^2 \qquad 3.48$$

we finally get:

$$R = \begin{vmatrix} \bar{\nabla}_0 \bar{D} & \bar{D}^2 \\ \bar{D}^2 & \bar{D} J \bar{D} \end{vmatrix}$$

$$\bar{\beta} = (\bar{\nabla}_0^2 , \bar{\nabla}_0 \bar{D}) \qquad 3.49$$

where all terms, except R_{22}, are known. By sampling the minimized function we can express this missing term as:

$$\bar{D} J \bar{D} = \frac{2}{h^2} [f(\bar{x}_0 + h\bar{D}) - f(\bar{x}_0) - h\bar{\nabla}_0 \bar{D}] \qquad 3.50$$

The coefficients α_1 and α_2, resulting from the solution of 3.45, can be arbitrarily rescaled, since we are only interested in the direction of

search, the stepsize being found by the one-dimensional minimization procedure outlined in previous section. A most convenient representation of a direction of search $\bar{\nabla}$, renormalized to avoid numerical overflows, is given by:

$$\bar{\nabla} = \left(\frac{\bar{D}\, J\, \bar{D}}{|\bar{D}|^3} - \frac{\bar{\nabla}_0 \bar{D}}{|\bar{\nabla}_0|^2 |\bar{D}|} \right) \bar{\nabla}_0 + \frac{1}{|\bar{D}|} \left(\frac{(\bar{\nabla}_0 \bar{D})^2}{|\bar{\nabla}_0|^2 |\bar{D}|^2} - 1 \right) \bar{D} \qquad 3.51$$

Although primarily designed to accomodate the narrow valleys superimposed on the least-squares statistic by the spectroscopic data, the gradient+derivative method usually gives much better results than the simple steepest descent, providing faster fitting despite the necessity of calculating two sets of derivatives per step of minimization. Since two linearly independent vectors define a two-dimensional space, the gradient+derivative method is very suitable to deal with the decoupled correlated pairs of the matrix elements (note that, as could be expected, the solution of the model case discussed above is found in a single step of minimization).

III.5.6 QUADRATIZATION OF THE S STATISTIC BY REDEFINION OF VARIABLES

The minimization methods outlined in previous subsections are built on the assumption that the minimized function can be locally described by the first or second order approximation, therefore their efficiency is strongly dependent on the extent to which this assumption is justified. Generally, the Coulomb excitation data analysis problem cannot be parametrized in such a way that the least-squares statistic S (3.24) becomes a strictly quadratic function. Some hints as how to improve the efficiency of minimization come, however, from considering the extreme cases, most important of which is a perturbation-type process, characterized by direct dependence of the excitation probabilities on the product of squares of the matrix elements directly connecting a given level to the ground state. Assuming in addition a cascade-like decay with negligible feeding from above and negligible branching, we expect the γ-decay intensities to be proportional to the product of squares of the level-dependent subsets of transitional matrix elements, thus the γ-yields part of the S statistic can be expressed as a quadratic function of the logarithms of γ yields versus the logarithms of the matrix elements (note that he same holds for the spectroscopic data, although the signs of the E2/M1 mixing ratios and known E2 matrix elements are to be disregarded). While expressing the dependent variables in logarithmic scale is straightforward, the same operation for the matrix elements would mean enforcing the sign identical to that of an initial guess. To avoid this problem the logarithmic transformation of the matrix elements is only taken in the first order of Taylor expansion, resulting in the actual minimization still performed in the matrix elements space with the direction of search being modified. To derive such an approach, let us consider the modification of a single matrix element, M, having an initial value of M_o, during a single step of minimization. A transformation to the logarithmic scale yields the tranformed derivative of a minimized function f with respect to M:

$$\frac{\partial f}{\partial \ln M} = |M_0| \frac{\partial f}{\partial M} \qquad 3.52$$

which, using the steepest descent method, gives a new value of M according to:

$$\ln|M| = \ln|M_0| - h|M_0|\frac{\partial f}{\partial M} \qquad 3.53$$

Expanding $\ln|M|$ into Taylor series around M_0 and retaining only the first order term we finally get:

$$M = M_0 - hM_0^2 \frac{\partial f}{\partial M} \qquad 3.54$$

which defines the modified direction of search. When the gradient+ derivative method is used, both vectors must be combined according to 3.52 and multiplied by $|M_0|$ to obtain the transformed direction of search.

A scale change of the matrix elements is, in principle, mainly justified if the logarithmic scale is simultaneously used for the dependent variables (γ yields etc.). However, even if the dependent variables are not transformed, the change of scale for the matrix elements, resulting in the relative, rather than absolute, variations , can improve the efficiency of the minimization. A typical situation in which fitting the relative changes is efficient is the one when a strong dependence on a small matrix element determines the stepsize, h, common for a whole set, thus inhibiting the modification of much larger matrix elements if the absolute changes are used. Using the relative changes, however, one brings the sensitivity to all matrix elements to a common range, thus improving the simultaneous fit.

The minimum of a logarithmically transformed S function does not, in general, coincide with the minimum of the original least-squares statistics. The minimization procedure uses only the direction of search resulting from the transformation of the dependent variables, if requested, still monitoring the original S statistics. The tranformation of the dependent variables should be therefore switched off when the current solution is close to the minimum of S.

III.5.7 SELECTION OF PARAMETERS FOR MINIMIZATION

The gradient-type minimization, as used in GOSIA, tends to vary the parameters according to their influence on the least-squares statistic S. It is easily understandable, since the most efficient decrease of S is primarily obtained by varying the parameters displaying the strongest influence, measured by the current magnitude of the respective components of a gradient. With the stepsize, h, being common for the whole set of parameters, it is clear that unless the strong dependences are already fitted (which results in reduction of their derivatives) the weak dependences will be practically not activated. This is a serious concern in the Coulomb excitation analysis, since the sensitivity of the S function to different matrix elements may vary by orders of magnitude. The attempt to perform the minimization using a full set of the matrix elements usually means that most of them will came into play only after some number of steps of minimization but all the necessary derivatives are to be calculated from a very beginning, enormously increasing the time spent on computation without any significant improvement compared to the much faster minimization performed initially for only a subset of matrix elements. To speed up the process of fitting, GOSIA offers a wide range of both user-defined and automatic ways of reducing a number of parameters according to the current status of the minimization. The user may first decide to fix some of the matrix elements included in the initial setup, but found to have no influence on the processes analyzed. Secondly, the user may specify a subset of the matrix elements to be varied during a current run overriding the selection made initially. The selection of the free variables for a current run can be also made by the minimization procedure itself, based on the magnitudes of the absolute values of the gradient components evaluated during a first step of the minimization compared to the user-specified limit. The direction of the search vector, being either a gradient or a gradient+derivative vector, is always normalized to unity, allowing the user

to define the limit below which the matrix elements will be locked for a current run if the absolute values of the respective derivatives are below this limit. In addition, some precautions are taken against purely numerical effects, most notably againt the situation in which the numerical deficiency in evaluating the derivative causes a spurious result. The minimization procedure in GOSIA stops if either of three user-defined conditions is fulfilled: first, the value of the S function has dropped below the user-specified limit; second, the user-specified number of steps has been exceeded; third, the user-given convergence limit has been achieved, i.e. the difference between two subsequent set of matrix elements (taken as a length of the difference vector) is less than this limit. First two conditions fulfilled terminate a current run, while after the convergence limit has been hit the minimization is resumed if it was specified to lock a given number of the matrix elements influencing the S function to the greatest extent to allow the weaker dependences to be fitted (the details of the usage of the user-defined steering parameters are given in Chapter IV). To further reduce the numerical deficiency, GOSIA monitors the directions of two subsequent search vectors and fixes itself the matrix element having the largest gradient component if two subsequent directions are almost parallel, which usually signifies that the spurious result of the numerical differentiation of S with respect to this matrix element inhibits the fitting of the less pronounced dependences. A warning message is issued if this action was taken.

An additional reduction of the free variables can be done by coupling of the matrix elements, i.e. fixing the ratios of a number of them relative to one "master" matrix element. This feature is useful if the experimental data available do not allow for a fully model-independent analysis, therefore some model assumptions have to be introduced to overdetermine the problem being investigated. The "coupled" matrix elements will retain their ratios, as defined by the initial setup during the fitting, a whole "coupled" set treated as a single variable.

Finally, GOSIA requires that the matrix elements are varied only within the user-specified limits, reflecting the physically acceptable ranges. The matrix elements are not allowed to exceed those limits, neither during the minimization nor the error calculation.

III.5.8 SENSITIVITY MAPS

As a byproduct of the minimization GOSIA provides optionally the information concerning the influence of the matrix elements on both the γ yields and excitation probabilities. The compilation of those maps is, however, time-consuming and should be requested only when necessary. The yield sensitivity parameters, α^{y}_{ik}, define the sensitivity of the calculated γ yield k with respect to the matrix element i as:

$$\alpha^{y}_{ki} = \frac{\partial \ln Y_k}{\partial \ln |M_i|} = \frac{M_i \partial Y_k}{Y_k \partial M_i} \qquad 3.55$$

The excitation probability sensitivity parameters , α^{p}_{ki}, are expressed similarly, the yields being replaced by the excitation probabilities. The code allows six most pronounced dependences to be selected for each experimentally observed yield for the printout, while a number of the matrix elements for which the most important probability sensitivity parameters are printed out can be selected by the user.

By definition, the sensitivity parameters provide (to the first order) a relationship between the relative change of the excitation probabilities (or the calculated γ yields) and the relative change of the matrix elements according to:

$$\frac{\Delta p_k}{p_k} \approx \alpha^{p}_{ki} \frac{\Delta M_i}{M_i} \qquad 3.56$$

thus supplying the locally valid information on the dependence of experimental data on matrix elements. An identical relationship holds for the yield sensitivity parameters, although the code only calculates them only for the γ detector labeled as #1 for each experiment, thus the angular distribution of the γ rays, affected for example by the mixing ratios, is not fully accounted for. It is suggested that a γ detector yielding the most

complete and accurate yields should be defined as a first one in the description of an experiment to assure that the yield sensitivity maps are calculated for all the yields observed.

The sensitivity parameters are not strongly dependent on the actual matrix elements, therefore the sensitivity maps can be treated as an indication of the features of the excitation/deexcitation process at any stage of minimization. As an extreme case it should be noted that if the lowest-order perturbation theory applies, i.e. the excitation probability of a given state is proportional to the product of the squares of matrix elements connecting this state with the ground state, then the probability sensitivity parameter will equal 2 for all such matrix elements and will vanish for all others, no matter what the actual values are. The same holds for the yield sensitivity parameters, provided that the γ decay follows a simple cascade with no branching (the feeding from above can be neglected as a consequence of assuming the applicability of the lowest-order perturbation approach).

The sensitivity maps provide an useful information which can be used during fitting to define the current sets of correlated matrix elements to be varied, to check to what extent the different sets of experimental data are independent and, finally, to ascertain which matrix elements included in the initial setup have significant influence on the processes analyzed. The data obtained during the compilation of the yield sensitivity map are also used to generate the correlation matrix, selecting the subsets of matrix elements being strongly correlated for the error estimation (see Section III.6). It should be noted, however, that the compilation of the sensitivity maps is time-consuming, thus it should be requested only periodically when needed. The sensitivity maps are also helpful when planning an experiment, in which case a set of simulated γ yields can be used as experimental data for a dummy minimization run (simulated yields can be created by GOSIA using OP,POIN - see IV.18). A comparison of the sensitivity parameters for different (existing or planned) experiments give an indication to what extent the additional sets of data provide the qualitatively new information.

III.6. ESTIMATION OF ERRORS OF THE FITTED MATRIX ELEMENTS

The most commonly used methods of estimating the errors of the fitted parameters (in our case the matrix elements) resulting from the least-squares minimization are derived using the assumptions which not necessarily apply to the Coulomb excitation analysis. Usually, the errors of the fitted parameters are evaluated either using the curvature matrix or by requesting an increase of the least-squares statistic dependent on the number of degrees of freedom and the value of this statistic at the minimum. An approach based on the second-order approximation is not applicable because this approximation is in general not valid even in the vicinity of the fitted set of matrix elements, not to mention the problems resulting from the so-called "nuissance parameters", i.e. the parameters which can be formally introduced, but have no influence on the observed processes. The inclusion of such parameters prohibits a straightforward inversion of the second-derivative matrix. Moreover, the curvature matrix approximation assumes that the fit is perfect, i.e. the gradient at the solution point vanishes, thus only the second-order term describes the behavior of the least-squares statistic. Practically, however, we have to assume that a fitting procedure must be stopped at some point even though a number of the matrix elements having a weak influence on the Coulomb excitation process is far from their best values. This is not important from the point of view of extracting the information contained in the experimental data but can considerably disturb the error estimation of the significant dependences when the second-order approximation is used. The unavoidable presence of the nuisance parameters also prohibits the error estimation procedures based on the assumption that the least-squares statistic should obey the χ^2 distribution with a given number of degrees of freedom. It should be noted that the concept of the number of degrees of freedom is implicitly based on the assumption that all the parameters are of about equal significance, which is obviously not true in our case since the sensitivity of the

observed γ yields to the various matrix elements differs by the orders of magnitude. It is clearly seen by noticing that to describe a given experiment one can arbitrarily add any number of unobserved levels connected by any any number of the matrix elements having no influence on either Coulomb excitation or γ deexcitation, thus arbitrarily changing the number of parameters and, consequently, the number of degrees of freedom. Finally, any procedure based on the number of degrees of freedom will result in ascribing the errors of the fitted matrix elements according to the subjective feeling what still is a valid parameter of the theory and what is not. The error estimation formalism used in GOSIA, described in subsequent sections, has been therefore derived without employing neither local quadratic approximation nor the concept of the degrees of freedom to provide a reliable (however in general non-analytic) method of calculating the errors of the fitted parameters.

III.6.1. DERIVATION OF THE ERROR ESTIMATION METHOD

Let us assume that a set of observables, Y_k, measured with known and fixed experimental errors, σ_k, is used to determine the values of a set of parameters, x_i. We also assume that the observables are related to the parameters by an error-free functional dependence, i.e. that if the experiments were error-free each experimental point Y_k could be exactly reproduced as:

$$Y_k = f_k(\bar{x}) \qquad 3.57$$

where f_k stands for the functional description of the k-th observed data point using a given set of parameters, represented as a vector. However, since we have to assume the experimental uncerntainties, we can only determine the parameters by requesting that the least- squares statistics (as defined by 3.24) is minimized with respect to the set of parameters. In other words, the assumption that a set of n parameters is sufficient to

reproduce N experimental observables (N≥n), is equivalent to assuming that only a certain values of observed data forming a n-dimensional hypersurface in the space of observables are allowed and the fact that the measured set of observables does not correspond exactly to any set of parameters is only due to the experimental errors. From this point of view the extraction of the parameters based on a set of observables reduces to determining which point on a hypersurface of the "allowed" experimental values (referred to as a "solution locus") corresponds to the measured values. While the assignment of the closest point on a solution locus defines a "best" set of parameters (as shown below), the distribution of the probability that different points belonging to the solution locus actually represent the set of observables defines the errors ascribed to the parameters. It can be shown that both the "best" set of the parameters and the errors of the parameters can be found examining the least-squares statistic if the "perfect theory" approach is assumed. Such an approach, actually employed in GOSIA, is presented below.

To simplify the notation it is convenient to introduce the normalized observables, y_k, defined as:

$$y_k = \frac{Y_k}{\sigma_k} \qquad 3.58$$

and to assume that the functional dependence also includes the normalization relative to the fixed experimental errors σ_k. Treating both the set of normalized observables and the set of normalized functional dependences as vectors, we can compactly define the unnormalized least-squares statistic, χ^2, as:

$$\chi^2 = [\ \bar{f}(\bar{x}) - \bar{y}\ ]^2 \qquad 3.59$$

where we have used a symbol χ^2 to distinguish the unnormalized statistic from the normalized statistic S, as defined by Eq. 3.24. Assuming that the normalized observables, y_i, are independent and normally distributed (the width of the distribution equal to unity, as a result of the normalization to the known experimental errors) one finds that the probability of the observed set $\bar{y}$ is an experiment-distorted reflection of a "true" set $\bar{y}'$ is

proportional to:

$$P(\bar{y}') \approx \exp(-\frac{1}{2}(\bar{y} - \bar{y}')^2) \qquad 3.60$$

An assumption of the "perfect" theory allows only the "true" sets of experimental data which can be described by the functional dependence f, belonging to the solution locus. Therefore only the sets $\bar{y}'$ which can be expressed as:

$$\bar{y}' = \bar{f}(\bar{x}) \qquad 3.61$$

are to be taken into account. Substituting 3.61 into 3.60 one gets:

$$P(\bar{f}(\bar{x})) \approx \exp(-\frac{1}{2}\chi^2) \qquad 3.62$$

Note that in this "geometrical" picture χ^2 has a meaning of the square of the distance from the observed set of data to a point belonging to the solution locus, thus the least-squares minimization is equivalent to finding a point on the solution locus closest to the experimentally observed set of data. Such a point has the highest probability of reflecting an error-free measurement, as long as the assumption of a perfect theory is in effect. Eq. 3.62 gives the probability that the observed set of data corresponds to a given point on the solution locus per the element of volume of the solution locus, thus the transition to a probability of a given set of parameters per unit of volume in the parameter space requires that the density function, given by:

$$\rho(\bar{x}) = \frac{dV}{dx_1 dx_2 \ldots dx_n} \qquad 3.63$$

is used, with dV standing for the volume element of the solution locus as a function of the parameters x_i. The probability distribution in the parameter space can be subsequently written as:

$$\frac{dP(\bar{x})}{dx_1 dx_2 \ldots dx_n} = C\,\rho(\bar{x})\,\exp(-\frac{1}{2}\chi^2(\bar{x})) \qquad 3.64$$

with a normalization constant C resulting from the condition that the integral of the probability distribution over a whole space of parameters is equal to unity. Eq. 3.64 defines the probability distribution of simultaneous assignment of a whole set of parameters. Practically, however, we are rather interested in ascribing the errors to the individual parameters, therefore we have to reconstruct the one-dimensional probability distributions corresponding to the individual parameters. Such a distribution for parameter i, with no assumptions made as to the "true" values of the remaining parameters, will be given by:

$$\frac{dP(x_i)}{dx_i} = \int \frac{dP(\bar{x})}{dx_1 dx_2 \ldots dx_n} dx_1 dx_2 \ldots dx_{i-1} dx_{i+1} \ldots dx_n \qquad 3.65$$

the integration extending over all allowed values of the parameters except of the parameter i. Using 3.65 the error bars of a given parameter can be found by requesting that the probability that the "true" value of this parameter (evaluated by integrating the distribution 3.65) is contained within the error bars equals to an adopted confidence limit of 68.3% corresponding to the standard deviation obtained using the Gaussian distribution. Since neither the perfect minimum nor the symmetry of χ^2 around the minimum is assumed, it is reasonable to define the upper and lower error limits independently. This is explicitly given by requesting that:

$$\frac{\int_{x_i}^{x_i+\delta x_i} \frac{dP(x_i)}{dx_i} dx_i}{\int_{x_i}^{x_i(\max)} \frac{dP(x_i)}{dx_i} dx_i} = .683 \qquad 3.66$$

where δx_i stands for the upper error limit, while $x_i(\max)$ denotes the maximum allowed value of x_i. A similar formula is used to determine the lower error limit with the maximum allowed value of x_i replaced by the

minimum allowed value of this parameter.

Until now the derivation of the error estimation formalism has rigorously followed the initial assumptions. The error estimation using 3.66 is, however, not practical when dealing with a multidimensional parameter space and the non-analytic description of the functional dependence used to relate the parameters to the observed data. First, it is technically impossible to evaluate the density function, $\rho(\bar{x})$, if the analytic functional dependence is not known, as in the case of the multiple Coulomb excitation. It can be argued that if the parametrization of the processes observed is reasonable, the density function should be only weakly dependent on the actual set of parameters compared to the dependence of the χ^2 function (otherwise, the parametrization would be unstable). Assuming that the χ^2 exponent in 3.66 drops sharply in the vicinity of the error limit while no drastic change of the density function takes place, one can take for granted that within a reasonable accuracy an effect of weighting the Gaussian distribution with the density function can be safely neglected. Second, it is easily seen that the reconstruction of the one-dimensional probability distribution according to Eq. 3.65 is not feasible if the analytic form of the functional dependence is not known. We are therefore forced to adopt a "worst case" approach, i.e. to use an approximation yielding the overestimated error bars but allowing a reduction of the multidimensional problem to one-dimensional without performing the numerical integration in multidimensional space. To construct such an approach we introduce a concept of a "maximum correlation curve" defined as a curve in the parameter space for which an effect of varying a given parameter is to the greatest extent balanced by the changes of the correlated parameters to minimize an overall change of the χ^2 function. Introducing the above approximations the error criterion 3.66 can be rewritten as:

$$\frac{\int_{x_i}^{x_i+\delta x_i} \exp(-\frac{1}{2}\chi^2(x_i)\,dl(\bar{x})}{\int_{x_i}^{x_i(\max)} \exp(-\frac{1}{2}\chi^2(x_i)\,dl(\bar{x})} = .683 \qquad 3.67$$

where l stands for the "maximum correlation" path and the probability distribution is treated as a function of the i-th parameter only, the dependence on other correlated parameters being defined by the path of integration, l. This simplification results in overestimation of the error bars, corresponding to the confidence limit of at least 68.3%.

The error estimation formalism, presented above, fits well the needs of Coulomb excitation analysis. It is not sensitive to the redundant parameters, which will simply display no influence on χ^2 statistic. It allows to easily introduce physical limits of the matrix elements just by normalizing the probability distribution to its integral between those limits (note that in case of insignificant matrix elements this will yield the errors of 68.3% of the full range - GOSIA issues a warning if the integration is stopped on the limit before the criterion 3.67 was fulfilled). Finally, neither the purely quadratic behaviour of χ^2 nor the perfect minimum are explicitly assumed.

III.6.2 NUMERICAL ESTIMATION OF ERRORS

The error estimation in GOSIA is performed in two separate steps. First, the "diagonal" errors, i.e. the errors of individual matrix elements with all the others kept fixed, are found. This part of error calculation is relatively fast and thus has been separated from the "full", or correlated, error estimation. The calculation itself consists of a straightforward numerical solution of 3.67, the fourth-order Runge-Kutta integration method used to numerically evaluate the integrals involved. The probability distribution is renormalized to its value at the central set of matrix elements to avoid under- and overflows, i.e. $\Delta\chi^2$ is used instead of χ^2. As mentioned above, the diagonal error calculation is not very time-consuming, therefore it can also be used to speed up the minimization provided that the strong influences were already fitted. Running the diagonal errors, one can detect the matrix elements being still far their best values judging from the pronounced assymetries of the error bars. In addition, GOSIA notifies the user every time a better value of the statistic S has been found. This information can be used to "manually" predict a better solution without performing a time-consuming minimization of the weak dependences. Also, in some cases, the improvement of χ^2 found during the error calculation can be so large that the Gaussian distribution associated with the error estimation cannot be handled due to the machine-dependent overflow of the exponential involved. GOSIA detects such situations using an user-defined capacity of the computer, allowing to indicate which subsets of the matrix elements are to be refitted to improve the minimum.

The diagonal error calculation is usually repeated a few times until the minimum of the least-squares statistic S is found satisfctory from a point of view of individual matrix elements. The following "full" error calculation differs from the diagonal error calculation only by applying Eq. 3.67 along the predicted path of maximum correlation. Although, in general, this path is a curve in a space of the parameters, we are forced, for

practical reasons, to approximate it by a straight line. To make this approximation as reliable as possible, the information resulting from the diagonal error calculation is used by GOSIA to determine the way the probability distribution is sampled. An estimate of the diagonal error for a given matrix element is first used to evaluate an appropriate stepsize for the Runge-Kutta integration algorithm. Since the influence of a given matrix element is not a priori known a common stepsize is used for the diagonal error estimation. This approach is subsequently refined by adjusting the stepsize for each matrix element individually during the full error calculation based on the diagonal error range. It may, in some cases, cause a slight decrease of the error range if there is no significant correlation and the stepsize assumed for the diagonal error calculation was actually not correct taken into account the sensitivity of the χ^2 statistic to a given matrix element. The diagonal error bars are also used to define how the maximum correlation curve is approximated by the straight line in a space of the parameters. This operation is perfomed by assuming that the matrix element for which the correlated error is estimated is varied to the value corresponding to its central value ± an appropriate diagonal error and fixed at this value, while the one-step gradient minimization of the remaining matrix elements is done to find the correlation axis. The maximum correlation direction is then defined as a vector difference of the resulting set of the matrix elements and the central point. In this way, a correlation curve is approximated at a range consistent with the order of magnitude of the final error. It should be, however, noted that performing the one-step gradient minimization to find the correlation axis is very time-consuming if all the matrix elements are taken into account. Moreover, since the gradient method will only affect the values of the matrix elements strongly correlated with the one investigated, the calculation of the derivatives with respect to all others is simply redundant and does not yield any improvement in predicting the correlation axis. To speed up the full error calculation GOSIA offers a mechanism of reducing the number of matrix elements being taken into account by predicting the subsets of mutually correlated matrix elements. This requires that at a final stage of minimization the yield sensitivity map is compiled and the full set of the

sensitivity parameters α^{γ}_{ki} (3.55) is stored on a permanent file. A separate program, SELECT, uses the map of the sensitivity parameters to predict the correlation. Each two matrix elements are correlated if they affect the same data points, thus, for each matrix element M_l the correlation with a matrix element M_k can be measured by:

$$c_{lk} = \sum_i | \alpha^{\gamma}_{ki} \alpha^{\gamma}_{li} | \qquad 3.68$$

the summation extending over all observed γ yields. The absolute values are taken to prevent the neglect of the correlation due to coincidental cancellation of the opposite sign terms. For each matrix element, indexed by the row index l, SELECT identifies those matrix elements M_k having the values of c_{lk} greater then 10% of the maximum value of c_{lk} in this row. As a result, SELECT produces a binary matrix whose elements are either 0, if no strong correlation was predicted, or 1. The matrix elements explicitly correlated by the spectroscopic data are assumed to be correlated by definition. The correlation matrix is then used during the full error calculation to fix the matrix elements for which the correlation was not predicted when searching for the correlation axis.

GOSIA issues the messages if lower values of the S statistic have been found. The set of the matrix elements producing an overall best value of S is stored on a permanent file, which could be eventually used to improve the minimization as a starting guess. However, it should be remembered that the uncorrected fast approximation used during the error estimation can be a source of inaccuracies, thus the small changes in the S statistic can usually be disregarded.

III.7 IDENTIFICATION OF ERRONEOUS DATA POINTS

Fitting a large set of parameters, as in case of the Coulomb excitation analysis, one must be aware of a possible existence of the local minima, which can cause the fitting procedure to be trapped in an erroneous solution. While there is no general method of distinguishing a local minimum from a global one some judgement is still possible based on the value of the normalized least-squares statistic S and the comparison of experimental and fitted data. A local minimum could be created artificially by including the erroneous pieces of data, such as incorrectly assigned γ yields, or, even if there were no mistakes in the data, could result from the local dependence on the parameters. The information provided by GOSIA during the minimization and error estimation is usually quite sufficient to determine whether the solution is acceptable. To further facilitate the identification of the local solutions GOSIA is equipped with a "troubleshooting" module, designed to detect the inconsistencies within the data set. This module uses the information obtained at a current stage of minimization concerning the dependence of the observed γ yields on matrix elements. Only the γ yields observed in the detectors labeled #1 for each experiment are used, as a result of the convention that the γ detector providing a most complete and reliable set of data should be defined as a first one. The troubleshooting routine first calculates the normalized S statistic disregarding the other γ detectors and the spectroscopic data, assuming the independent, code-calculated normalization, thus overriding the user-specified normalization constants. A large difference between a value of S calculated this way and the value resulting from the minimization points out to either wrong relative normalization or a problem with the reproduction of the γ-ray angular distribution, which may be due to the errors in assigning the angular positions of the γ detectors (the inconsistencies within the spectroscopic data are easy to notice comparing the calculated and experimental values). A next step is to select the experimental γ yields

data which locally inhibit the minimization with respect to the individual matrix elements. Keeping in mind the gradient method used for the minimization it is easily seen that a "perfectly consistent" set of data used to form a least-squares statistic, which can be shortly written in form:

$$\chi^2 = \sum_i \delta_i^2 \qquad 3.69$$

is characterized by the fact, that all individual components of the derivative with respect to a given matrix element M_k

$$\frac{\partial \chi^2}{\partial M_k} = 2 \sum_i \delta_i \frac{\partial \delta_i}{\partial M_k} \qquad 3.70$$

should be of the same sign, which means that the overall direction found to improve the minimum with respect to this matrix element is the same as resulting from the separate pieces of data. The inconsistent pieces of data may, in turn, produce large terms of opposite sign, which consequently causes a small value of the derivative due to cancellation. In such situation a given matrix element will not be varied. As a measure of this effect we introduce a parameter r_k, defined for each matrix element M_k as:

$$r_k = \log \frac{\sum_i \left| \delta_i \frac{\partial \delta_i}{\partial M_k} \right|}{\left| \sum_i \delta_i \frac{\partial \delta_i}{\partial M_k} \right|} \qquad 3.71$$

This parameter equals 0 if all the terms summed are of the same sign and becomes large when the cancellation effect is dominant. The numerator of 3.71 can be treated an an indication of the influence of a given matrix element M_k (the "strength" of this matrix element) and is listed in the output of the troubleshooting routine separately. The routine further selects the data points having the largest positive and negative contributions to the derivative for all the matrix elements for which

calculated r_k exceeds an user-specified limit. This information may be helpful to pinpoint the erroneous data points, e.g. the misassigned γ transitions. Sometimes, mostly for weakly overdetermined cases, the local minima and the saddle points may occur even if all data are correct. The information provided by the troubleshooting module can then be used to modify the setup of the matrix elements to be fitted or to temporarily switch off some γ yield data to allow the minimization procedure to find a way out from such an erroneous solution.

IV. INPUT INSTRUCTIONS FOR THE CODE GOSIA

IV.1 ORGANIZATION

Input, execution and control of the code GOSIA is achieved by specifying a given sequence of option commands. These option commands are activated using the input format OP,---- where ---- designates the four-character alphanumeric name of the option command. Some options are used for input or selection of input needed for specific tasks while other options execute appropriate modules of the code.

The code GOSIA can operate in either of two mutually exclusive modes. The first, activated by the option OP,COUL, performs the calculation of Coulomb excitation probabilities and γ-ray yields for a fixed set of the matrix elements. No fitting of matrix elements to experimental data is performed if OP,COUL has been selected. The other mode, activated by the command OP,GOSI, should be used if a least-squares fit of matrix elements to experimental data is desired. The user is free to use any other option commands in conjunction with either the OP,COUL or the OP,GOSI commands consistent with an obvious logic. For example, the code cannot calculate Coulomb excitation amplitudes if the level scheme is not defined, it also can not execute the fit-related commands if OP,COUL has been selected. The input to the option commands OP,COUL and OP,GOSI contains suboptions for which the prefix OP, is not appended to the name.

A summary of all available options is given below. Detailed descriptions of each option and suboption command are given in alphabetical order in the subsection of this chapter listed next to the name of each option. Details of the file manipulation procedures are given in Chapter VI. The names of the option commands are truncated to four characters. Full, self-explanatory names are given in parentheses in the following description.

CONT (CONTROL) (IV.3)

Suboption of OP,COUL and OP,GOSI which is used to control and select various optional features of the code for both execution and output. This option can be omitted in which case default parameters will be used.

OP,CORR (CORRECT) (IV.4)

Execution option to modify the experimental data to correct for the difference between the integrated yield calculations and the point values used for the calculation of Coulomb excitation cross sections and γ-ray yields, as described in detail in III.4.

OP,COUL (COULEX) (IV.5)

Activates the simple excitation/deexcitation mode. No fit of matrix elements to the data is made with this option in contrast to OP,GOSI. Consequently, the appreciable input required for the fit procedure can be skipped. OP,COUL contains the following suboptions:

LEVE
(Section IV.13)
ME
(Section IV.15)
EXPT
(Section IV.8)
CONT
(Section IV.3)

OP,ERRO (ERRORS) (IV.6)

Activates the error estimation module of the code. Also, it can be used to test the goodness of the solution, as discussed in detail in Chapter VIII.

OP,EXIT
(EXIT)
(IV.7)

Terminates the job and causes the final output to be compiled.

EXPT
(EXPERIMENT)
(IV.8)

Suboption of OP,COUL and OP,GOSI which is used to input the experimental conditions for each of the experiments to be analyzed.

OP,FILE
(IV.9)

Optionally allows to declare permanent files to be attached to the job in the input rather than in the job control stream.

OP,GDET
(GE DETECTORS)
(IV.10)

Creates the files which contain the data needed to calculate the solid angle attenuation factors (I.2.3). Output files should be attached to the job when OP,YIEL is encountered.

OP,GOSI
(GOSIA)
(IV.11)

This alternative option to OP,COUL is used when a fit of matrix elements is to be made to Coulomb excitation data. The suboptions for this option are the same as for OP,COUL (however, note that the input to ME differs from that used for OP,COUL):

LEVE
(Section IV.13)
ME
(Section IV.16)
EXPT
(Section IV.8)
CONT
(Section IV.3)

OP,INTG (INTEGRATE) (IV.12) — Execution option used to integrate the deexcitation γ-ray yields, resulting from Coulomb excitation, over energy loss of the incident beam in the target and over the solid angles of the particle detectors.

LEVE (LEVELS) (IV.13) — Suboption of OP,COUL and OP,GOSI which is used to read in and catalog the level scheme of the investigated nucleus.

OP,MAP (MAP) (IV.14) — Causes the q-parameter maps (III.2) to be calculated and stored on a permanent file.

ME (IV.15) — (OP,COUL Version) Suboption of OP,COUL which is used to input and catalog the matrix elements.

ME (IV.16)	(OP,GOSI Version) Suboption of OP,GOSI which is used to establish the matrix element setup for fitting.
OP,MINI (MINIMIZE) (IV.17)	Executes the least-squares fit of the matrix elements to the experimental data.
OP,POIN (POINT) (IV.18)	Execution option to calculate the Coulomb excitation and deexcitation γ-ray yields at fixed scattering angle and bombarding energy.
OP,RAND (RANDOM) (IV.19)	Used to overwrite a given set of matrix elements by a set of random values lying within specified limits.
OP,RAW (IV.20)	Used to input data necessary if efficiency-uncorrected (raw) γ yields and/or yields resulting from summing several γ spectra are to be used as experimental data.
OP,RE,A (RELEASE) (IV.21)	Releases all matrix elements previously fixed and voids all coupling of matrix elements for the current minimization run.

OP,RE,C
(RELEASE)
(IV.22)

Releases all previously fixed matrix elements but preserves couplings.

OP,RE,F
(RELEASE)
(IV.23)

Voids coupling of matrix elements while retaining fixed ones.

OP,REST
(RESTART)
(IV.24)

Causes the program to use, as a starting point, a set of matrix elements stored on disk by a previous calculation in place of the set given as input.

OP,SIXJ
(IV.25)

Creates a table of Wigner 6-j symbols used by the sum rules code SIGMA (Chapter V). OP,SIXJ is case-independent, thus it can be executed without defining the level and matrix elements scheme. It can also be inserted anywhere in the input sequence.

OP,STAR
(START)
(IV.26)

Execution option to calculate only the Coulomb excitation amplitudes and cross sections, not the γ-ray yields. This comprises a subset and consequently an alternative to OP,POIN. This option can be used with either OP,COUL or OP,GOSI.

OP,TITL
(TITLE)
(IV.27)

Reads in the user-given title to be reprinted as a header of the output (maximum 80 alphanumeric characters). Can be repeated if more than one line is needed.

OP,TROU
(TROUBLE)
(IV.28)

Performs an analysis at the local minimum to pinpoint erroneous experimental data. This option must be inserted immediately before OP,EXIT.

OP,YIEL
(YIELDS)
(IV.29)

Used for input of data required if it is necessary to calculate the γ-ray deexcitation of the Coulomb excited nucleus. OP,YIEL is mandatory if OP,GOSI has been selected, in which case it is also used to specify additional spectroscopic information, i.e. branching ratios, mixing ratios, lifetimes and known E2 matrix elements, as well as relative γ detector efficiencies and upper limits of the unobserved transitions. The experimental deexcitation yields are supposed to reside on a separate permanent file attached to the job. Section IV.29 describes the structure of such a file.

IV.2 INPUT FORMATS

As a rule the input should be given in free format mode (READ*). This implies that the number of entries should correspond to the number of variables in the respective read list, different entries being separated by either a comma or a space. Floating-point values can be given as integers (the decimal point is not required and the conversion is automatic). Integers may not be given as floating point numbers. Blanks are not equivalent to zeros, unlike fixed-field formats, therefore zeros must be typed in explicitly. Some exceptions to this general input format will be stressed in the descriptions of various options. A wrong sequence of input entries is usually detected when a number is encountered instead of an expected alphanumeric option code. In this case a message UNRECOGNIZED OPTION --- is issued and the job aborted (--- designates an unrecognized string). This means that the sequence of the input entries is wrong somewhere between the last recognized option command and the entry reprinted.

IV.3 CONT
(CONTROL)

This suboption of either OP,GOSI or OP,COUL is used to override default settings of the job performance controls and to specify optional features of the program. CONT can be omitted if the default settings of the control parameters are satisfactory. CONT can be used anywhere in the OP,COUL and OP,GOSI input stream, usually as the last suboption specified. The input format is as follows:

CONT

. Input control parameters needed for the job.

.

.

END, . Marks the end of CONT input.

The control switches are specified by a three-character alphanumeric string followed by a comma and, in some cases, by a floating point number X (as a convention, X will be used as the initial symbol for floating point entries while symbols beginning with I are specified to be integer). Even if X has obviously the meaning of an integer it should be entered as a floating point number, the conversion being done by the code. Some of the switches require additional input. The available control switches are as follows:

.....

ACC,X. Sets the accuracy parameter used as an internal check of the Adams-Moulton routine to 10^{-X}. The default value is X=5. The step-size is either doubled or halved depending on whether the maximum deviation is less than 0.02×10^{-X} or greater than 10^{-X}. Do not use too large a value of X, as it slows down the calculation considerably with little increase in accuracy for X much larger than 6. Instead use the switch INT, to achieve maximum accuracy. See III.1 for details.

.....

ACP,X. Sets the convergence test parameter for the exp (A) expansion (III.2) to 10^{-X}. Default value is X=5.

.....

CCF, This switch overrides OP,MINI or OP,ERRO commands and causes GOSIA to terminate execution after calculating and storing the internal correction factors. This allows to split the minimization or error estimation jobs, which can be helpful when using unreliable or overloaded computer systems.

.....

CRF, This option causes GOSIA to read in the internal correction factors from file TAPE1 instead of recalculating them. This is a valuable time saver for restarting the minimization and error calculations using the OP,REST command. The internal correction factors are stored on TAPE1 automatically when calculated by the code.

.....

CRD,X. This switch defines which experiments use circular particle detectors. CRD, simplifies the input to OP,INTG.
The additional input is as follows:

IE(1) The indices, according to the input sequence to EXPT, of
IE(2) those X experiments involving circular detectors.
. Note that the axial symmetry option in the EXPT input should
. be used rather than CRD, if the circular detector is
IE(X) symmetric with respect to the z (i.e. beam) axis.

.....

DIP,X. Sets the E1 dipole polarization parameter to be X/1000. (See 1.18). Default value is 5.

END, Mandatory CONT flag marking the end of CONT input.

FIX, This switch provides the easy way to override matrix elements setup specified by ME input. When FIX, is encountered all matrix elements are fixed and only those specified by subsequent input are released for minimization or error estimation. Further input required:

IM The number of matrix elements to be released.
I(1) Indices of the matrix elements to be released (defined
I(2) by the sequence of the ME input).
.
.
I(IM)

Using FIX, it is possible to reduce easily the number of free matrix elements without modifying the ME input.

FMI, Fast minimization switch. Causes the code to terminate the job immediately after the OP,MINI step was completed, without compiling the final output. FMI, provides substantial time saving when the final output is not needed since the compilation of the final OP,MINI output involves full Coulomb excitation calculation. The remainder of the input, including the repeated OP,MINI commands is ignored if the FMI, switch has been selected. FMI, cannot be used when the SEL, switch is set.

INR, Independent normalization switch. Overrides the relative normalization of γ detectors and different experiments as specified in OP,YIEL input. With INR, switch set,the code will calculate the best normalization factors (i.e. the ones providing the minimum value of χ^2 for a given set of matrix elements) for each single γ detector independently.

.....

INT,X. Overrides the default accuracy check parameter,IS,of Adams-Moulton integration routine for specified experiments. The accuracy check is made every IS steps,with a resultant possible change in integration stepsize. The default value is IS=1,thus the stepsize may be adjusted after each complete integration step. Setting IS=1000 effectively switches off the stepsize control since 1000 steps exceeds the range of integration (according to 3.1),forcing the code to retain maximum accuracy. X has the meaning of the number of experiments for which the default is to be altered. Additional input consists of X records,IE_n being the experiment number and IS_n the accuracy control parameter for this experiment. The experiments are numbered according to the sequence of the EXPT input, thus this control switch can only be used after the suboption EXPT definition.

IE_1, IS_1
.
.
.
IE_X, IS_X

.....

LCK, This switch allows to fix a series of matrix elements without modifying the initial setup, e.g. it can be used to keep the matrix elements belonging to a given multipolarity fixed during minimization. It requires further input as follows:

I,I1
I,I1 Ranges of matrix elements to be fixed.
.
.
0,0 Two zeros end input.

.....

NCM,X. Causes the kinematics calculation to be performed assuming final state of the excited nucleus is the state with user-given index equal to X. Default value is 2.0. The states of an excited nucleus are numbered according to the sequence of the LEVE input.

.....

PRT, This overwrites the default options specifying the printout. It requires additional input as follows:

I,I1
.
. I is the print option code and I1 is the user-specified
I,I1 setting. The 0,0 ends the input of the print options.
0,0 The following table lists all the available codes:

CODE	DEFAULT VALUE	OTHER POSSIBLE VALUES	CONSEQUENCES OF OPTION
1	1	0 -1	Prints out level scheme,input matrix elements and kinematics (1). 0 inhibits such printout,while -1 can be used to suppress kinematics only. When 0 is selected, the sequence: CONT PRT, 1,0 0,0 END, should be inserted before the LEVE and ME suboptions of either OP,COUL or OP,GOSI to set an appropriate flag.
2	1	0	Reprint of experimental γ yields to be fitted (1). 0 suppresses this printout.
3	1	0	Prints out experimental branching ratios and a comparison of experimental and calculated values (1). 0 inhibits this printout.

4	-2	0 or any positive integer	Prints out the yield sensitivity (α_y parameters) map (see III.5) after every I1 number of minimization steps if I1 is positive. Note that compilation of this yields sensitivity map is time consuming since it requires calculation of derivatives with respect to all matrix elements. Consequently, it should be compiled only when necessary. I1=-2 causes the compilation of this map when the OP,EXIT command is encountered after at least one execution of the OP,MINI command. I1=0 specifies no compilation or printout of this sensitivity map.
5	1111	Any positive integer	Prints out the value of χ^2/N, where N is the number of data points, after every specified I1 number of minimization steps. If I1=1 then χ^2/N will be printed after every step.
6	11111	Any positive integer	Printout of the gradient will occur every I1 minimization steps. Default value effectively inhibits this printout.
7	0	1	Specifies printout of excitation amplitudes and population when OP,EXIT is encountered after at least one OP, MINI command (1). I1=0 specifies no such printout.

8	1	0	I1=1 specifies a comparison of experimental and calculated yields. I1=0 specifies no such printout. This table will not be compiled if FMI, switch was used, even if I1=1.
9	0		Unused - free to be assigned.
10	1	0	I1=1 specifies printout of kinematics for each integration meshpoint. I1=0 inhibits such printout.
11	1	0	I1=1 specifies printout of γ yields for each integration meshpoint. I1=0 inhibits such printout.
12	1	0	I1=1 specifies printout of q-parameter maps. I1=0 inhibits such printout.
13	1	0	I1=1 specifies printout of normalization constants as defined by equation 4-18. I1=0 inhibits such printout.
14	1	0	I1=2 specifies printout of the deorientation effect attenuation coefficients. I1=0 inhibits such printout.

15	1	0	I1=1 specifies printout of mean lifetimes. I1=0 inhibits such printout.
16	0	1	I1=1 causes all possible calculated yields to be printed in the tables comparing the experimental and calculated yields. I1=0 causes the printout of the experimental and calculated yields only for the observed transitions and unobserved transitions for which the calculated values exceed the upper limits specified in the OP,YIEL input.
17	0	Any positive integer	Causes printout of the probability sensitivity maps (the α_p parameters defined in III.5). I1 specifies the number of matrix elements having the largest influence to be printed for each level with the corresponding α_p values.
18	0	1	Causes the printout of the interpolated internal conversion coefficients. I1=0 inhibits this printout.
19	0	1	I1=1 causes the printout of excitation amplitudes when executing commands other than OP,STAR (e.g. OP,INTG).

20	0	1	I1=1 causes the printout of efficiency-uncorrected yields and respective efficiencies if OP,RAW is used. This output is produced on TAPE23. Note that the γ-ray energies printed out are Doppler-shifted, according to the user-given geometry and calculated kinematics Modified energies are used to calculate the detection efficiencies.

SEL, Creates a file (TAPE18) containing the information needed by the program SELECT to generate the correlation matrix used for the error calculation - see the description of OP,MINI and OP,ERRO. This switch is only active when OP,MINI is executed with a default setting of the print parameter 4 (see the description of the print parameters defined by the PRT, switch below).

SKP, This causes the code to skip selected experiments during the minimization procedure, i.e., the code does not take into account the selected experiments. This switch can be quite useful since often a subset of the experiments is sensitive only to a subset of matrix elements. The SKP, switch requires additional input:

IE The number of experiments to be skipped.

I(1)
I(2)
. The indices of experiments to be skipped (experiments are numbered according to the sequence in which they appear in the EXPT input).
.
I(IE)

SMR, This control switch causes the input file for the SIGMA program (See Section V) to be generated when OP,ERRO is executed. This switch is ignored if OP,ERRO is not executed.

TEN, Causes GOSIA to write the statistical tensors in the system of coordinates defined by Fig. I.3 on TAPE17 when either OP,STAR or OP,POIN is executed. The tensors written are the pure Coulomb excitation tensors, as defined by 1.30, and can subsequently be used by the external programs to examine the γ-decay process (e.g. to study the deorientation effect). The structure of the statistical tensors file is described in Chapter VI.

VAC, This switch is used when it is desired to change the default parameters used to evaluate the vacuum deorientation effect (I.2.1). It requires the following additional input:

I,X(I) where I= 1,2,...,7 specifies the parameter to be overwritten, X(I) being the new value. Two zeros end this input. The parameters are defined as in 1.53 . The index value I is as follows:

I	X(I)	Default Value
1	J_1	3
2	Γ	$0.02(ps^{-1})$
3	Λ^{∞}	$0.0345(ps^{-1})$
4	τ_c	3.5(ps)
5	g	Z/A
6	K	6.10^{-6}
7	x	0.6

A common g factor is assumed for all nuclear levels. Note that g=Z/A often is a poor estimate. The known g factors of the lowest states can be used to give a better estimate.

Note that since the lifetimes are given in picoseconds the field strength parameter K is 10^{-12} times the true value in gauss (the default values corresponds to 6.10^{6} gauss).

The deorientation effect can be switched off (if, for example, the influence of deorientation on the result is to be tested) by specifying:

```
VAC,
3,0.
6,0.
0,0.
```

.....

WRN,X. This switch causes a warning message to be printed with the comparison of experimental and calculated yields for those yields for which the experimental and calculated values differ by more than X standard deviations. The default setting is X=3.

IV.4 OP,CORR
(CORRECT)

This execution-only option requires no input other than the command itself. It uses the file of original experimental yields (see Section IV-30), read from TAPE3, and writes on TAPE4 a set of yields which have been modified to correct for the difference between the yields calculated using full integration and the yields calculated using "mean" values of bombarding energy and scattering angle for each experiment (see Equation 3.23). The modified (corrected) experimental yields, on TAPE4, then are used as data for the minimization and error estimation procedures. The OP,INTG and OP,CORR commands must be run as one job with the OP,CORR command following OP,INTG in the sequence of option commands. The values of the mean energy and scattering angle used for the point calculations are those specified for each experiment in the EXPT input.

Note that NTAP (specifying the file containing the experimental yields in OP,YIEL) must equal 3 when using the OP,CORR command (i.e. the file containing the original uncorrected experimental yields must be TAPE3).

IV.5 OP,COUL
(COULEX)

This option is used to calculate the Coulomb excitation cross sections and yields of deexcitation γ-rays when no fitting of matrix elements to data is required. This option essentially is a truncated version of OP,GOSI which it replaces when fitting of matrix elements to data is not desired. The advantage of OP,COUL over the alternate OP,GOSI is that the considerable input of data required for the fitting procedure can be omitted. The OP,COUL command is used to input the information defining the nucleus studied and the experiments for which the Coulomb excitation calculations are to be performed. The OP,COUL command should occur immediately following OP,TITL since the input to OP,COUL is used by almost all modules of the program. The input to OP,COUL comprises four different sub-options:

LEVE — Read and establish the level scheme of the investigated nucleus. See Section IV.13.

ME — Read and catalog the matrix elements. See Section IV.15. Note that this sub-option input differs from that of the version used with OP,GOSI.

EXPT — Input of experimental parameters. See Section IV.8.

CONT — Used to control and select various optional features of the program for both execution and output. This suboption can be omitted in which case default parameters of the code will be used. See Section IV.3.

A blank record is necessary to terminate the input to OP,COUL.

IV.6 OP,ERRO
(ERRORS)

The module of GOSIA activated by OP,ERRO is designed primarily for estimating the error bars to be assigned to the set of matrix elements corresponding to the minimum value of χ^2. However,this option can also be helpful in checking the existence of better solutions by providing a relatively fast way of scanning the χ^2 hypersurface. Error estimation is performed in two separate stages - first,the "diagonal",or uncorrelated errors are found, next, the diagonal errors are used in the estimate of the "overall", or correlated errors. This procedure is described in detail in Section III.6, see also Chapter VIII for some recommendations concerning the use of OP,ERRO.

The input to OP,ERRO is as follows:

OP,ERRO
IDF,MS,MEND,IREP,IFC,RMAX

where:

IDF — Mode flag. IDF=0 sets diagonal error calculation mode,IDF=1 causes overall error estimation.

MS,MEND — The range of matrix elements indices for which error estimation is to be performed, i.e. the calculation will be carried out for matrix elements with indices fulfilling MS ≤ INDEX ≤ MEND. MS can also be entered as 0 or -1. MS=0 implies that the calculation will be performed for all matrix elements (excluding fixed ones - see below), thus providing a short form of specifying the full range. MS=-1 can be used only for "overall" error calculation (IDF=1). This allows the user to select an arbitrary set of the matrix elements defined by additional input required only if MS=-1. In this case the input to OP,ERRO is as follows:

```
OP,ERRO
1,-1,0,IREP,IFC,RMAX
MS_1,MEND_1
   .
   .
MS_n,MEND_n
0,0
```

where MS_i and $MEND_i$ define the range of matrix elements indices similarly to MS and MEND when both are positive. MS_i=$MEND_i$ selects a single matrix element. Two zeros terminate this portion of input. This feature allows to repeat the overall error estimation for a subset of matrix elements or to include the matrix elements which previously have been skipped without modifying the ME setup.

A given value of MEND is redundant if MS=0 or MS=-1 has been selected.

IREP Repetition flag, assuming values of 0,1 or 2. IREP=0 implies a new calculation, i.e. no previously stored errors are read in and the error file will be created. Obviously, IREP=0 should be used in conjunction with IDF=0 for a first calculation of the diagonal errors. IREP=1 causes previously stored errors to be read in and used for the continuation of the error estimation. The errors are stored on file TAPE15, which is updated during each execution of OP,ERRO. IREP=2 means that the sum-rules file, TAPE3, has already been created during a previous "overall" errors calculation and causes the code to read it in and update it during the current run. The CONT switch SMR, should be set for both creation and update of TAPE3. Note that in this case the experimental yields must reside on TAPE4 to avoid a multiple definition of the input/output files. TAPE3 is created with IREP=1 and updated with IREP=2 only if SMR, was specified. IREP=2 reduces to IREP=1 if the SMR, switch was not encountered. Both TAPE15 and TAPE3 are required by the sum-rules code SIGMA - see Section V.2.2.

The proper combination of MS,MEND and IREP makes it posssible to split the time-consuming error estimation into several runs which is important when running GOSIA on heavily loaded or unreliable computers.

IFC — IFC=0 specifies that the correlation matrix is to be used to reduce the number of matrix elements taken into account to calculate the correlated errors (see Section III.6). The correlation matrix is created by the external program SELECT. To prepare the input information for SELECT it is necessary to execute OP,MINI with CONT switch SEL, and the default value of the print parameter 4, i.e. 4,-2. This should be done at a final stage of minimization prior to the error calculation. The information for SELECT is written by GOSIA on TAPE18 which should be attached to SELECT also as TAPE18. No other input is necessary. The output from SELECT is written on TAPE10 and should be attached to the OP,ERRO job as TAPE18.

IFC=1 implies that the correlation matrix will not be used. In this case it is not necessary to create and attach TAPE18. It is however strongly recommended that IFC=1 be used only for small cases with all matrix elements of similar significance. Otherwise, selecting IFC=1 will dramatically increase the execution time with no effect on the result.

IFC is redundant if IDF=0.

RMAX — The largest floating point number available on a given computer. RMAX is used to prevent possible overflows during the scan of a probability distribution (see III.6).

Note: Fixed matrix elements will not be varied during the error calculation. Matrix elements cannot be coupled when OP,ERRO is executed. Use release options (OP,RE,A and OP,RE,F) to remove couplings and unwanted fixing of matrix elements introduced in the ME setup.

IV.7 OP,EXIT

This option causes the code to terminate the execution and to compile the final printout as specified by the CONT PRT, print options. OP,EXIT may be inserted anywhere in the input stream and the execution will terminate after the completion of the last executable OP,--- command encountered before OP,EXIT. The remainder of the input stream will be ignored, thus OP,EXIT allows to execute various modules of the code without removing the irrelevant portions of the input. No additional input is required.

IV.8 EXPT (Mandatory suboption of OP,COUL and OP,GOSI)

This suboption provides input of the experimental conditions used for the various experiments to be analyzed. The experiments are defined by mean values of projectile energy and scattering angle, which are used for "point" excitation/deexcitation calculations. The realistic approach must include integration of γ yields over finite ranges of bombarding energy and scattering angles. This feature is provided by OP,INTG which should be used to reproduce observed γ yields. As described in Chapter III, GOSIA uses "point" energy and scattering angles to execute all modules except for the integration module activated by OP,INTG. The options OP,INTG and OP,CORR are used to convert experimental γ yields to "point" values. Mean values of bombarding energy and scattering angle used by OP,CORR are the ones given in the EXPT input.
The input to EXPT is as follows:

EXPT
NEXP, Z_1, A_1
$\pm Z_n$, $\pm A_n$, E_p, $\pm\theta_{LAB}$, M_c, M_a, IAX, ϕ_1, ϕ_2, IKIN, LN
. . .
. . .
. . .

NEXP records equal to the number of experiments.

The experiments will be numbered by the code according to the sequence of these records from 1 to NEXP.

Detailed explanation of entries is given below.

NEXP — The number of experiments defined in the input. Each experiment corresponds to a particular combination of bombarding energy, scattering angle, experimental detector arrangement and (Z,A) of the nucleus exciting the nucleus

being investigated. (NEXP≤50).

Z_1 Charge number of the investigated nucleus (Integer format).

A_1 Mass (in units of amu) of the investigated nucleus.

Z_n Charge number of the uninvestigated nucleus. A positive value signifies target excitation, i.e., $Z_n = Z_{projectile}$. A negative value signifies projectile excitation, i.e., $Z_n = Z_{target}$ (Integer format).

A_n Mass (in the units of amu) of the uninvestigated nucleus. A_n will thus correspond to the projectile mass if Z_n is positive and target mass if Z_n is negative. A negative sign appended to A_n signifies that this is a "thick" target experiment, that is, the beam is completely stopped in the target. This latter option has the time saving feature of switching off some irrelevant calculations such as the deorientation effect and recoil velocity correction.

E_P The mean projectile bombarding energy, in the laboratory frame of reference, to be used for calculating the Coulomb excitation yields for the particular experiment. Input in units of MeV.

θ_{LAB} The mean scattering angle (degrees) of the projectile in the laboratory frame of reference. θ_{LAB} must be positive if the projectile is detected. A negative sign should be given with the true value of the <u>projectile</u> scattering angle if the recoiling target nucleus has been detected to ensure the selection of the proper kinematics. Note that by definition θ_{LAB} is always positive, the sign being only used by the code to set appropriate flags.

M_C Controls the number of magnetic substates to be included in the full Coulomb excitation calculations. For a given ground state polarization M_o, the magnetic substates in the range (M_o-M_c, M_o+M_c) will be included for each level. The code takes care of the obvious limitations in magnetic substates set by the spins of the states. $M_c=0$ corresponds to the conservation of magnetic quantum number as occurs for backscattering.

M_A Controls the number of magnetic substates to be included in the approximate Coulomb excitation calculation. The meaning of M_A in the same as for M_C, namely magnetic substates in the range (M_o-M_a, M_o+M_a) will be included for all states for a given ground state polarization M_o). The only allowed values of M_a are 0 or 1.

IAX The axial symmetry flag which can take values of 0 or 1 only. Zero defines axial symmetry of the particle detector in which case further input is simplified and the calculations are speeded up. Unity implies that axial symmetry is not assumed.

ϕ_1, ϕ_2 The azimuthal angular limits of the particle detector (in degrees). The coordinate system used has the z axis in the direction of the incoming beam. The x and y axes can be defined in any convenient way provided that the angles of all detectors are given relative to the same cooordinate system. Note that ϕ_2 must be larger than ϕ_1.

IKIN The kinematics flag which can take values of 0 and 1 only. If $A_{Projectile} > A_{Target}$, IKIN specifies which of the two possible kinematic solutions to choose. IKIN=0 implies that the solution having the larger center-of-mass scattering angle is chosen. Redundant if $A_{Projectile} < A_{Target}$.

NOTE : if use INR (under CONT p. 109) then it overrides the relative normalization of γ-detectors and ϕ Expt as specified in OP,YIEL input.

LN Normalization constant control which specifies that the given experiment has a normalization constant coupled to that for experiment LN. The normalization constant is the factor normalizing the calculated yields to the experimental for a given experiment (See the description of the input YNRM in OP,YIEL, Section (IV.29). Experiments are numbered according to the sequence of records read in under EXPT. Therefore, if LN is equal to the record number defining a particular experiment then an independent normalization is assumed. If LN does not equal the record number defining a given experiment then the program requires a user-given relative normalization between the current experiment and experiment LN which is input using the OP,YIEL command.

This input is useful for experiments where several scattering angles are measured simultaneously and therefore the relative normalization for the different scattering angles is known for this common experiment. The code will fit one absolute normalization constant to the coupled experiments.

As an example consider two experiments to study ^{72}Ge. One experiment involves Coulomb excitation of a ^{72}Ge target by a 50 MeV ^{16}O beam studied at a laboratory scattering angle of 160° using an annular particle detector. The second experiment involves projectile excitation of a 170 MeV ^{72}Ge beam on a ^{208}Pb target studied at a scattering angle of 150° by a particle detector subtending an azimuthal ϕ range from -30° to 30°. The sample input is as follows:

```
EXPT
2,32,72
8,16,50,160,3,1,0,0,0,0,1
-82,208,170,150,3,1,1,-30,30,0,2
```

Three magnetic substates are included for the full Coulomb excitation calculation and 1 magnetic substate for the approximate calculations for both experiments. Experiment 1 was done using an axially symmetric geometry, therefore ϕ_1 and ϕ_2 are redundant. Independent normalization of both experiments is desired; therefore, the LN indices correspond to the experiment record numbers. In both cases $A_{projectile} < A_{target}$, thus IKIN is redundant.

IV.9 OP,FILE

This option allows to define the permanent files necessary for a current job in the GOSIA input rather than in an external job control stream. The use of OP,FILE is optional, but when used it should be the first command in the input stream, so the full output goes to the user-defined file. The input to OP,FILE is as follows:

```
OP,FILE
I1,I2,I3
NAME
  .
  .
0,0,0
```

where:

I1 - Unit number (TAPE number). I1=22 is the ouput file.

I2 - Status indicator. I2=1 indicates STATUS=OLD, I2=2 implies STATUS=NEW, while I2=3 corresponds to STATUS=UNKNOWN.

I3 - I3=1 to indicate formatted file, I3=2 means unformatted (binary) file. All files used by GOSIA are formatted, except of TAPE1 (internal correction coefficients file) which should be declared as unformatted.

NAME - user-assigned filename.

IV.10 OP,GDET
(GE DETECTORS)

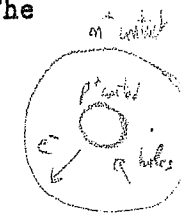
This option is used to create a file (TAPE9) which contains the data needed to reproduce the γ-energy dependence of the solid angle attenuation factors for the coaxial Ge or detectors (see Section I.2.3). For each γ detector a calculation following the formalism presented in Section I.2.3 is carried out at several γ-energy meshpoints, then the energy dependence is fitted using a rational approximation according to Eq. 3.15. The fitted coefficients stored on TAPE9 are automatically read in when OP,YIEL or OP,INTG is encountered. This means that OP,GDET should be executed once before the execution of either OP,YIEL or OP,INTG.

The input to OP,GDET is as follows:

NPD — A number of physically different γ detectors being used for a whole set of experiments defined in EXPT. The physically identical detectors are understood as the ones having an identical crystal geometry and being placed at the same distance from the target. In addition, if graded absorbers were used, the physically identical detectors are assumed to be equipped with the same sets of graded absorbers. (NPD≤50)
NPD should be given with a minus sign appended if OP,RAW is to be used, i.e. if any of the experiments defined contains not efficiency-corrected spectra. In this case an additional file, TAPE8, is created. TAPE8 contains the absorber information, needed to reproduce the efficiency curves - see OP,RAW (IV.20).

r,R,L,d

$l_1, l_2 \ldots l_7$ Specifies the geometry and the graded absorbers setup for each of the physically different detectors. This sequence should be repeated NPD times. All entries are given in centimeters. The entries are defined as follows:



r The radius of the inactive p-core (the inner radius of a crystal)

R The radius of the active n-core (the outer radius of a crystal).

L The length of a crystal.

d The distance from a target to the face of a crystal.

$l_1 \ldots l_7$ The thicknesses of the commonly used graded absorber materials, with the subscripts 1 through 7 corresponding to Al, C, Fe, Cu, Ag/Cd/Sn, Ta and Pb, respectively. The absorption coefficients for these materials are defined in GOSIA, for the energy meshpoints used, as internal data.

It should be noted that if Ta or Pb absorber layers were used it is assumed that the γ transitions having an energy below the cutoff of the absorption curve are of no interest, therefore the energy-dependence fit is made only using a subset of meshpoints corresponding to the γ energies above 60 keV if Cd/Sn layer was employed, above 80 keV if a Ta layer was employed and above 100 keV if a Pb layer was employed. It is also assumed that the symmetry axis of the crystal is aligned with the center of the target. Moreover, the effect of the in-flight decay, which changes the geometry as seen by a decaying nucleus, is not taken into account for the estimation of the solid angle attenuation factors. The significance of this correction is in all cases far below the level of the experimental accuracy.

IV.11 OP,GOSI
(GOSIA)

This alternate option to OP,COUL is used when fitting matrix elements to Coulomb excitation data. The OP,GOSI command is used to input the information defining the nucleus studied and the Coulomb excitation experiments to be used in the least-squares fit procedure. The OP,GOSI command shall occur immediately following OP,TITL since the input to OP,GOSI is used by almost all the other option commands of this program. OP,GOSI requires the same input sequence of suboptions as OP,COUL, the only difference being that a different version of ME is used. That is, the input comprises the following four suboptions:

LEVE (LEVELS)	Read and establish the level scheme of the investigated nucleus. See Section IV.13.
ME	Read and catalog the matrix elements. See section IV.16. Important: note that the input to ME under OP,GOSI differs from the version used for OP,COUL.
EXPT	Input of experimental parameters. See Section IV.8.
CONT (CONTROL)	Used to control and select various optional features of the program for both execution and output. This option can be omitted in which case default parameters of the code will be used. See section IV.3.

A blank record is necessary to terminate the input to OP,GOSI.

IV.12 OP,INTG
(INTEGRATE)

This command produces the most accurate calculation of the yields of deexcitation γ-rays following Coulomb excitation to be used for realistic comparison with experimental data. This option includes integration over solid angle of the particle detectors, energy loss in the target as well as full correction for the recoil velocity of the deexciting nucleus and the deorientation effect.

OP,INTG comprises two distinct stages. The first stage calculates the yields of deexcitation γ-rays integrated over azimuthal angle ϕ for each energy and scattering angle meshpoint. This calculation of the meshpoint yields should be repeated for each experiment according to the order the experiments appear in the EXPT input. GOSIA stores the calculated meshpoint yields on internal files. The second stage uses the data stored on these internal files to integrate over bombarding energy and the range of scattering angles subtended by the particle detectors which is performed by interpolating between the γ yields calculated at each meshpoint. It is permitted to integrate over any arbitrary (θ,ϕ) shape for the particle detector including the case of several (≤ 4) ϕ ranges for each θ value. An option is included to simplify integration over circular detectors because of the frequent use of such a geometry. The input for the circular detector is a sligthly modified subset of the normal input.

The full input to OP,INTG is described below followed by the input for the circular detector option. Since the input to OP,INTG is long a summary of the input is given at the end of this section to serve as a quick reference.

IV.12.1 NORMAL INPUT TO OP,INTG

OP,INTG

NE,±NT,E_{min},E_{max},θ_{min},θ_{max}

NE — The total number of energy meshpoints at which full Coulomb excitation calculations will be performed (NE≤11).

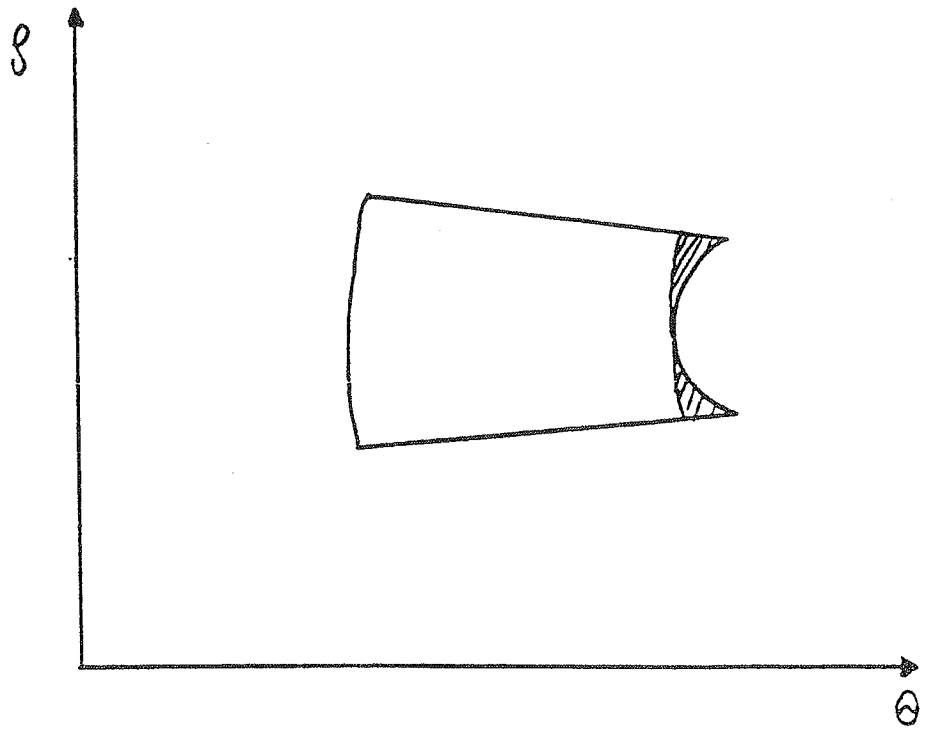
NT — The total number of θ meshpoints at which the full Coulomb excitation calculations will be performed. Negative value of NT specifies that the (θ,ϕ) shape of the detector will be determined by the user - see below.

E_{min},E_{max} — The minimum and maximum bombarding energies (in MeV) between which the integration is to be performed.

θ_{min},θ_{max} — The minimum and maximum angles (in degrees) between which the integration is to be performed. Note, θ angles are always positive and correspond to laboratory scattering angles of the detected particle, that is, the angle of the scattered projectile if it is detected and the angle of the recoiling target nucleus if it is detected. The above input string is modified if the circular detector flag CRD in CONT is activated for this experiment, as described later.

$E_1, E_2, \ldots E_{NE}$	Energy meshpoints at which the exact Coulomb excitation calculations are performed (MeV). These must exceed or at least equal the range over which the integration is to be performed to obtain reliable Lagrange interpolation.
$\theta_1, \theta_2, \ldots \theta_{NT}$	Projectile scattering angles (degrees) in the laboratory frame, used as meshpoints. Note, if the target is detected then the projectile scattering angle corresponding to the detected recoiling target angle must be input with a negative sign to set the flag specifying the target nucleus detected. The input angles must correspond to the detected particle angular range which exceeds or at least equals the range of angles subtended by the detector to obtain reliable Lagrange interpolation. Do not input these angles for the circular detector option.
NFI	The number of ϕ ranges for each θ_i meshpoint needed to describe the $\theta(\phi)$ dependence.
$\phi_1, \phi_2, \ldots$	NFI pairs of ϕ angles describing the ϕ range for given θ_i.

The above two records must be input for each θ meshpoint specified. NFI should not exceed 4. In most cases NFI=1, then the pair of ϕ angles simply specifies the lower and upper ϕ limits for a given θ meshpoint. However, for some geometries, such as for rectangular shaped detectors, it is necessary to include more than one ϕ range for some θ values. For example, a rectangular detector placed with its normal at 45° to the incident beam has (θ,ϕ) contours shown in adjacent figure:



The contours for the largest θ are subdivided into two ranges of ϕ as shown by the cross hatched areas in the figure. Thus, in this case NFI=2 for any θ meshpoint in the cross hatched area.

Do not input NFI and the ϕ ranges if either the circular detector option or axial symmetry is specified.

This ends the input required to calculate the γ-ray yields integrated over azimuthal angle ϕ at the specified set of meshpoints. This part of input must be repeated for all experiments defined in EXPT.

The second stage of the input is required for the integration and once again has to be entered for all experiments:

NP	Number of stopping powers to be input, $3 \leq NP \leq 20$. If NP=0 then the stopping power table is taken from the previous experiment and the following input of energy and dE/dx values can be omitted for this case. This is useful where experiments differ only with regard to range of scattering angles or bombarding energies.

$E_1, E_2, .., E_{NP}$ The energy meshpoints (in MeV) at which values of the stopping power are to be input.

$(\frac{dE}{dx})_1 \; .. (\frac{dE}{dx})_{NP}$ Stopping powers in units of MeV/(mg/cm^2). Interpolation between the energy meshpoints of the stopping power table is performed during integration. Consequently it is important to ensure that the range of energy meshpoints of the stopping power table exceed the range of energies over which the integration is to be performed.

NI1,±NI2 The number of equal subdivisions of energy (NI1) and projectile scattering angle (NI2) used for integration. Lagrange interpolation is performed to interpolate between the (E_i, θ_i) meshpoints at which the full Coulomb excitation calculations of the deexcitation γ-ray yields were performed (See Section III.4). Both NI1 and NI2 should be even and not exceed 100. If odd values are given the program increases them to the next larger even number. However, the $\Delta\phi$ input will be confused if NI2 is negative and odd.
Important: NI2 can be negative and must be negative if NT is specified to be negative. Conversely, NI2 must be positive if NT is positive. If NI2 is negative then the following input must be provided:

$\Delta\phi_1, \Delta\phi_{|NI2|+1}$ where $\Delta\phi_i$ is the total range of ϕ (in degrees) for each equal subdivision of projectile scattering angle. That is, $\Delta\phi_i$ equals the sum of all ϕ ranges for a given subdivision θ value if the azimuthal angular range also is

subdivided into non-contiguous regions. Note that there is an important difference in how the interpolation over scattering angle is performed depending on whether NT and NI2 are both positive on both negative. For the positive sign the program interpolates between the calculated yields at each θ meshpoint. This produces excellent results if the ϕ dependence of the particle detector is a smooth function of projectile scattering angle, θ.

The negative sign option should be used if the ϕ dependence is more complicated or if ϕ changes rapidly with θ. When the negative sign is used the program stores for each meshpoint the calculated yields per unit angle of azimuthal range, i.e., the calculated yields divided by the total ϕ range specified at that angle for the exact calculation. The program then interpolates these yields per unit of ϕ between the meshpoints. These interpolated values are then multiplied by the appropriate $\Delta\phi$ for each subdivision meshpoint prior to integration. Note that the code uses NI2 equal subdivisions of projectile scattering angles. This is not the same as equal division of geometric angle of the detector if the recoiling target nucleus is detected.

The circular detector option (CONT CRD,) incorporates a feature to calculate automatically the azimuthal angular range $\Delta\phi$ at each subdivision of scattering angle θ. Consequently, do not input $\Delta\phi$ values when using the circular detector option.

The integration-related portion of the input must be repeated for each experiment defined in EXPT.

It is recommended to use as small a number of meshpoints as possible because the full Coulomb excitation calculations performed at the meshpoints are time-consuming. In many cases the required accuracy can be achieved by requesting a large number of subdivisions between the meshpoints, the values in subdivision points being found by fast interpolation.

IV.12.2 CIRCULAR DETECTOR OPTION

The input for a given experiment differs slightly if the circular detector option is selected. This option is activated by the flag CRD, in the CONT suboption of either OP,COUL or OP,GOSI. For such experiments the input to OP,INTG is as follows:

NE,NT,E_{min},E_{max},θ,ϕ,$\theta_{1/2}$	In this case θ and ϕ are the angular coordinates of the center of a circular particle detector subtending the half-angle $\theta_{1/2}$. The remaining entries are identical to the ones described in the previous section.
$E_1,E_2,\ldots,E_{NE}$	The energy meshpoints for the full Coulomb excitation calculation, analogous to those described in the previous section.

The above input is used in the first stage, that is, in the meshpoint calculation. The input of the second stage, that is, the integration section, should look as follows:

NP	Number of stopping powers to be input.
$E_1,E_2,\ldots,E_{NP}$	Energy meshpoints for the stopping powers in MeV.
$(dE/dx)_1,\ldots,(dE/dx)_{NP}$	The values of the stopping powers, analogous to the normal input. If NP=0 the values of this table will be those from the previous experiment.
NI1,NI2	Number of subdivisions of energy (NI1) and projectile scattering angle (NI2) used during the integration. Both shall be even numbers and shall not exceed 100.

IV.12.3 SUMMARY OF INPUT TO OP,INTG - NORMAL INPUT

OP,INTG

NE,NT,E_{min},E_{max},θ_{min},θ_{max}

$E_1, E_2, \ldots, E_{NE}$

$\pm\theta_1, \pm\theta_2, \ldots, \pm\theta_{NT}$

NFI

$\phi_1, \phi_2, \ldots, \phi_{2NFI-1}, \phi_{2NFI}$

This portion of input is to be entered for each experiment defined in EXPT, unless axial symmetry or circular detector option have been used.

NP

$E_1, E_2, \ldots, E_{NP}$

$(dE/dx)_1, (dE/dx)_2, \ldots, (dE/dx)_{NP}$

NI1,±NI2

$\Delta\phi_1, \Delta\phi_2, \ldots, \Delta\phi_{|NI2|+1}$

This portion of input must again be given for each experiment.

IV.12.4 SUMMARY OF INPUT TO OP,INTG - CIRCULAR DETECTOR OPTION

. OP,INTG

NE,NT,E_{min},E_{max},θ,ϕ,$\theta_{1/2}$

E_1,E_2,...,E_{NE}

This input should be defined in the part of the input related to the calculation of the meshpoints. The remainder, listed below, should be included in the integration-related section.

NP

E_1,E_2,...,E_{NP}

$(dE/dx)_1$,$(dE/dx)_2$,...,$(dE/dx)_{NP}$

NI1,NI2

IV.13 LEVE
(LEVELS)

Mandatory suboption of both OP,COUL and OP,GOSI

This suboption is used to define the level scheme of the investigated nucleus. Each level of the investigated nucleus is defined by a single record. The input is as follows:

LEVE	
I_1,IP_1,S_1,E_1	Each record describes one level,the number of
I_2,IP_2,S_2,E_2	records being equal to the number of levels of
I_3,IP_3,S_3,E_3	the investigated nucleus to be included in the
...	calculations.
0,0,0,0	Terminates input to LEVE.

I	Is a user-given state number. Each nuclear level will be referred to in the code by its I value. By convention, index of the ground state must be 1.
IP	Can be given values of +/-1. Positive parity is designated by +1 and negative parity by -1.
S	Is a floating point number specifying the spin quantum number of the state.
E	Is a floating point number specifying the excitation energy of the state in MeV.

The input to LEVE is terminated by four zeros.

IV.14 OP,MAP

This execution option causes the calculation and storage of the maps of the q-parameters (see Section III.2). Maps for $\Delta m = \pm 1$ transitions will be calculated only if the inclusion of the magnetic substates was requested for the approximate calculations by setting M_A=1 in the input to EXPT. The maps will be read correctly if the input to EXPT is subsequently changed to M_A=0. However, the maps will be read incorrectly if OP,MAP was executed with M_A=0 and subsequently M_A was changed to 1. The maps are stored on TAPE7 and read from TAPE7. Both minimization and error calculation require that TAPE7 is attached to the job if OP,MAP was not executed during the same run.

No input other than the command is required for OP,MAP.

IV.15 ME (OP,COUL)

Mandatory suboption of OP,COUL

This suboption of OP,COUL is used to input and catalog the matrix elements. The suboption LEVE must precede ME since the catalog of matrix elements is performed using the level scheme and state indices assigned using the LEVE command.

The input is as follows:

ME	
λ,0,0	Specify multipolarity λ.
INDEX1,INDEX2,ME	List of matrix elements for multipolarity λ.
INDEX1,INDEX2,ME	
INDEX1,INDEX2,ME	
λ_1,0,0	Specify multipolarity λ_1.
INDEX1,INDEX2,ME	List of matrix elements for multipolarity λ_1.
INDEX1,INDEX2,ME	
INDEX1,INDEX2,ME	
.	
.	
.	
0,0,0	Terminates ME input.

The matrix elements for each multipolarity are given separately. The set of matrix elements for a given multipolarity is preceded by a single record defining the multipolarity λ, i.e.

λ,0,0

where λ=1 through 6 for E1 through E6 respectively while λ=7 for M1 and λ=8 for M2. The ME data sets for each multipolarity must appear in increasing order for λ=1 through λ=8. Unused multipolarities can be skipped in the input. The matrix elements for each multipolarity are read in as

INDEX1,INDEX2, ME — INDEX# is the user given state number as defined in the LEVE input

ME = <INDEX2||E(M)λ||INDEX1> i.e., the reduced multipole matrix element defined by equation 1.16

Note that the definition of reduced matrix element does not include the i^1 term for the Eλ matrix elements used in the original Winther-deBoer semiclassical Coulomb excitation code (WI66). The Eλ matrix elements are given in units of e.barns$^{\lambda/2}$ i.e., e$(10^{-28}m^2)^{\lambda/2}$ The Mλ matrix elements are given in units of μ_n.barns$^{(1-1)/2}$. Within a given multipolarity, only matrix elements in the upper triangle, i.e. INDEX2≥INDEX1, should be given. Matrix elements in the lower triangle are set by the program. Within a given multipolarity both INDEX1 and INDEX2 columns must appear in increasing order (odometer ordering). The header of the next multipolarity ends input for a given multipolarity. A single record of 3 zeros ends the input to ME.

RESTRICTIONS:

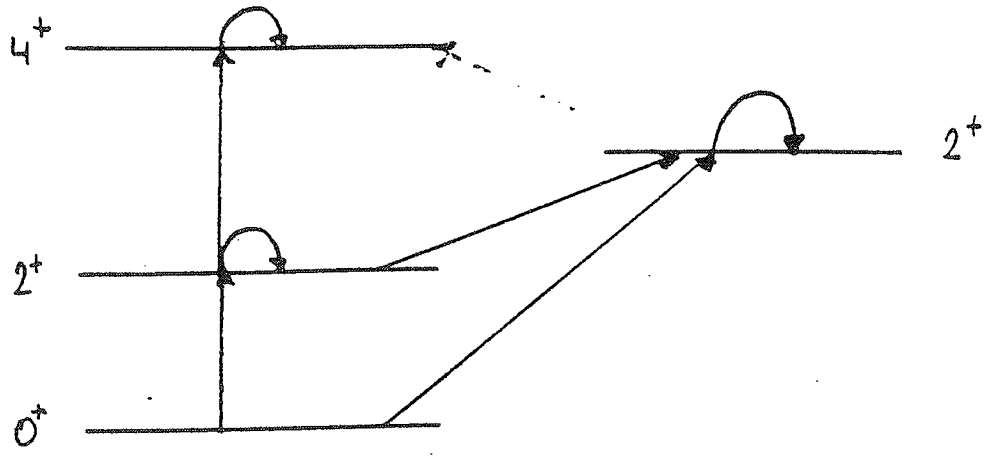
Note that the sequence of matrix elements is uniquely set by the input conventions. An error message will be printed and the job aborted if any of the following restrictions are violated.

a. Multipolariaties must appear in order from lowest to highest starting with Eλ and then Mλ.

b. Matrix elements must belong to the upper triangle, i.e., INDEX2 ≥ INDEX1.

c. INDEX values must be in increasing order, i.e. odometer order.

EXAMPLE: An example of the use of the suboptions LEVE and ME for a OP,COUL calculation is given below. Consider the following nuclear level scheme:



The 2_1^+-2_2^+ coupling is assumed to be of mixed M1 and E2 character. Definition of this nuclear system should be as follows:

```
OP,TITL
Example of definition of nucleus
OP,COUL
LEVE
1,1,0,0                    Ground state is given index "1".
2,1,2,0.500
3,1,4,1.000
4,1,2,0.750
0,0,0,0                    Ends LEVE input.
ME
2,0,0                      E2 matrix elements. All E2 matrix elements
1,2,1.0                    equal to 1.0 e.barns.
1,4,1.0
2,2,1.0                    INDEX1 and INDEX2 in increasing order.
2,3,1.0
2,4,1.0
3,3,1.0
4,4,1.0
7,0,0                      Terminates input for E2. Starts input for
2,4,1                      M1 matrix element equal to 1μN.
0,0,0                      End ME input.
```

IV.16 ME (OP,GOSI)

Mandatory suboption of OP,GOSI

This suboption of OP,GOSI is used both to input and to catalog the starting set of matrix elements as well as to set constraints on the variation of these matrix elements for the least-squares search procedure. The suboption LEVE must precede ME since the catalog of the matrix elements is performed using the level scheme and state indices assigned using the LEVE command.

Although similar in many respects, the input to the OP,GOSI version of ME is more extensive than that required by the OP,COUL version of ME (Section IV-15). The OP,GOSI version of ME differs from the OP,COUL version in the following respects:

a) Restrictions are placed on the range over which each matrix element is allowed to vary during the least-squares search procedure. These restrictions are used to prevent the code from finding unphysical solutions. Moreover, these restrictions limit the range of coupling coefficients ζ over which the ζ-dependence of the q-parameters is fitted.

b) Specifications are given defining which matrix elements are to be treated as free variables, and which are to be kept fixed or varied conserving a preset coupling with other matrix elements. This allows a reduction in the number of unknowns by using other knowledge such as lifetime, branching ratio or multiple mixing ratio data to restrict the number of free parameters used in the least-squares search. Note that lifetimes, branching ratios, multiple mixing ratios and E2 matrix elements also can be included explicitly in the data set used for the least-squares search (See OP,YIEL, Section IV.29). Restrictions on matrix elements can be overridden by the OP,RE,A , OP,RE,C and OP,RE,F options or, conversely, additional restrictions can be imposed using the FIX or LCK command of the suboption CONT without changing the ME input. Input

from the OP,GOSI version of ME requires a five-entry record.
A summary of the input format is a follows:

ME	
λ_1,0,0,0,0	Specify multipolarity.
INDEX1,±INDEX2,ME,R_1,R_2	List of matrix elements
" " "	for multipolarity λ_1 plus
" " "	lower (R_1) and upper (R_2) limits.
λ_2,0,IF$_2$,0,0	Specify multipolarity.
INDEX1,±INDEX2,ME,R_1,R_2	List matrix elements for multipolarity λ_2.
" " "	
A 0, 0, 0, 0, 0	Terminates input.

Matrix elements for each multipolarity are input as a set preceded by a single record defining the multipolarity, i.e., λ,0,0,0,0 λ=1 through 6 from E1 through E6 respectively, while λ=7 for M1 and λ=8 for M2.

Matrix elements are input as:

INDEX1,±INDEX2,ME,R_1,R_2	INDEX# is the user-given state number as defined in the LEVE input.
ME=<INDEX2||E(M)λ||INDEX1>	The multipole matrix element defined by equation 1.16. It is given in units of e.barns$^{1/2}$ for Eλ matrix elements and μ_N.barns$^{(1-1)/2}$ for Mλ matrix elements. The sign assigned INDEX2 plays no role in the definition of the matrix element. A negative sign signifies coupled matrix elements as discussed below.
R_1 and R_2	The lower and upper limits,respectively, between which the given matrix element ME is allowed to vary. Obviously $R_2 \geq R_1$. Equality of R_1 and R_2 implies that this given matrix element is kept fixed at the

value ME. Note that in this case, i.e., $R_1=R_2$, R_1 need not be equal to ME. For example record 1,2,0.5,2,2 is equivalent to 1,2,0.5,0.5,0.5

Fixing matrix elements as in the first example is recommended because of two features of the code. First, when an OP,RE command is used the limits of fixed matrix elements are set as $R_2=|R_2|$ and $R_1=-|R_2|$. If fixing is done as in the second example the matrix element will be allowed to vary only in one direction i.e., between ±0.5. Secondly, when fitting the q-parameters, the ζ-ranges are set according to the actual limits R_1,R_2. If fixed matrix elements are released at a later stage in the analysis then there is less risk of incorrect extrapolation if the approach used in the first example is employed rather than later extending the limits without recalculating the q-parameter maps. Note that neither R1 nor R2 should be exactly zero, use a small number instead.

A negative sign assigned to INDEX2 specifies that the matrix element defined by the pair of indices INDEX1, INDEX2 is not a free variable but is a coupled one. In this case R_1 and R_2 are no longer upper and lower limits but the pair of indices of the matrix element to which this matrix element is coupled. The code automatically assigns upper and lower limits to the coupled matrix elements using the upper and lower limits given to the one to which it is coupled while preserving the ratio of the initial values of the coupled matrix elements. These upper and lower limits calculated by the code are used by the code if this coupling is subsequently released. The ratio of coupled matrix elements set by the initial values is preserved in the least squares search if the coupling is not released.

As an example consider the pair of matrix elements

1,2,2.0,-4,4
2,-3,1.,1,2

The second statement signifies that the matrix element connecting state 2 to 3 is coupled to the matrix element connecting states 1 and 2 in the ratio

$$\frac{M(2\to3)}{M(1\to2)} = +0.5$$

This ratio will be preserved in the least squares search if this coupling is not released. Limits (R_1,R_2) of -2,+2 will be assigned by the code to the matrix element connecting states 2 and 3. These limits are useful if the coupling of these matrix elements is subsequently released.

The convention of coupling matrix elements already described is valid only within a single multipolarity. The coupling of matrix elements belonging to different multipolarities is performed by using $100\lambda + R_2$ as input for the index R_2 of the "slave" matrix element where lambda is the multipolarity of the master matrix element. The convention that λ=7 for M1 and λ=8 for M2 is still valid.

An important restriction is that there can be only one "master" matrix element with a number of slaves coupled to it if a group of matrix elements are specified to be mutually related. For example, a valid sequence is

```
1,2,2.,-4,4                    E2 set of matrix elements
2,-3,2.,1,2
     .
     .
2,-3,0.5,1,202                 M1 set of matrix elements.
```

This describes the coupling of both the M1 and E2 matrix elements of the 2→3 transition to the E2 matrix element connecting states 1 and 2. The E2 matrix element connecting states 1 and 2 will be treated as a variable, any changes of this matrix element will cause appropriate changes in both the M1 and E2 matrix elements connecting states 2 and 3. An <u>invalid</u> sequence is

```
1,2,2.,-4,4                    E2 matrix elements
2,-3,1.,1,2
     .
     .
2,-3,.5,2,203                  M1 matrix elements
     .
```

This is invalid because it couples the M1 matrix element to the E2 matrix element 2-3 which already is a "slave". Coupling of a set of matrix elements to a fixed one is allowed, it will simply fix the whole set. Nevertheless, it is not allowed to fix the master matrix element using $R_1=R_2$ of a sign opposite to the matrix element.

For example use of the statement

1,2,2.0,-4,-4

will cause a flip of the signs of all matrix elements coupled to the above matrix element. The correct statement is:

1,2,2.0,4,4.

Note it is useful to reiterate that it is not necessary to change the ME input in order to alter constraints etc. in the fitting of matrix elements. The commands OP,RE,A; OP,RE,C; and OP,RE,F can override some constraints introduced by ME setup, while the FIX and LCK commands of suboption CONT allow addition of new constraints.

RESTRICTIONS

Failure to comply with the following restrictions may cause erroneous results or an error message will be printed and the job aborted:

a) Multipolarities must appear in order from lowest to highest starting with Eλ then Mλ.

b) Matrix elements must belong to the upper triangle, i.e. INDEX1≤INDEX2.

c) INDEX values must be in increasing order, i.e. odometer ordering.

d) The limits $R_2 \geq R_1$.

e) Neither R_1 nor R_2 should be exactly zero.

f) Do not set $R_1=R_2$ with a sign opposite to the matrix element if couplings are made to other matrix elements.

To illustrate a typical input consider the example discussed in the previous section, but here used under the OP,GOSI command. Let us assume that the number of experimental data is insufficient to perform a completely model-independent analysis. Then some model is used to couple all the diagonal quadrupole matrix elements to the $0_1^+-2_1^+$ transition matrix element. In addition, the E2/M1 mixing ratio for the $2_2^+-2_1^+$ transition is fixed. The sample input then will be as as follows:

```
OP,TITL
NUCLEUS DEFINITION FOR OP,GOSI
OP,GOSI
LEVE
1,1,0,0                          ground state is given index 1
2,1,2,0.500
3,1,4,1.00
4,1,2,0.750
0,0,0,0                          ends LEVE input
ME
2,0,0,0,0                        E2 header
1,2,1.,-2,2                      free variable
1,4,1.,-2,2                      free variable
2,-2,1.,1,2                      coupled to 1→2
2,3,1,-3,3                       free variable
2,4,1,.01,5                      free variable
3,-3,1,1,2                       coupled to 1→2
4,-4,1,1,2                       coupled to 1→2
7,0,0,0,0                        ends E2 input, starts M1 input
2,-4,1,2,204                     coupled to 2→4 E2
0,0,0,0,0                        ends ME input
```

In this example there are only four variables, i.e. the 1→2,2→3,1→4 and 2→4 E2 matrix elements. All the diagonal matrix elements are kept equal to the E2 matrix element connecting 1→2, the same holds for the 2→4 M1 matrix element which is equal to the 2→4 E2 matrix element.

IV.17 OP,MINI
(MINIMIZE)

This command causes execution of the least-squares fitting of matrix elements to the experimental data. Refer to Section III.5 for an explanation of the procedures used for the least-square search. The starting set of matrix elements used by OP,MINI depends on the other option commands specified. If OP,RAND is specified then OP,MINI uses the set of random numbers generated by OP,RAND as the set of starting matrix elements. If OP,REST is specified then the starting set of matrix elements is read from TAPE2. If neither OP,RAND nor OP,REST are specified then the matrix elements input using the suboption ME are used as a starting set. Completion of an OP,MINI command causes the set of matrix elements resulting from minimization to be written onto TAPE2. This current set can be used as a new starting point for continued minimization.

The OP,MINI command provides various switches to allow those matrix elements satisfying certain criteria to be locked during the current minimization procedure. This reduction of the number of free variables can greatly speed up the minimization procedure. The FIX command in the suboption CONT provides another mechanism for fixing matrix elements (see Section IV.3).

The input to OP,MINI comprises the title plus one record, i.e.

OP,MINI
IMODE,NPTL,CHILIM,CONV,TEST,LOCKF,NLOCK,IFBL,LOCKS,DLOCK

where:

IMODE

Mode selector. IMODE should be defined as a four-digit number IJKL where:

I=1 or 2. I=1 specifies that the fast approximation will be used to calculate both S (Eq.3.24) and its partial derivatives.
I=2 implies that S will be calculated using the full Coulomb excitation formalism while its derivatives still will be estimated using the fast approximation. I=1 is recommended for almost all applications. The time required to complete the minimization step using I=2 is about an order of magnitude greater than when using I=1. The use of I=2 should be reserved for small cases or for cases requiring extreme accuracy in locating the minimum. The TEST switch, described below, provides a more efficient way of retaining high accuracy than I=2.

J=0 or 1. J=0 selects the simple steepest descent minimization while J=1 selects the gradient and gradient derivative method (see Section III.5).

K=0 or 1. K=0 implies that the absolute changes in matrix elements will be used to improve the minimum while K=1 requests the use of the relative changes. To first order K=1 corresponds to using the logarithms of matrix elements as independent variables instead of the matrix elements themselves, as when K=0.

L=0 or 1. L=0 specifies that the experimental yields, branching ratios etc. will be used as dependent variables to construct the S function while L=1 requests that a logarithmic scale will be used for dependent variables.

There are no restrictions concerning the selection of the above switches and any combination can be used. Proper selection of IMODE can speed up the minimization procedure appreciably and is case-dependent

NPTL — The maximum number of steps of minimization allowed.

CHILIM — The S criterion to stop minimization. That is, the minimization terminates if S < CHILIM.

CONV — The convergence criterion to stop minimization when $|\bar{M}_{i+1}-\bar{M}_i|<$CONV when $\bar{M}_i$ denotes the vector of matrix elements at the i-th step of minimization. This convergence criterion also is used by the iterative search for the minimum along the gradient direction. This iterative procedure is stopped when the absolute difference between two subsequent iterations is less than CONV. Minimization may be resumed after the CONV criterion is fulfilled if LOCKF=1 (see below).
Note: any of the above three criteria, namely NPTL, CHILIM and CONV, stops minimization if fulfilled. The LOCKF switch resumes minimization only when the calculation was terminated because convergence was achieved. A reasonable value for CONV is 10^{-4}.

TEST — Specifies recalculation of the internal correction factors every time S drops by a factor of TEST. In the limit TEST≤1 the internal correction coefficients will be calculated at each step of minimization which corrects for the discrepancy between the value of S calculated using the fast approximation and S coming from the full formalism. Note that this is faster than using I=2 since only one full calculation is required

per step for TEST≤1 whereas each sampling of the minimized function during the one-dimensional search along the gradient direction will require a full Coulex calculation using the I=2 option.

LOCKF — Can equal 0 or 1. LOCKF=0 implies that minimization will be terminated if the convergence limit CONV is satisfied. LOCKF=1 causes the program to fix the NLOCK matrix elements having the most significant S derivatives. This switch provides a different subspace of matrix elements, this can be useful when trapped in a local minimum or when the matrix elements having weak influence on S should be allowed to vary. As described in Section III.5, GOSIA will lock the matrix element having the most significant S derivative if the search directions in two consecutive steps are close to being parallel, even if LOCKF=0.

NLOCK — The number of matrix elements having the largest derivatives of S to be locked if LOCKF=1 and the convergence limit CONV is satisfied. See LOCKF.

IFBFL — May equal 0 or 1. If IFBFL=0 then the derivatives are calculated using only the forward difference method whereas IFBFL=1 causes the forward-backward difference method to be used for calculation of the derivatives. The IFBPL=1 option is justified only in the vicinity of the minimum when the forward difference method may produce spurious results since the IFBFL=1 option is a factor of two slower than the IFBFL=0 option.

LOCKS — May equal 0 or 1. If LOCKS=1 then the code fixes, at the first stage of minimization, all matrix elements M_i for which the absolute value of the partial derivative of S with respect to M_i is less than DLOCKS (the gradient is always normalized to unity), i.e:

$$\left|\frac{\partial S}{\partial M_i}\right| < \text{DLOCKS}$$

This allows an automatic reduction of the number of variables for which derivatives need to be calculated to only those having a significant influence.
LOCKS=0 switches off this option.

DLOCKS — Specifies the limit of the derivative below which a matrix element will be fixed if LOCKS=1.

IV.18 OP,POIN
(POINT)

This option command causes execution of a calculation of the γ-ray yields for one scattering angle and one bombarding energy as specified for each experiment in EXPT. OP,POIN can be used to simulate 'corrected' experimental γ yields. In this mode OP,POIN also generates a 'corrected experimental yields file' on TAPE4, which can be used subsequently for simulating the real experiments (e.g. to analyze the influence of the matrix elements on the supposedly observed yields). Note: when executing OP,POIN one should set experimental yields file selector (NTAP in OP,YIEL input) to 0 - see IV.29.

The input to OP,POIN is as follows:

OP,POIN

IFL,YLIM — IFL=0 specifies the normal calculation, IFL=1 the 'simulation' calculation. YLIM is redundant if IFL=0, for IFL=1 it specifies that all transitions whose yield divided by the yield of the normalizing transition (defined in OP,YIEL) exceeds YLIM will be treated as 'experimentally observable' and will be included in the TAPE4 file. OP,POIN will also produce a file containing γ detector efficiency information if OP,RAW was executed and PRT, flag 20 was set to 1 (TAPE23). Note that the decay energies in TAPE23 output are Doppler-shifted.

IV.19 OP,RAND
(RANDOM)

This option generates a set of random matrix elements which replaces the set defined previously for the current job. Each matrix element in the random set is created assuming a uniform distribution of random numbers lying between the limits specified for each matrix element in the input to ME. This option is used to eliminate bias in the analysis and to test the uniqueness of a the least-squares fit to a given data set by retrying the minimization starting from a number of sets of random matrix elements.

The input requires only one number:

SEED	A floating-point seed number for the internal random number generator. SEED should be larger than unity and less than 32000. Note that FORTRAN random number generators are reproducible, giving the same sequence of random numbers when called. Therefore SEED should be different for repeated runs, otherwise the results will be identical.

IV.20 OP,RAW

This option allows to define γ-intensities for some, or all, experiments as "raw", i.e. not detector efficiency-corrected. In addition the raw γ intensities can be summed over a set of γ detectors. This feature is important when analyzing data from multidetector arrays (crystal balls). Spectra from the γ detectors symmetric with respect to the recoil direction, identically Doppler-shifted, can be added to increase statistics and to reduce the number of datasets to be processed (such sets of data will be referred to as "clusters"). GOSIA can handle such data provided that the efficiency calibration of the individual detectors is input. This information should be given using OP,RAW. OP,RAW should be executed if at least one experiment involves raw data or clusters. OP,RAW should immediately follow OP,YIEL (IV.29). If OP,RAW is to be used the first entry of OP,GDET (IV.10) should be negative to produce additional file, TAPE8, required by OP,RAW. Do not use OP,RAW if all γ intensities are efficiency-corrected.

Energy-dependent efficiency calibration for each individual γ detector is assumed to follow a functional form used by the code GREMLIN (see Appendix), available on request from NSRL.

The input to OP,RAW is as follows:

IEXP	Number of experiment to be labeled as raw (according to the sequence of CONT suboption EXPT).
A1,A2,...A8	Parametrization of efficiency curves for all γ detectors
A1,A2,...A8	used in experiment IEXP. Parameters A1 through A8
.	correspond to a0,a1,a2,a3,f,N,b,c, as defined in
.	Appendix. Use f=0 to switch off F factor and c=0 to
.	switch off W factor. These sets of parameters should
.	be ordered according to the sequence of "logical" γ
.	detectors, as defined in OP,YIEL (IV.29) input. Doppler
.	shift of the γ energies is taken into account.

A1,A2,....A8

NC	Number of clusters.
ID1	Number of γ detectors for cluster #1.
I1,I2,...I(ID1)	Indices of "logical" detectors forming cluster #1,
.	according to the sequence defined in OP,YIEL.
0	IEXP=0 ends input.

The sequence ID1... should obviously be repeated NC times to define every cluster, unless NC=0 (no clusters). The whole input is to be defined for every raw experiment.
The use of OP,RAW imposes an important constraint on how the experimental γ yields should be ordered in either TAPE3 or TAPE4. The sequence of γ yields data sets should follow the HIGHEST "logical" detector index within a cluster. Single detectors can be handled as if they were one-detector clusters, without labeling them as clusters.

Example:

Three γ detectors were used and the spectra from the detectors labeled 1 and 3 in OP,YIEL assignment were added. In this case there are two clusters, namely composite detector 1+3 and single detector 2. The input to OP,RAW should then be as follows:

```
OP,RAW
1          experiment #1 labeled as raw
A1....A8 for logical detector 1
A1....A8 for logical detector 2
A1....A8 for logical detector 3
1          one cluster
2          two detector in this cluster
1,3        logical detectors forming this cluster
0          ends OP,RAW input
```

In this case the experimental γ yields from detector 2 should precede these from 1+3 cluster (highest logical detector index for the data from detector 2 is 2, while for 1+3 cluster it is 3).

IV.21 OP,RE,A
(RELEASE,A)

This option voids all coupling of matrix elements and releases fixed ones. As described in ME (Section IV.16) matrix elements are fixed by specifying identical upper and lower limits R1=R2. When a fixed matrix element is released these upper and lower limits are set equal to -|R2| and |R2|, respectively. Consequently, it is useful to use |R1|=|R2|>|ME| when fixing matrix elements to ensure that the released matrix element can be varied within an appropriate range.

IV.22 OP,RE,C
(RELEASE,C)

This option releases fixed matrix elements but retains the couplings of matrix elements. No additional input is required.
As described in IV.16 and IV.21, when fixed matrix elements are released the upper and lower limits are set equal to |R2| and -|R2|, respectively.

IV.23 OP,RE,F
(RELEASE,F)

This option voids the coupling of matrix elements but retains the fixing of matrix elements. No additional input is required. As described in section IV.16, the upper and lower limits assigned to a coupled matrix element on its release are calculated from the corresponding limits assigned to the master matrix element using the ratio of initial values of the coupled matrix elements.

IV.24 OP,REST
(RESTART)

This option causes a set of matrix elements to be read from file TAPE2 which then replaces the set defined by the input to ME for the current job. This option enables continuation of a minimization or performing any other operation using the latest set of matrix elements instead of the one appearing in the ME setup. Note that each OP,MINI command causes its final set of matrix elements to be written on file TAPE2.

OP,REST provides a possibility to manually overwrite some of the matrix elements stored on TAPE2 for the current job. This feature can be the useful time-saver when, for example, better estimates of some matrix elements have been found during a preliminary diagonal errors calculation. The input to OP,REST should be given as:

OP,REST	
I_1,V_1	Index of the matrix element (according to
I_2,V_2	the sequence of ME) to be overwritten (I)
...	and its new value (V).
0,0	Two zeros terminate input. A sequence:
OP,REST	
0,0	leaves the values stored on TAPE2 unchanged.

IV.25 OP,SIXJ

This stand-alone option creates a 6-j table to be used by the quadrupole sum-rules program SIGMA (see Chapter V). OP,SIXJ is not related to an investigated nucleus, thus it can be inserted anywhere in the input stream, even as the only option command. The output is written to a file TAPE14. No further input is required.

Note: The execution of OP,SIXJ will cause GOSIA to stop the job after the 6-j symbol table has been written. The remainder of the input will be ignored.

IV.26 OP,STAR
(START)

Execution command to calculate Coulomb excitation amplitudes and probabilities, not the γ-ray yields, at the energy and scattering angles specified in the EXPT input. This comprises a subset and consequently an alternative to OP,POIN. The OP,STAR requires no input.

Note that OP,STAR is (besides the OP,SIXJ and OP,GDET commands) the only executable option which does not require the γ-ray deexcitation related information provided using OP,YIEL and thus can immediately follow OP,COUL or OP,GOSI commands.

IV.27 OP,TITL
(TITLE)

This option requires one input record consisting of up to 80 alphanumeric characters. This string is reprinted as a run title. OP,TITL should appear as the first option command, or follow OP,FILE command if used, since execution is immediate. Otherwise, the title will not appear as a header of the output. OP,TITL can be skipped. If more than one title line is wanted this command can be repeated as many times as desired.

IV.28 OP,TROU
(TROUBLE)

This troubleshooting option can be used to pinpoint erroneous experimental data and to check if the minimization is trapped in a local minimum. As described in detail in section III.7, this module analyzes the contribution to χ^2 of the deexcitation γ-ray yields to ascertain if there is an inconsistency in the data. The parameter r_k defined in equation 3.71 is a measure of the consistency of the data. That is, it identifies if the current minimum of χ^2, with respect to a given matrix element, results from cancellation of large and opposite contributions due to inconsistent data or whether all the data are consistent.

The input consists of one record:

NS,RL — NS is the number of experimental yields giving the largest positive and negative components of the derivative of χ^2 with respect to a given matrix element to be selected and printed out. This information will appear in the output if for this given matrix element r_k exceeds RL. χ^2 function is defined by Eq. 3.69.

NOTE:

1) OP,TROU must be the last option before OP,EXIT
2) OP,TROU must be used in conjunction with the yields sensitivity map, i.e. print control parameter IPRM(4) in CONT (Section IV.3) must assume its default value equal to -2.

IV.29 OP,YIEL
(YIELDS)

This option is mandatory if it is desired to calculate the yields of deexcitation γ-rays following Coulomb excitation. The first part of this option is used to input the internal conversion coefficients and the description of the γ-ray detectors. This first section is used in conjunction with either OP,COUL or OP,GOSI. The second part of this option is used in conjunction with OP,GOSI to input additional information required for the least-squares fitting such as normalization constants, γ-ray branching ratios, lifetimes, E2/M1 mixing ratios and diagonal or transitional E2 matrix element data to be included in the fit. The input to OP,YIEL must be complete and consistent with the option of the code selected.

OP,YIEL defines the "logical" γ detectors, which are referred to everywhere in the input except of OP,GDET. Different logical detectors may be in fact the same "physical" ones. This distinction allows to reduce the number of experiments defined in all cases the setup used is symmetric with respect to the beam axis. As an example, let us consider the experiment in which two particle detectors are placed at symmetrically to the beam axis at angles (θ,ϕ) and $(\theta,\phi+\pi)$, respectively. Gamma rays are detected in coincidence with scattered particles in one Ge detector placed at position (θ_g,ϕ_g), so the scan of event-by-event data yields two γ spectra. A straightforward approach is to define two experiments, differing only by the placement of the γ detector with respect to the scattered particles. Instead, one can define only one experiment (keeping in mind that the Coulomb excitation depends on ℓ, but not on ϕ) and two logical detectors, one at (θ_g,ϕ_g) and another at $(\theta_g,\phi_g+\pi)$. Both are identified as the same "physical" detector, but different sets of γ yields (both spectra resulting from the scan) are assigned to them. Such a manipulation saves almost 50% of CPU time since evaluation of deexcitation γ yields requires negligible computation time compared to the excitation calculation.

GOSIA allows also to define logical detector clusters (see OP,RAW-

IV.20), i.e. sets of γ yields which result from summing the raw spectra, therefore the number of experimental data sets is not always equal to the number of logical detectors. Further description will refer to the "logical" detectors simply as γ detectors, which should be distinguished from either "physical" detectors or data sets.

A resume of the input to OP,YIEL is as follows:

OP,YIEL

IFLAG	Assumes the values of 0 or 1. IFLAG=1 means that the correction to the angular distribution of the γ-rays due to a finite distance traveled by the decaying nucleus will be included in the calculation (see Section III.3). IFLAG=0 switches off this correction.
N1,N2	Number of energies (N1) and multipolarities (N2) to define the internal conversion coefficients.
$E_1, E_2, \ldots, E_{N1}$	Energy meshpoints for internal conversion coefficients (in MeV), common for all multipolarities.
I1	Multipolarity I1.
CC(I1,1)..CC(I1,N1)	Internal conversion coefficients for multipolarity I1 at each energy meshpoint (N1 entries).
I2 CC(I2,1)..CC(I2,N1)	This sequence should be repeated for all multipolarities defined, i.e. N2 times.
NANG(I)..NANG(NEXP)	Number of γ-ray detectors for each of the NEXP experiments. NANG(I) can be entered as its true value with a negative sign, which means that the γ detector setup is identical to that of the previous experiment, for example if the experiments differ only by the scattering angle. In this case the next three records need not be entered.

IP(1)..IP(NANG(I)) Identifies the γ detectors used in a given experiment according to the sequence the "physical" detectors were defined in the input to OP,GDET (Section IV.10). For example, if IP(L)=K, then it is understood that the L-th detector used in the current experiment is the K-th detector defined in the OP,GDET input. This assignment of "physical" detectors to the "logical" ones is the only instance the "physical" detectors are referred to. Everywhere else the γ detectors are the "logical" detectors.

$\theta_1,\ldots\theta_{NANG(I)}$ θ angles for γ detectors used in experiment I.

$\phi_1,\ldots\phi_{NANG(I)}$ ϕ angles for γ detectors used in experiment I.

The above sequence, starting from the definition of IP should be repeated for each of NEXP experiments defined, except of the experiments for which NANG is negative. The experiments must be ordered according to the sequence they appear in EXPT input.

NS1,NS2 The transition from NS1 to NS2 to be used as the normalization transition where NS1 and NS2 are the state indices.

End of input for OP,COUL. The remainder of the input is required only if OP,GOSI was specified.

NDST	Number of data sets in experiment 1. Usually equal to NANG(1), unless detector clusters were defined in OP,RAW
$UPL_1 \ldots UPL_n$	Upper limits for all γ detectors used in experiment 1.
$YNRM_1 \ldots YNRM_n$	Relative normalization factors of γ detectors used in experiment 1.
. . .	
. . .	The above three records should be repeated for all experiments according to the sequence of EXPT, except for those assigned the negative value of NANG. Subscript n=NDST denotes the number of data sets.
NTAP	Specifies file containing experimental yields. NTAP=0 is used when this file is not necessary, e.g. when running OP,STAR or OP,POIN under OP,GOSI. Otherwise NTAP=3 or 4 corresponding to file TAPE3 or TAPE4, respectively. NTAP must equal 3 if OP,CORR is executed and must equal 4 if OP,ERRO is executed.
NBRA,WBRA	Number and weight of branching ratios.
I1,I2,I3,I4,B,DB	NBRA records of branching ratios.
. . .	I1→I2/I3→I4 = B±DB
. . .	where I1,I2,I3,I4 are state indices, B is the branching ratio with error DB.
NL,WL	Number and weight of mean lifetimes.
INDEX,T,DT	T±DT is the mean lifetime of level INDEX.
. . .	NL records, lifetimes in picoseconds
NDL,WDL	Number and weight of E2/M1 multipole mixing ratios.
IS,IF,DELTA,ERROR	$\delta \frac{E2}{M1}$ (IS→IF) = DELTA * ERROR

. . .	NDL records
NAMX,WAMX	Number and weight of known E2 matrix elements.
I1,I2,ME,DME	ME±DME is the E2 matrix element (units e.barns)
. . .	and error for the transition I1→I2 (I1≤I2).
. . .	NAMX records.

The known E2 matrix element data end the input to OP,YIEL when OP,GOSI has been selected.
A more detailed description of the input is presented below:

IFLAG — Determines whether the effect of the finite distance traveled by the decaying nucleus on the γ-ray angular distribution is to be included (IFLAG=1) or not (IFLAG=0). This effect, taken into account as a first-order correction (see Section III.3), is important only for the long-living states and should not be included in the cases where all the lifetimes are supposed to be in the subnanosecond range to speed up the calculations. Also, the first-order correction may be inhibited if it is necessary to change the sign of some matrix elements, in which case the lifetimes calculated during the minimization may assume unreasonable values if the matrix elements determining the lifetime of a level happen to be close to zero during the search procedure. In such cases GOSIA will automatically reset IFLAG to 0 if IFLAG was input as 1. It is recommended to use IFLAG=1 only at the final stage of the minimization, when the signs of the matrix elements are already defined. IFLAG=1 should not be used in conjunction with OP,RAND.

N1,N2

N1 is the number of energies used as meshpoints for input of the internal conversion coefficients. Energy meshpoints are presumed to be identical for each multipolarity. At least one point below the lowest transition energy and one point above the highest are required for reliable interpolation of internal conversion coefficients. Use a reasonable range of internal conversion coefficients to ensure a reliable interpolation. Check the interpolated values at least once by requesting the print-out of internal conversion coefficients (refer to print controls described in Section IV.3). Note that the Lagrangian interpolation used is not able to take into account the discontinuities which may be present at low γ energies due to the cutoff edges. Since the interpolation uses two points on both sides of the decay energy, make sure that the discontinuity is separated from the closest decay energy by at least one meshpoint. This assures that the interpolation "sees" the monotonic dependence.

N2 is the number of multipolarities for which internal conversion coefficients are given. This must be consistent with the number of multipolarities used for the matrix element setup in ME.

$E_1, E_2, E_3, \ldots E_{N1}$

Input of the energies used as meshpoints for the internal conversion coefficients. Units of MeV.

I1	Multipolarity of the internal conversion coefficients. I1=1.. 6 for E1...6 respectively. I1=7 for M1 and 8 for M2.
$CC_1(I1), CC_2(I1), ..CC_{N1}(I1)$	Internal conversion coefficients for multipolarity I1 at the energy meshpoints given above. Repeat the multipolarity, I1, and internal conversion coeffient records CC for all N2 multipolarities.
NANG(1)...NANG(NEXP)	NANG is the number of γ detectors for each experiment. NANG is limited to ≤200. In many cases, a series of logically different experiments is in fact performed during one "physical" run, for example when position-sensitive parallel-plate particle detectors are used, providing the data for a wide range of scattering angles. For this type of experiments the physical setup of the γ detectors remains unchanged, therefore repeating the γ-detector related input would be redundant. To reduce the unnecessary input, one can enter NANG(I) as the true value of the γ detectors used with a negative sign. It will be understood that the γ detector setup is the same as for the previous experiment in the EXPT input sequence. In this case the next three records should not be input.
IP(1),IP(2)..IP(NANG(I))	The definition of the "physical" γ detectors used in an experiment I according to the sequence of OP,GDET.
$\theta(1), \theta(2), ...\theta(NANG(I))$ $\phi(1), \phi(2), ...\phi(NANG(I))$	The angular coordinates (θ,ϕ) in degrees of each γ detector in the same coordinate

frame as used for the EXPT input for this experiment.
The z axis always is in the direction of the incident beam. It is recommended that for each experiment the γ-ray detector giving the best quality data be selected as detector number one. This is because only γ-ray detector number one is taken into account for certain features of the code, namely, generation of the yield sensitivity maps, i.e.

$$\left(\frac{\partial \ln(\text{YIELDS})}{\partial \ln(\text{ME})}\right)$$

and the consistency tests performed by the troubleshooting routine OP,TROU.

The sequence of input records starting from the definition of IP must be repeated for all experiments I=1,NEXP as defined in EXPT input, unless NANG is negative for a given experiment I.

NS1,NS2 — The transition from the state with index NS1 to the state with NS2 is chosen as a normalizing transition. Make sure that the energy of state NS1 is higher than that for state NS2. The transition is common to all experiments. It is used for setting upper limits of unobserved γ-ray transitions and for printout compiled by OP,POIN.

The input to OP,YIEL required by OP,COUL ends at this point. The remainder of the input is related to the least-squares fitting and needs to be entered only for OP,GOSI.

NDST

Number of data sets, equal to the number of γ detectors if no detector clusters were defined in OP,RAW. NDST≤32, while up to 20 clusters per experiment can be defined.

$UPL_1 \ldots UPL_n$
$YNRM_1 \ldots YNRM_n$

The number of entries in each record corresponds to the number of data sets for each experiment defined, i.e. n=NDST.
The sequence of these two records should be repeated for all experiments according to the sequence in which the experiments appear in the EXPT input.
These three records should not be input if NANG(I) is negative.
UPL_i is the γ-ray yield upper limit for detector i for unobserved transitions taken relative to the normalizing transition NS1→NS2 selected by the previous record. If the calculated yield of any unobserved γ-ray transition, divided by the yield of the normalizing transition, exceeds UPL, then it is included in the calculation of the least squares summation used for the fit. Otherwise, the many transitions which are below the limit of detection by a particular experiment are not included in the least squares fit procedure. (See Section III.6).

$YNRM_i$ is the relative normalization factor for detector i used in experiment IEXP. GOSIA does not require the absolute normalization for a given experiment, instead, the code finds itself the best normalization constant correlating calculated and experimental γ yields. For each γ detector i used in

experiment IEXP the calculated and experimental γ yields are correlated by:

$$Y_i^{exp} = Y_i^{calc} * C_i(IEXP)$$

where $C_i(IEXP)$ is the normalization constant for experiment IEXP and detector i. The code fits the common normalization factor for all γ detectors used in a given experiment IEXP, C(IEXP), related to the individual γ detectors' normalization factors $C_i(IEXP)$ by:

$$C_i(IEXP) = C(IEXP) * YNRM_i(IEXP)$$

Different experiments may have known relative normalization, e.g. when different projectile scattering angle slices are defined as experiments. In this case the physical setup, i.e. the location of γ detectors etc. is the same for a whole group of experiments and their relative normalization is set only by the Rutherford cross sections and the efficiencies of the particle detectors for specified scattering angle ranges. The known relative normalization may be used by specifying the proper LN indices in the EXPT input, then the code will use a given $YNRM_i(IEXP)$ values to fit the common C(IEXP) value for the whole subgroup of experiments, the definition of $C_i(IEXP)$ for individual γ detectors remaining the same. Note that it is possible to request independent normalization for each individual γ detector by using the CONT switch INR,. In this case the YNRM input is redundant.

The normalization constants calculated using

user-supplied information are printed by the code along with the recommended relative YNRM values calculated independently for each γ detector.

Consider the example of ^{72}Ge discussed in the description of EXPT (see section IV.8). Assume that there are two γ-detectors for each experiment and that a correction needs to be made to the detection efficiency of the second detector. An input of the form:

```
2
0.05,0.10
1,0.7
2
0.02,0.03
1.,0.6
```

means that unobserved transitions will contribute to the least-squares sum when their calculated yield intensities exceed:

EXPT #	γ-Detector #	
1	1	5% of normalization transition
1	2	10% of normalization transition
2	1	2% of normalization transition
2	2	3% of normalization transition

and the normalization constants are:

EXPT #	γ-Detector #	
1	1	C1 calculated by the code
1	2	0.7 * C1
2	1	C2 calculated by the code
2	2	0.6 * C2

NTAP

Specifies the number of the file on which the experimental yields reside. NTAP can have values of 3 or 4 corresponding to TAPE3 or TAPE4. The file of original experimental yields is modified to correct for the difference between full Coulomb excitation calculations, integrated over detector solid angles and target thickness, and point calculations at fixed scattering angle and incident energy. This modified file of experimental data is used for the least squares minimization and error estimation in conjunction with point calculations. This correction is performed by the OP,CORR command (see Section III.4 and Section IV.4) which reads the unmodified experimental yields from file TAPE3 and writes the corrected experimental yiels in TAPE4. Consequently, NTAP must equal 3 when OP,CORR is used. The least-squares minimization and error estimation require the corrected yields. In this case, NTAP should be consistent with the file assignment given in the computer control statements preceding this program. NTAP must equal 4 when OP,ERRO is executed with the CONT SWR, switch because TAPE3 is then reserved for the output needed by the

quadrupole sum-rules program SIGMA.
NTAP may equal 0 when experimental yields are not required, e.g. when running OP,STAR or OP,POIN under OP,GOSI. NTAP=0 implies that the code will not attempt to find and read in the experimental yields file.

NBRA,WBRA

Are the number of experimental branching ratios to be input and weighting factor, respectively. A maximum of 50 branching ratios can be input. If NBRA=0 then no further input of branching ratios is required. The weighting factor, WBRA, is defined for all the branching ratios used in the least-squares summation. Thus, normally WBRA=1.0. It can be helpful, during minimization, to switch off (WBRA=0) or reduce the weight of the branching ratio data to eliminate a problem caused by trapping of the search in the narrow valleys resulting from accurate branching ratio data. For example, branching ratio data can cause the search to be trapped in a solution having the wrong sign for a given matrix element.

If NBRA is not zero then the input is as follows:

I1,I2,I3,I4,B,DB

. . .

Repeated NBRA times

. . .

where I is the level index specified in the LEVE input. The branching ratio B with error DB is defined by the ratio of γ-ray intensities:

$$\frac{I1 + I2}{I3 + I4} = B \pm DB$$

NL,WL

Are the number of experimental mean lifetimes to be input and the weighting factor. NL≤10. If NL=0 then no further lifetime records need to be input. The weighting factor,WL, is used for all the lifetime data in the least-squares summation. Normally, WL=1. The weighting factor can be set to a smaller number or zero if it is desired to reduce or switch off, respectively, the influence of the lifetime data.

INDEX,T,DT

. . .

. . .

NL records

INDEX is the index of the level, specified in the input to LEVE. T is the mean lifetime, in picoseconds (10^{-12}secs), of the level. Note, it is not the half-life $T_{1/2}=\ln(2.)*T$. DT is the error of the mean lifetime in picoseconds.

NDL,WDL

Are the number of experimental E2/M1 mixing ratios to be input and the weighting factor. NDL≤20. If NDL=0 no further mixing ratio records are required. The weighting factor, WDL, is used for all the data points in the least-squares summation. Normally, WDL=1.0. WDL can be made smaller or zero to reduce or switch off the influence of the mixing ratio data.

IS,IF,DELTA,ERROR

. . .

. . .

NDL records of mixing ratios

DELTA is the E2/M1 mixing ratio for the transition from level IS to level IF. It is defined as:

$$\text{DELTA} = \delta\left(\frac{E2}{M1}\right) = 0.835\ E_{\gamma}(\text{MeV})\ \frac{\langle IF||M(E2)||IS\rangle}{\langle IF||M(M1)||IS\rangle}$$

Note that the phase convention is that of Krane [KRA70]. See [KRA70] for a discussion of the various phase conventions. ERROR is the error in the mixing ratio. Note the error is assumed to be symmetric to assure continuity of the least squares function.

NAMX,WAMX

The number of experimental E2 matrix elements (NAMX) to be input and the weighting factor (WAMX). If NAMX=0 no more input is required. The weighting factor, WAMX, is common for all the matrix elements used in the least-squares summation. Normally WAMX=1.0. WAMX can be made smaller or zero to reduce or switch off the influence of these additional data, NAMX≤30

$INDEX_1$,$INDEX_2$,ME,DME

. . .

. . .

Repeat NAMX times.

$INDEX_n$ is the level index. Note the restriction $INDEX_1 \leq INDEX_2$. ME is the E2 matrix element, in units e.barns, while DME is the error, assumed to be symmetrical. In the fit procedure the sign of ME is ignored if INDEX1 is not equal to INDEX2.

The input of known E2 matrix elements concludes the input to OP,YIEL. The experimental deexcitation γ-ray yields are input separately as described in Section IV.30.

IV.30 INPUT OF EXPERIMENTAL γ-RAY YIELDS FROM COULOMB EXCITATION

The experimental γ-ray yields from the Coulomb excitation experiments are supposed to reside on a separate file being either TAPE3 or TAPE4. The structure of the file is as follows:

IEXP,NG,ZP,AP,EP,ND,WT	This header record appears before the experimental yields for each experiment and data set.
IEXP	This is the experiment number. The experiments must be input in the same order as used for EXPT and OP,YIEL.
NG	Number of data sets for experiment IEXP. NG is equivalent to the OP,YIEL NDST.
ZP	Charge number of the projectile.
AP	Mass number of the projectile.
EP	Bombarding energy of the projectile (MeV).
ND	Number of experimental γ-ray yields to be input for the specific IEXP and data set.
WT	The weighting factor assigned to a given data set (see Eq.3.25). Normally WT=1.0. This weight factor can be made less than one or zero to reduce or switch off respectively the influence of this particular data set.

All the entries of the header, except WT and ND, are used only for reprint

of experimental data, therefore using the values defined in EXPT and OP,YIEL inputs is not strictly required. Nevertheless, it is recommended to enter IEXP,ZP,AP,EP and NG according to the previous definition to make sure that the sequence of experimental yields is correct.

Each header should be trailed by ND records for that particular experiment and data set. The format is:

II,IF,Y,ΔY

where:

II	Initial level index.
IF	Final level index.
Y,DY	The arbitrarily normalized γ-ray yield for transition II→IF with absolute experimental error ±ΔY.

For unresolved doublets, consisting of the II1→IF1 transition plus the II2→IF2 transition, the input format is: (100*II1+II2), (100*IF1+IF2), Y_1+Y_2, $\Delta(Y_1+Y_2)$ where:

II1,II2	Are the initial level indices for transition 1 and 2.
IF1,IF2	Are the final level indices for transition 1 and 2.
Y_1+Y_2,$D(Y_1+Y_2)$	Is the summed yield of the unresolved transitions II1→IF12 and II2→IF2 with error $\pm\Delta(Y_1+Y_2)$.

There are no restrictions regarding the sequence of the experimental data within the single data set. Data sets within an experiment should be ordered according to the highest logical detector index. If no clusters are defined (see OP,RAW) this is equivalent to ordering the data sets according to the sequence of logical detectors defined in OP,YIEL.

V. QUADRUPOLE SUM RULES - PROGRAM SIGMA

The heavy-ion induced Coulomb excitation allows to measure essentially full sets of the E2 matrix elements for the low-lying states of the nuclei. It is interesting to ascertain to what extent these sets of data can be correlated using only a few collective degrees of freedom. The quadrupole sum rules [CLI72, CLI86] have been proven to be a powerful tool for extracting the collective parameters from the wealth of data produced by the Coulomb excitation. This procedure, outlined below, is completely model-independent, thus being specially suitable to be used on the data also obtained without recursion to the models. Conversion of the E2 matrix elements to the quadrupole invariants is performed by the separate code, SIGMA, which uses the information stored by GOSIA on a permanent file during error calculation.

V.1. FORMULATION OF THE QUADRUPOLE SUM RULES

The electromagnetic multipole operators are spherical tensors and thus zero-coupled products of such operators can be formed which are rotationally invariant, i.e., are identical in any instantaneous intrinsic frame and the laboratory frame. Let us, for practical reasons, consider only the E2 operators. We can always define an instantaneous "principal" frame in such a way, that:

$$\begin{aligned} E(2,0) &= Q\cos\delta \\ E(2,1) &= E(2,-1) = 0 \\ E(2,2) &= E(2,-2) = 1/\sqrt{2} \cdot Q\sin\delta \end{aligned} \qquad 5.1$$

where Q and δ are the arbitrary parameters, identical to Bohr's (β,γ) with recursion to the model, but in general completely model-independent. Using this parameterization the zero-coupled products of the E2 operators can be formed in terms of Q and δ, e.g.:

$$[E2 \times E2]^0 = \frac{1}{\sqrt{5}} Q^2$$

$$\{[E2 \times E2]^2 \times E2\}^0 = \frac{\sqrt{2}}{\sqrt{35}} Q^3 \cos 3\delta \qquad 5.2$$

which are the two lowest order products. It is straightforward to form any order product, the limit being set only by practical feasibility. On the other hand, one can evaluate the matrix elements of the E2 operators products by recursively using the basic intermediate state expansion:

$$\langle s|(E2 \times E2)^J|r\rangle = \frac{(-1)^{I_s+I_r}}{(2I_s+1)^{1/2}} \sum_t \langle s||E2||t\rangle\langle t||E2||r\rangle \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_t \end{Bmatrix} \qquad 5.3$$

which allows to express the rotational invariants built of Q and δ as the sums of the products of the reduced E2 matrix elements using the experimental values of these matrix elements. As an example, an expectation value of Q^2 can be found directly using 5.2 and 5.3:

$$Q^2 = \frac{\sqrt{5}}{(2I_s+1)^{1/2}} \langle s||(E2 \times E2)^0||s\rangle =$$

$$= \frac{(-1)^{2I_s}\sqrt{5}}{(2I_s+1)^{1/2}} \sum_r M_{sr}M_{rs} \begin{Bmatrix} 2 & 2 & 0 \\ I_s & I_s & I_r \end{Bmatrix} \qquad 5.4$$

where the shortened notation for the matrix elements:

$$M_{sr} = \langle s|| E2 ||r\rangle \qquad 5.5$$

is used. The Wigner's 6-j symbol $\begin{Bmatrix} 2 & 2 & 0 \\ I_s & I_t & I_r \end{Bmatrix}$ is equal to ([ROT59]):

$$\begin{Bmatrix} 2 & 2 & 0 \\ I_s & I_t & I_r \end{Bmatrix} = (-1)^{I_s+I_r} \frac{1}{\sqrt{5}} \frac{1}{(2I_s+1)^{1/2}} \delta_{I_sI_t} \qquad 5.6$$

The 6-j symbol 5.6 appears frequently in the sum rules and its simple

analytic form makes possible the simplification of the formulas resulting from the intermediate state expansion. The general phase rule for the reduced matrix elements M_{rs} can also be used to further simplify 5.4:

$$M_{rs} = (-1)^{J_s - J_r} M_{sr} \qquad 5.7$$

It can be easily seen that by inserting 5.6 and 5.7 into 5.4 one gets:

$$Q^2 = \frac{1}{2I_s+1} \sum_r M_{sr}^2 \qquad 5.8$$

The similar evaluation of $Q^3\cos 3\delta$ yields:

$$Q^3\cos 3\delta = \mp \frac{\sqrt{35}}{\sqrt{2}} \frac{1}{2I_s+1} \sum_{tu} M_{su} M_{ut} M_{ts} \begin{Bmatrix} 2 & 2 & 2 \\ I_s & I_t & I_u \end{Bmatrix} \qquad 5.9$$

where a negative sign corresponds to the integral spin system, while a positive sign corresponds to the half-integral spin system.

The higher order sum rules can be formed with the different J couplings, involving summation over the different sets of the reduced E2 matrix elements. This provides an important test for the self-consistency of the E2 experimental data, as well as for the convergence of the sum rules themselves. It is estimated [CL186] that about 90% of the non-energy-weighted E2 strength is contained within the low-lying, and thus Coulomb excitation accessible, level structure. The missing strength is primarily due to the giant dipole resonance which we have neglected so far. Assuming that this missing strength can be neglected one can expect that different J couplings should yield the similar results for the rotational invariants. Practically, however, the finite level system used in the analysis and the finite coupling scheme will result in the discrepancies between different J-coupled sum rules giving an estimate of the completeness of the data used. The simplest sum rule involving the different J coupling is given by the fourth-order product related to the expectation value of Q^4:

$$P^4(J) = \langle s|\{(E2 \times E2)^J \times (E2 \times E2)^J\}^0|s\rangle =$$

$$= \frac{(2J+1)^{1/2}}{2I_s+1} \sum_{rtu} M_{st} M_{tr} M_{ru} M_{us} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_t \end{Bmatrix} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_u \end{Bmatrix} (-1)^{I_s - I_r} \qquad 5.10$$

Three independent estimates of Q^4 can be evaluated using $P^4(J)$ for J=0,2,4:

$$Q^4(0) = 5P^4(0)$$

$$Q^4(2) = \frac{7\sqrt{5}}{2} P^4(2) \qquad 5.11$$

$$Q^4(4) = \frac{35}{6} P^4(4)$$

It is easily seen that the above expressions for Q^4 involve summation over the different sets of matrix elements, the selection rules being set by the 6-j symbols of 5.10. The expectation values of Q^2 and Q^4 can be used to build the Q-variance:

$$v^2(J) = Q^4(J) - [Q^2]^2 \qquad 5.12$$

having the physical meaning of the square of the softness in Q.
The matrix element of the fifth-order product

$$P^5(J) = \langle s|\{(E2 \times E2)^J \times [(E2 \times E2)^2 \times E2]^J\}^0|s\rangle \qquad 5.13$$

defines $Q^5\cos 3\delta$. There are three independent sum rules for J=0,2,4 coupling. Making an intermediate state expansion and reducing the resulting 6-j symbols with $I_s=0$ one obtains:

$$Q^5\cos 3\delta(J) = \mp C(J) \frac{1}{2I_s+1} \sum_{rtvw} M_{st} M_{tr} M_{rv} M_{vw} M_{ws}$$

$$\cdot (-1)^{I_w+I_s} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_t \end{Bmatrix} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_w \end{Bmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ I_w & I_r & I_v \end{Bmatrix} \qquad 5.14$$

where $C(0) = 5\frac{\sqrt{35}}{\sqrt{2}}$, $C(2) = C(4) = \frac{35}{2} \frac{\sqrt{35}}{\sqrt{2}}$

and a negative sign should be used for the integral-spin cases, while a positive sign corresponds to the half-integral spin cases.

The sixth order products of E2 operators define both the expectation value of Q^6 and the expectation value of $Q^6\cos 3\delta$. The matrix element:

$$P_0^6(J) = \langle s|\{([E2xE2)^J \times (E2xE2)^J]^0 \times (E2xE2)^0\}^0|s\rangle \qquad 5.15$$

is related to Q^6, while the matrix elements:

$$P_1^6(J) = \langle s|\{[(E2xE2)^2 \times E2]^J \times [(E2xE2)^2 \times E2]^J\}^0|s\rangle \qquad 5.16$$

and

$$P_2^6(J) = \langle s|(\{[E2xE2)^2 \times E2]^J \times [E2x(E2xE2)^2]^J\}^0|s\rangle \qquad 5.17$$

both define $Q^6\cos^2 3\delta$. Coupling scheme 5.15 yields for J=0,2,4:

$$Q^6(J) = C(J) \sum_{\substack{rtvwu \\ I_r=I_w}} \frac{1}{2I_r+1} M_{st} M_{tw} M_{wu} M_{ur} M_{rv} M_{vs}$$

$$\begin{Bmatrix} 2 & 2 & J \\ I_s & I_w & I_t \end{Bmatrix} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_v \end{Bmatrix} (-1)^{I_s-I_u} \qquad 5.18$$

where $C(0) = \frac{5}{2I_s+1}$; $C(2) = C(4) = \frac{35}{2(2I_s+1)}$

Knowing the expectation value of Q^6 one can construct the second statistical moment, the skewness, of Q^2:

$$s(Q^2(J)) = Q^6(J) - 3Q^4(J)Q^2 + 2(Q^2)^3 \qquad 5.19$$

The evaluation of $P_1^6(J)$ (5.16) and $P_2^6(J)$ (5.17) may involve the J=0,2,3 and 4 coupling schemes. However, J=3 coupling is insignificant from the point of view of Coulomb excitation since it favors strongly E2 matrix elements coupling the states with $\Delta I=\pm 1$ spin difference. These matrix elements are not well defined by the Coulomb excitation experiments. It is most clearly seen in case of even-even nuclei where the ground state spin is 0 and the preferable path of excitation involve the m=0 magnetic substates for all states. In this case, the 3-j symbol involved in the definition of the coupling parameters ζ_{kn} (1.17c) is:

$$\begin{pmatrix} I & 2 & I\pm 1 \\ 0 & 0 & 0 \end{pmatrix} = 0 \qquad 5.20$$

since $j_1+j_2+j_3 = (2I+2)\pm 1$ is odd (see e.g.[ROT59]). This means that the lowest significant coupling is the $\Delta m=\pm 1$ coupling being an order of

magnitude weaker than the $\Delta m=0$ coupling. Applying the first order perturbation theory 1.24, 1.26 one also finds that due to the antisymmetry of $Q_{2/1}(\omega)$ this mode of excitation is strongly inhibited. As a result, the E2 matrix elements connecting the even and odd spin states are measured with the large errors, unless some additional data, most important the branching ratios, are available.

Restricting ourselves to J=0,2 and 4 couplings we have from 5.16 and 5.17:

$$Q^6\cos^2 3\delta(0) = \frac{35}{2}\ P_1^6(0) = \frac{35}{2}\ P_2^6(0) \qquad 5.21$$

and $$Q^6\cos^2 3\delta(J) = 35\ (P^6_{1,2}(4) - \frac{\sqrt{5}}{4}\ P^6_{1,2}(2)) \qquad 5.22$$
$$J=2,4$$

with $$P_1^6(J) = \frac{5(2J+1)^{1/2}}{2I_s+1} \sum_{rutvw} M_{su}\, M_{ut}\, M_{tr}\, M_{rv}\, M_{vw}\, M_{ws}$$

$$\cdot \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_t \end{Bmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ I_s & I_t & I_u \end{Bmatrix} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_w \end{Bmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ I_w & I_r & I_v \end{Bmatrix} (-1)^{2I_s+I_t+I_w} \qquad 5.23$$

and $$P_2^6(J) = \frac{5(2J+1)^{1/2}}{2I_s+1} \sum_{rutrv} M_{su}\, M_{ut}\, M_{tr}\, M_{rv}\, M_{rw}\, M_{ws}$$

$$\cdot \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_t \end{Bmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ I_s & I_t & I_u \end{Bmatrix} \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_v \end{Bmatrix} \begin{Bmatrix} 2 & 2 & 2 \\ I_s & I_v & I_w \end{Bmatrix} (-1)^{I_s+I_r+I_t+I_w} \qquad 5.24$$

5.21 through 5.24 define three independent estimates of $Q^6\cos^2 3\delta$ - one involving the J=0 coupling, identical for both P_1^6 and P_2^6 and two involving the J=2 and J=4 couplings for P_1^6 and P_2^6, respectively. Using the value of Q^6 (5.18) the expectation from 5.22, which, combined with the expectation value of $\cos 3\delta$ can be obtained which define the softness in δ as the square root of the $\cos 3\delta$ variance:

$$v^2(\cos 3\delta) = \langle\cos^2 3\delta\rangle - \langle\cos 3\delta\rangle^2 \qquad 5.25$$

The expectation value of $\cos 3\delta$ can be extracted either from the

$Q^3\cos3\delta$ invariant or three possible values of $Q^5\cos3\delta$ provided that the expectation values of Q^3 and Q^5 are known. These values can be estimated using an interpolation between Q^2, Q^4 and Q^6. We use:

$$\langle Q^3\rangle = \left(\frac{1}{2}\left((Q^2)^{1/2} + (Q^4(0))^{1/4}\right)\right)^3 \qquad 5.26$$

$$\langle Q^5\rangle = \left(\frac{1}{2}\left((Q^4)^{1/4} + (Q^6(0))^{1/6}\right)\right)^5 \qquad 5.27$$

where the J=0 coupling for Q^4 and Q^6 is used because of the minimum number of the matrix elements involved, thus being preferable from a point of view of the completeness of the summation and the error propagation. For the same reason only the expectation value of $\cos3\delta$ extracted from $Q^3\cos3\delta$ is used for the softness in δ.

To summarize, the sum rules allow to find the expectation values of rotational invariants built of Q and δ. It is then possible to find the statistical distribution of Q^2 and $\cos3\delta$ i.e. the first statistical moments related to the softness in both parameters and the second statistical moment, the skewness (in our case calculated for Q^2 only). With various J-couplings which can be used to evaluate the higher-order invariants, the sum rules provide the test of the completeness of the data as well as of the self-consistency of the fitted E2 matrix elements.

V.2. PROGRAM SIGMA

A separate code, SIGMA, has been written to evaluate the sum rules. This program has been designed to use the information created by GOSIA (see V.3), although it can be used separately to calculate the centroids (i.e., the expectation values) of the rotational invariants only, with no error estimation. The following subsection outlines the algorithms used for the computation of the rotational invariants and resulting statistical distribution of Q and cos3δ and the method employed to estimate the errors of computed values.

V.2.1. COMPUTATION OF THE INVARIANTS

The most efficient way to evaluate the rotational invariants is to use the matrix multiplication formalism having the selection rules for different sum of products superimposed by masking the array of the E2 matrix elements with the appropriate 6-j matrices. Let us define (with s being a fixed target state index):

$$\bar{V}_L = \{M_{sr}\} \text{ "left-hand vector"} \qquad 5.28a$$

$$\bar{V}_R = \{M_{rs}\} \text{ "right-hand vector"} \qquad 5.28b$$

$$S_{rv}(J) = M_{rv} \quad \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_v \end{Bmatrix} \qquad 5.28c$$

$$S^{T}_{rv}(J) = M_{vr} \quad \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_v \end{Bmatrix} \qquad 5.28d$$

$$T_{rv}(J) = \left(\sum_w M_{rw} M_{wv} \quad \begin{Bmatrix} 2 & 2 & 2 \\ I_r & I_v & I_w \end{Bmatrix}\right) \quad \begin{Bmatrix} 2 & 2 & J \\ I_s & I_r & I_v \end{Bmatrix} \qquad 5.28e$$

$$T'_{rv} = \sum_w M_{rw} M_{wv} \quad (-1)^{I_w - I_s} \quad \frac{1}{2I_r+1} \delta_{I_r I_v} \qquad 5.28f$$

The rotational invariants can be expressed in terms of the operators 5.28 as (if the phase needs to be appended, r stands for the row index and v stands for the column index):

$$Q^2 = \frac{1}{2I_s+1}\ \bar{v}_L \cdot \bar{v}_L \qquad 5.29a$$

$$Q^3\cos 3\delta = \mp\ \frac{\sqrt{35}}{\sqrt{2}}\ \frac{1}{2I_s+1}\ \bar{v}_L \cdot S(2) \cdot \bar{v}_R \qquad 5.29b$$

$$Q^4(J) = C(J)\ \bar{v}_L \cdot S^T(J) \cdot [S(J)\ (-1)^{I_s+3I_r}] \cdot \bar{v}_R \qquad 5.29c$$

$$Q^5\cos 3\delta(J) = \mp\ C(J)\ \bar{v}_L \cdot S^T(J) \cdot T(J) \cdot \bar{v}_L \qquad 5.29d$$

$$Q^6(J) = C(J)\ \bar{v}_L \cdot S^T(J) \cdot T' \cdot S(J) \cdot \bar{v}_R \qquad 5.29e$$

$$Q^6\cos^2 3\delta(J) = c(J)\ \bar{v}_L \cdot [S(2)\ (-1)^{I_s+I_w}] \cdot S^T(J) \cdot$$

$$\cdot [T(J)\ (-1)^{I_s+I_w}] \cdot \bar{v}_R \qquad 5.29f$$

$$Q^6\cos^2 3\delta(J) = C(J)\ \bar{v}_L \cdot [S(2)\ (-1)^{I_s+I_r}] \cdot S^T(J) \cdot S(J) \cdot$$

$$\cdot [S(2)\ (-1)^{I_s+I_w}] \cdot \bar{v}_R \qquad 5.29g$$

where $C(J)$ are the appropriate constants as defined in the previous subsection and two formulas for $Q^6\cos 3\delta(J)$ correspond to the coupling schemes 5.16 and 5.17. The invariants are evaluated according to 5.29 from the right side, so that only the matrix-vector multiplications are performed, without any matrix-matrix multiplications.

V.2.2 ESTIMATION OF ERRORS IN SIGMA

The rigorous estimation of the errors of the function of the E2 matrix elements would require the knowledge of all sets of these matrix elements yielding a given value of this functions together with the probability of each such set. Technically it is of course out of question to apply this method to evaluate the errors of the rotational invariants. We are therefore forced to use a crude approximation, which is to assume that the set of the measured matrix elements is contained within an ellipsoidal contour (note that because of the correlation all matrix elements, not only E2, have to be taken into account). This contour is defined by a requested increase of the S statistic (3.24) and its orientation in the space of the matrix elements results from the correlations introduced by a method of measurement. One should be aware that the correlation of the matrix elements introduced by a functional form may be completely different from that resulting from the measurement. As an extreme example it is easily checked that the variance of Q^2 vanishes if there is only one state of a given spin, whatever values of the matrix elements are used. In this case, the error of the variance is zero, no matter what errors are assigned to the matrix elements.

The error contour, defined by the increase of the S statistic (3.24), is approximated by the quadratic formula:

$$\Delta S = \delta = \nabla_o \cdot \Delta\bar{M} + \frac{1}{2} \Delta\bar{M} \cdot J \cdot \Delta\bar{M} \qquad 5.30$$

where ∇_o is the gradient taken at the origin, $\bar{M}_o$, while J is the second derivatives matrix:

$$J_{ik} = \frac{\theta^2 S}{\theta M_i \; \theta M_k}$$

and

$$\Delta\bar{M} = \bar{M} - \bar{M}_o \qquad 5.31$$

It is easily checked that all points on the contour 5.30 can be parameterized by:

$$\Delta\bar{M} = \bar{M} - \bar{M}_o = \frac{2\delta\bar{e}}{\nabla_o\bar{e} + [(\nabla_o\bar{e})^2 + 2\delta\bar{e}\ J\ \bar{e}]^{1/2}} \qquad 5.32$$

where $\bar{e}$ is an arbitratry vector. Denoting a given function of matrix elements by $S(\mathbb{M})$ we have to locate the points $\mathbb{M}$ on the contour yielding the extremal values of $S(\mathbb{M})$. Let us consider the function $S(\mathbb{M})$ which can locally be appoximated by the linear expansion in $\mathbb{M}$:

$$\Delta_s(\mathbb{M}) = \nabla_s \cdot (\mathbb{M} - \mathbb{M}_s) \qquad 5.33$$

where we expand $S(\mathbb{M})$ in a vicinity of $\mathbb{M}_s$. To find the extrema of 5.33 on the coutour 5.30 we have to find the vectors $\bar{e}$ satisfying:

$$\frac{d}{d\bar{e}}\left(\frac{2\delta \cdot (\nabla_s \cdot \bar{e})}{\nabla_o\bar{e} + [(\nabla_o\bar{e})^2 + 2\delta\bar{e}J\bar{e}]^{1/2}}\right) = 0 \qquad 5.34$$

which yields:

$$\nabla_s(2\delta - \nabla_o\bar{e}) - \nabla_o(\nabla_s\bar{e}) - (\nabla_s\bar{e}) \cdot J\bar{e} = 0 \qquad 5.35$$

From 5.35 it is clear that the vector $\bar{e}$ must be a linear combination of $J^{-1}\nabla_s$ and $J^{-1}\nabla_o$. Inserting

$$\bar{e} = \alpha\ J^{-1}\ \nabla_s + \beta\ J^{-1}\ \nabla_o \qquad 5.36$$

to 5.35 we get, using the identity

$$\nabla_s\ J^{-1}\ \nabla_o = \nabla_o\ J^{-1}\ \nabla_s \qquad 5.37$$

resulting from the symmetry of J:

$$\alpha = \pm\left(\frac{2\delta + \nabla_o J^{-1}\nabla_o}{\nabla_s J^{-1}\nabla_s}\right)^{1/2} \quad ; \quad \beta = -1 \qquad 5.38$$

which is valid for any arbitratily chosen origin $\mathbb{M}_o$. However, in our case we can assume that $\mathbb{M}_o$, the vector of fitted matrix elements, is a close

approximation of the minimum, thus $\nabla_o \approx 0$. Neglecting the terms containing ∇_o we finally get:

$$\bar{M} = \bar{M}_o \pm \left(\frac{2\delta}{\nabla_s J^{-1} \nabla_s}\right)^{1/2} J^{-1} \nabla_s \qquad 5.39$$

where a positive sign corresponds to the maximum of 5.33 on the contour 5.30 and a negative sign corresponds to its minimum. This formula gives an exact solution for any linear function of $\bar{M}$. For non-linear functions 5.39 can be used iteratively following the scheme:

$$\begin{aligned} \nabla_s^{(o)} &= \nabla_s(\bar{M}_o) \Rightarrow \bar{M}^{(1)} \\ \nabla_s^{(1)} &= \nabla_s(\bar{M}^{(1)}) \Rightarrow \bar{M}^{(2)} \end{aligned} \qquad 5.40$$

until the convergence is achieved. This procedure is used in SIGMA to estimate the errors of Q^2, $\cos 3\delta$ and their statistical moments. Because of the fact that the implementation of the sum rules is only possible for the cases in which virtually all the E2 matrix elements for low lying states are known, implying that the underlying Coulomb excitation problem is well overdetermined, it is reasonable to assume least-squares statistic increase $\delta=1$. The J matrix is estimated using the gradients computed by GOSIA during the calculation of correlated errors (see III.6) and stored on a permanent file. Applying the quadratic approximation 5.1 and assuming $\bar{M}_o$ = minimum (i.e. $\nabla_o=0$) one can write:

$$\nabla(\bar{M}) = J\,(\bar{M} - \bar{M}_0) \qquad 5.41$$

During the correlated errors calculation GOSIA evaluates the gradients in points $\bar{M}$ for which only one matrix element at the time is perturbed from its central value. This means that $\bar{M} - \bar{M}_o$ has only one non-zero component, thus 5.41 defines k-th column of J if M_k has been perturbed. Two estimates of J_{ki} are available using positive and negative values of ΔM_k. In addition, J_{ki} can be evaluated using the i-th component of the gradient at perturbed M_k or using the k-th component of the gradient with perturbed M_i. Since the

quadratic approximation 5.1 is not fully adequate, the averaging procedure must be used to cancel the difference between various estimates and to preserve the symmetry of J. Furthermore, for the matrix elements M_k for which the full error calculation was not performed only the diagonal element J_{kk} is assumed to be non-zero, i.e., the correlation is neglected. The estimate of J_{kk} is this case results from:

$$\Delta S = 1 = \frac{1}{2} J_{kk} \Delta M_k \qquad 5.42$$

where ΔM_k is the average diagonal error of M_k, i.e., the mean value of the negative and positive deviations.

The method presented above allows to estimate the errors of the collective parameters and their distributions with the reasonable efficiency. One must be, however, aware of the scope of the approximations used, which do not allow to treat the estimated errors very rigorously, providing only a crude estimate of the accuracy the sum rules are determined with.

V.2.3. INPUT INSTRUCTIONS

SIGMA reads in the input file and in addition three permanent files created by GOSIA, referred to as TAPE1, TAPE2 and TAPE3. The input file selects the mode of calculation and should be given as:

IL

NST

I(1)
I(2)
.
.
.
I(NST)

only if 0< NST ≤ 75

IL may be either 0 or 1. IL=1 will cause the printout of the matrix elements (by their indices) involved in the evaluation of 14 invariants calculated for each state. The invariants are numbered from 1 to 14 according to the sequence they appear in first column of the output table (see the sample output at the end of this chapter). IL=0 will cause no compilation of this list.

NST selects the mode of error calculation. Three special values of NST - NST=-1, NST=0 or NST=99 require no further input. NST=-1 is used if only the invariants and the resulting statisical moments (given in the second column of the output table) are to be calculated and no error estimation is requested. In this mode SIGMA can be used independently of GOSIA and the information concerning the level scheme and coupling scheme, normally produced by GOSIA, must be provided by the user (see the description of the TAPE files below). NST=0 implies that the error calculation is to be performed only for Q^2, three values of $v(Q^2)$ and four

values of cos3δ for all states, while NST=99 specifies the errors to be estimated for every statistical moment for all states. The reason for this distinction is that the statistical moments based on the sixth-order invariants are usually not meaningful due to the number of the matrix elements involved and the resulting error propagation. Also, calculation of these invariants is most time-consuming. Usually, it is practical to calculate all the errors only for few lowest-lying states. This can be achieved using "mixed" calculation mode, specified by $0<NST\leq 75$. In this case, NST has the meaning of a number of states for which the "full" calculation is to be done, while for the remaining states the "fast" mode, corresponding to NST=0 will be used. In this mode the list of state indices (NST records) must follow.

Note that the errors quoted are the errors of statistical moments (column 2 of the output table), not of the invariants listed in the first column.

Permanent Files:

TAPE1: This file contains the errors of the matrix elements and is written by GOSIA as TAPE15. It is not required if NST=-1.

TAPE2: This file is written by GOSIA during full error calculation on TAPE3 if the CONT switch SMR, is set. TAPE2 contains the level scheme, the coupling scheme and the set of gradients used to evaluate the J matrix. If SIGMA is to be used independently of GOSIA, (i.e., only if NST=-1) a part of this file must be prepared by the user. The format of this portion of TAPE2 should be the following:

NS, NME, NI, NF	number of states=NS
	number of matrix elements=NME
	index of a first E2 matrix element=NI
	index of a last E2 matrix element=NF

INDEX(1), SPIN(1), ENERGY(1)	
.	
.	Level scheme
.	NS records
.	
INDEX(NS), SPIN(NS), ENERGY(NS)	
IME(1), INI(1), INF(1)	Coupling scheme. IME is the index
.	of matrix element, INI is the index
.	of an initial state, INF is the index
.	of a final state. GOSIA convention
.	applies to the ordering of the
IME(NME), INI(NME), INF(NME)	matrix elements (see IV.15).
	NME records.
IME(1), ME(1)	Values of the matrix elements.
.	NME records.
.	
.	
.	
IME(NME), ME(NME)	
0,0	Two zeros terminate input.

TAPE3: Contains the table of the 6-j symbols used for the calculation of the invariants. This table can be created by GOSIA with OP,SIXJ (see IV.25). GOSIA writes the table on TAPE14.

VI. FILE ASSIGNMENTS

The following chapter provides an overview of the file assignments in GOSIA, SIGMA and SELECT. A permanent or temporary file is referred to as TAPEn, where n designates the code-declared file number. An actual name for such a file depends on the operating system of a given computer, for example the CDC/NOS file TAPE1 will be named FOR001 under VAX/VMS. To allow the possibility of examining the contents of the permanent files generated by all three codes a free format FORTRAN write (i.e. WRITE(n,*)) is used. The only exception is the internal correction factors file TAPE1 (see Section III.5) which may be frequently updated during the least-squares fit, therefore to speed up the input/output operations the binary format (i.e. WRITE(1)) has been chosen instead.

The short description of the files being used by GOSIA, SIGMA and SELECT is presented in sections VI.1, VI.2 and VI.3, respectively. The files are classified as input files, i.e. the ones which must be attached to the current job, output files, i.e. the ones which are created by the job and should be saved as permanent files for further use, and internal files, used to transfer the data between some of the modules of GOSIA. The internal files need not be attached to the job or saved after the execution. Both GOSIA and SIGMA require an input file which should be provided by the user in the READ* format, while no such a file is needed to run SELECT.

Section VI.4 provides a series of examples of the typical command sequences together with the lists of the input, output and internal files employed during the execution.

VI.1 FILE ASSIGNMENTS IN GOSIA

TAPE1 Contains the internal correction factors (see Section III.5) created and updated when OP,MINI is executed. TAPE1 is required as an input file if the CONT switch CRF, was selected. CRF, causes GOSIA to read the internal correction factors from TAPE1 instead of calculating them when OP,MINI is encountered. Obviously, TAPE1 is to be saved after a previous run to use the time-saving CRF, switch when resuming the minimization. The internal correction factors are updated (and stored on TAPE1) every time the TEST criterion of the OP,MINI input (IV.17) is fulfilled, thus the internal correction coefficients stored on TAPE1 will correspond to the last set of matrix elements for which the update, defined by TEST, was done. In addition, the internal correction coefficients can be calculated using the CONT switch CCF, for a given set of matrix elements. In this case TAPE1 should be saved and defined as an input file for the subsequent run using the CONT CRF, switch.

TAPE2 Contains the set of matrix elements resulting from the last minimization run. TAPE2 is overwritten after completion of each OP,MINI command. The values of the matrix elements stored on TAPE2 can be used instead of those specified in the ME input using the OP,REST command before the selected executable option. An existing permanent file must be assigned to TAPE2 if OP,REST is used.

TAPE3 The function of TAPE3 depends on the command being executed. TAPE3 is the input file of the original, uncorrected experimental γ yields for OP,CORR (the output file of the

corrected yields will be written on TAPE4). Note that if OP,CORR is to be executed the OP,YIEL input entry NTAP (see Section IV.29) must equal 3. TAPE3 can also be assigned instead of TAPE4 as an input file of the corrected yields for OP,MINI and OP,ERRO, if the value of NTAP is 3. To avoid a possible input/output assignment conflict it is, however, recommended to use TAPE4 when executing OP,ERRO, since TAPE3 is reserved as an output file for the code SIGMA if the CONT switch SMR, is set. In this case TAPE3 is created during a first run of OP,ERRO with IDF=1 and IREP=1 (see Section IV.6) and updated if IDF=1 and IREP=2.

TAPE4 Contains the corrected yields written when OP,CORR is executed. TAPE4 should then be an input file of the experimental yields for both OP,MINI and OP,ERRO with the OP,YIEL entry NTAP=4. As discussed above, TAPE3 can also be assigned for this purpose. TAPE4 is also written when OP,POIN is executed with IFL=1 (see Section IV.18) to create the simulated "experimental" yields

TAPE7 Contains the maps of the q-parameters to be used by the fast Coulomb excitation calculation (see Section III.2). TAPE7 is written by OP,MAP and read automatically when either OP,MINI or OP,ERRO command is encountered. This means that the existing permanent file containing the q-parameter map should be attached to the minimization or error calculation jobs as TAPE7 unless OP,MAP has been executed before during the same run.

TAPE8 Contains the absorption coefficients needed to reproduce γ energy dependence of the detector efficiency. Created if NPD in OP,GDET is negative, which is connected to the use of "raw" spectra as defined by the input to OP,RAW.

TAPE9 Contains the parameters needed to approximately reproduce the γ-energy dependence of the Ge detector solid angle attenuation coefficients Q_k (see Section III.3). TAPE9 is written when OP,GDET is executed and automatically read in when OP,YIEL is encountered, which implies that TAPE9 should be attached to any job involving the calculation of γ yields.

TAPE14 An output file for OP,SIXJ. Contains the table of Wigner's 6-j symbols to be used by SIGMA. TAPE14 also serves as an internal file when OP,INTG, OP,CORR, OP,TROU or OP,MINI with the calculation of the sensitivity maps (see Section III.5) are executed.

TAPE15 Contains the current set of errors of the matrix elements calculated by OP,ERRO. TAPE15 is written by OP,ERRO if IREP=0 (see Section IV.6) and read, updated and overwritten if IREP=1. Internal for OP,INTG, OP,CORR and OP,TROU.

TAPE17 An output file for OP,ERRO, containing the best (i.e. yielding the lowest value of χ^2) set of matrix elements found during the scan of the χ^2 hypersurface (see Section III.6). Also serves as the output file to write the statistical tensors after Coulomb excitation using the CONT switch TEN, in conjunction with either OP,STAR or OP,POIN (see Section IV.3). The structure of this file, which may be used by external programs to examine the γ decay following the Coulomb excitation is as follows:

N

ρ_{00}

$\rho_{20}, \rho_{21}, \rho_{22}$

$\rho_{40}, \rho_{41}, \rho_{42}, \rho_{43}, \rho_{44}$

$\rho_{60}, \rho_{61}, \rho_{62}, \rho_{63}, \rho_{64}, \rho_{65}, \rho_{66}$

where N is the level index as defined by the sequence of the input to LEVE. The tensors for the ground state N=1 are not stored, thus $2 \leq N \leq NMAX$ where NMAX is the number of levels included. This sequence is repeated for each experiment according to the sequence of the input to EXPT. Note that because of the symmetry $\rho_{km} = (-1)^m \rho_{k-m}$ only the components with $m \geq 0$ are stored.
TAPE17 is also used as an internal file by OP,TROU and OP,INTG.

TAPE18 An input file for the program SELECT and for OP,ERRO if the correlation matrix is to be used to reduce the number of correlated matrix elements during a full error calculation (IDF=1 and IFC=0 in the OP,ERRO input - see Section IV.6, see also Section III.6). TAPE18 should be first created using the CONT switch SEL, and the default setting of the print parameter 4 (i.e. -2) while executing OP,MINI. TAPE18 should then be attached to the execution of SELECT, the result being written as TAPE10. The latter file can then be attached to the OP,ERRO job as TAPE18.
Internal for OP,TROU.

TAPE22 Output printer file. Unit 22 is used instead of default FORTRAN unit 6 to avoid merging the output with system messages (e.g. underflow warnings) on some systems. During minimization the current value of CHISQ is also output on TAPE6. Dependent on the system and execution mode it will appear either on the screen or in log file, which usually can be viewed during execution. This helps to decide whether or not interrupt the job if no progress is made.

TAPE23 Lists the Doppler-shifted γ-ray energies and detector efficiencies when OP,POIN is executed in conjunction with OP,RAW.

VI.2 FILE ASSIGNMENTS IN SIGMA

SIGMA requires three input TAPE files - TAPE1, TAPE2 and TAPE3. All three files are written by GOSIA. However, if no error estimation of the invariants is desired it is not necessary to attach TAPE1 and only a part of TAPE2 is needed - see Section V.2.2 for details. SIGMA produces no output files other than the printer output. The input file assignments are the following:

TAPE1 Contains the errors of the matrix elements, equivalent to the GOSIA output file TAPE15.

TAPE2 Equivalent to the GOSIA output file TAPE3 written during the calculation of the full errors (OP,ERRO with IDF=1 and the CONT switch SMR,).

TAPE3 The table of the 6-j symbols created by GOSIA as TAPE14 using OP,SIXJ.

TAPE6 The printer output file.

VI.3 FILE ASSIGNMENTS IN SELECT

SELECT requires one input TAPE file, TAPE18, written by GOSIA and no user-given input. The file assignments are as follows:

TAPE6 The printer output file.

TAPE10 Output file, containing the "correlation matrix", i.e. the square matrix, indexed by the indices of the matrix elements and having the elements either equal to 0 (no correlation detected) or to 1 (correlation detected). This matrix should be attached to the OP,ERRO job when calculating the correlated errors as TAPE18.

TAPE18 Input file, containing the information written by GOSIA also on TAPE18 during the execution of OP,MINI with the CONT switch SEL, set and the print parameter 4 equal to -2.

VI.4 EXAMPLES OF THE FILE ASSIGNMENTS FOR TYPICAL JOBS

This section provides some examples of the file assignments necessary to run the typical jobs. The schematic examples of the input streams, ordered according to the usual sequence of the jobs run to analyze a given case, are followed by the list of the input and output files. The dots designate the irrelevant portions of the input. The user-given input file and the printer output file (TAPE22 in GOSIA, TAPE6 in SIGMA and SELECT) are not listed. OP,TITL is always optional and can be skipped. It is also assumed that for all the jobs involving
minimization or error calculation (i.e. starting from VI.4.5.) the corrected experimental yields reside on file TAPE4.

VI.4.1. COULOMB EXCITATION AMPLITUDES

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
EXPT
 .
 .
CONT
 .
 .
END,

OP,STAR
OP,EXIT
```

Input: None

Output: None

Comments: This job can be run with both OP,GOSI and OP,COUL. Adding the CONT switch TEN, will cause creation of the output file TAPE17 (. the statistical tensor file).

VI.4.2. CREATION OF THE GE DETECTORS FILE

```
OP,TITL
 .
OP,GDET
 .
 .
OP,EXIT
```

Input: None

Output: TAPE9 (TAPE8)

Comments: The file TAPE9 is needed as input for all jobs involving the calculation of the γ yields. It is not necessary to select OP,COUL or OP,GOSI to run OP,GDET. TAPE8 is necessary only if OP,RAW is to be used.

VI.4.3 CALCULATION OF THE γ YIELDS

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
```

```
EXPT
 .
 .
CONT
(TEN,)
 .
 .
END,

OP,YIEL
 .
 .
OP,POIN
IFL,YLIM
OP,EXIT
```

Input: TAPE9

Output: TAPE4 if IFL=1, TAPE17 if the CONT switch TEN, is selected.

Comments: This job can be run with either OP,COUL or OP,GOSI. The OP,YIEL entry NTAP must equal 0.

VI.4.4 CALCULATION OF THE INTEGRATED γ YIELDS AND GENERATION OF A "CORRECTED" EXPERIMENTAL YIELDS FILE

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
```

```
EXPT
 .
 .
CONT
 .
 .
END,

OP,YIEL
 .
 .
OP,INTG
 .
 .
OP,CORR
OP,EXIT
```

Input: TAPE3,TAPE9
Output: TAPE4
Comments: The OP,YIEL entry NTAP must equal 3 (i.e. the original experimental yields must reside on TAPE3). OP,INTG can be executed without a subsequent OP,CORR, in this case NTAP must equal 0, TAPE3 need not be attached and no output file is written.

VI.4.5 CALCULATION OF THE q PARAMETER MAP

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
```

```
ME
 .
 .
EXPT
 .
 .
CONT
 .
 .
END,

OP,YIEL
 .
 .
OP,MAP
OP,EXIT
```

Input: TAPE4,TAPE9

Output: TAPE7

Comments: The maps of the q-parameters can be calculated without entering the decay-related information contained in the input to OP,YIEL. However, these maps are only needed for the fitting of the matrix elements, so the deexcitation data are usually already included in the input.

VI.4.6. MINIMIZATION RUN - INITIAL STAGE

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
EXPT
 .
 .
CONT
FMI,
PRT,
4,0
 .
 .
0,0
 .
 .
END,

OP,YIEL
 .
 .
OP,MINI
 .
 .
OP,EXIT
```

Input: TAPE4,TAPE7,TAPE9

Output: TAPE1,TAPE2

Comments: In this example it is assumed that the q-parameter map (TAPE7) has been generated during a previous run. OP,MAP can be executed before OP,MINI in the same run in which case TAPE7 should not be attached as an input file, but will appear as an output file instead. The PRT, entry 4,0 switches off the time-consuming calculation of the sensitivity map and is recommended during the initial stage of the minimization. To further speed up the fitting procedure one can also use the CONT switch FMI, if the printout of the comparison of the fitted and experimental data is not crucial. Usually one needs this table only periodically, so it is recommended to generate it separately when needed, by setting a high value of CHILIM in MINI command to inhibit actual minimization. This procedure is also more reliable, since it refreshes the normalization constants.

VI.4.7. MINIMIZATION - FINAL STAGE

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
EXPT
 .
 .
CONT
CRF,
SEL,
```

```
 .
 .
END,

OP,YIEL
 .
 .
OP,REST
 .
 .
OP,MINI
 .
 .
OP,EXIT
```

Input: TAPE1,TAPE2,TAPE4,TAPE7,TAPE9
Output: TAPE1,TAPE2,TAPE18
Comments: The CONT switch SEL, in conjunction with the default setting of the print parameter 4 (i.e. -2) causes the generation of an output file TAPE18, containing the information used by the code SELECT to create the correlation matrix, subsequently used during the error calculation. OP,REST causes GOSIA to use the values of the matrix elements stored on TAPE2 instead of those given in the ME input. The internal correction factors file TAPE1 may be updated if the TEST criterion is fulfilled.

VI.4.8 SELECT - CORRELATION MATRIX GENERATION

No user-given input is required to run SELECT. The only files needed are:

Input: TAPE18, created by GOSIA as TAPE18, as described above.
Output: TAPE10, containing the correlation matrix.

VI.4.9. DIAGONAL ERROR CALCULATION

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
EXPT
 .
 .
CONT
CRF,
 .
 .
END,

OP,YIEL
 .
 .
OP,REST
 .
 .
OP,ERRO
O,MS,MEND,O,O,RMAX
OP,EXIT
```

Input: TAPE1,TAPE2,TAPE4,TAPE7,TAPE9

Output: TAPE15

Comments: This example assumes the first diagonal error calculation, so IREP=0 and TAPE15 is not attached as an input file. To resume the diagonal error calculation the input to OP,ERRO should be modified as follows:

```
OP,ERRO
0,MS,MEND,1,0,RMAX
```

and the file TAPE15 should be attached as an input file. TAPE15 will be updated and overwritten.
It is also assumed that the internal correction factors (TAPE1) and the current set of matrix elements (TAPE2) are those generated by the last OP,MINI run.

VI.4.10. CALCULATION OF THE CORRELATED ERRORS

```
OP,TITL
 .
OP,GOSI
LEVE
 .
 .
ME
 .
 .
EXPT
 .
 .
CONT
CRF,
SMR,
```

```
.
.
END,

OP,YIEL
 .
 .
OP,REST
 .
 .
OP,ERRO
1,MS,MEND,1,0,RMAX
OP,EXIT
```

Input: TAPE1,TAPE2,TAPE4,TAPE7,TAPE9,TAPE15,TAPE18

Output: TAPE3,TAPE15,TAPE17 if sets of matrix elements yielding better values of χ^2 were found during the run.

Comments: The above example assumes that the file for the sum-rules code SIGMA (TAPE3) is to be created and that the correlation matrix (TAPE18) is to be used during the error calculation. If more than one run is necessary to perform the full error calculation one should modify the input to OP,ERRO as follows to resume the job:

```
OP,ERRO
1,MS,MEND,2,0,RMAX
```

and attach TAPE3 as an input file. TAPE3 will be updated and overwritten by the current job.

VI.4.11. 6-j SYMBOLS TABLE

```
OP,TITL
 .
OP,SIXJ
OP,EXIT
```

Input: None

Output: TAPE14

Comments: OP,SIXJ can be inserted anywhere in the command sequence, in which case the input files required by the preceding options must be attached.

Date: *September 2, 1987*
From: *Alexander Kavka*
To: *Coulex group members*

APPENDIX

EFFICIENCY CALIBRATION CODE

A new program is available to simplify the routine procedure of gamma-detector efficiency calibration. It is called GREMLIN ("Gamma-Ray Efficiency Measurement and Line INtensity calculation") and resides on the NSRL VAX in the directory [KAVKA]. If any changes are made in this code, the linking command is

$LINK GREMLIN,[KAVKA.SILVIA]POLFIT

GREMLIN performs two separate tasks:

1) Least-squares fit of an efficiency-calibration function to a set of peak areas from calibration spectra.

2) Calculation of γ-ray intensities from peak areas, using such a fitted function.

The code is interactive, and its prompts and questions are hopefully sufficient to guide the user. Therefore, this memo provides no real input instructions, with one exception: it describes the structure of the input files containing the calibration points.

Option 1: EFFICIENCY CALIBRATION

1.1 Input of calibration points

A maximum of 500 calibration points can be entered, grouped in up to 9 independently normalized data sets. Typically, these will originate from runs with different calibration sources, but there can just as well be several sets from the same source. If there is more than one data set, the code will automatically fit normalization parameters.

GREMLIN will ask for calibration points for each data set separately. For each set the input can be from a disk file or from the keyboard, and consists of one record for each calibration line. A record looks as follows:

$$E, \quad I, \quad \Delta I, \quad A, \quad \Delta A$$

where E is the γ-ray energy, $I \pm \Delta I$ the relative intensity, and $A \pm \Delta A$ the measured peak area. Note that two data sets cannot be in one file.

However, the input is simplified in the case of ^{152}Eu or ^{182}Ta sources, because the energies and intensities of major ^{152}Eu and ^{182}Ta transitions are stored in DATA statements in the

program. These values were taken from R.A. Meyer: *Multigamma-Ray Calibration Sources* (Lawrence Livermore Laboratory 1978). The record format is then

$$A, \quad \Delta A$$

If keyboard input was chosen, the code will display each tabulated energy and intensity and ask for the area and error. In an input file, the ^{152}Eu or ^{182}Ta lines must be given according to the following table:

line number	^{152}Eu (keV)	^{182}Ta (keV)
1	121.783	31.737
2	244.692	65.722
3	295.939	67.750
4	344.276	84.680
5	367.789	100.106
6	411.115	113.673
7	443.967	116.421
8	488.661	152.430
9	564.021	156.390
10	586.294	179.397
11	688.678	198.350
12	778.903	222.108
13	867.388	229.322
14	964.131	264.078
15	1005.279	927.983
16	1085.914	1001.696
17	1112.116	1113.414
18	1212.950	1121.299
19	1299.124	1157.505
20	1408.011	1189.051
21	1528.115	1221.406
22		1231.019
23		1257.421
24		1273.735
25		1289.158

Any unobserved line that is to be excluded from the fit must be entered as $A = \Delta A = 0$, at the keyboard as well as in a file.

Data for other sources than ^{152}Eu and ^{182}Ta can easily be added to the code in the future, should the need arise. Similarly it is trivial to include additional ^{152}Eu and ^{182}Ta lines in the lists.

1.2 Experimental and theoretical efficiency

For each calibration line GREMLIN calculates the relative efficiency and root-mean-square error:

$$\varepsilon = \frac{A}{I} \qquad \Delta\varepsilon = \varepsilon\sqrt{\left(\frac{\Delta A}{A}\right)^2 + \left(\frac{\Delta I}{I}\right)^2}$$

and makes a transformation to the variables which are then internally used for the fit, i.e.

$$x \equiv \log\frac{E}{E_0} \qquad y \equiv \log\varepsilon \qquad \Delta y = \frac{\Delta\varepsilon}{\varepsilon}$$

The logarithms are of base e and $E_0 = 50$ keV.

The function that GREMLIN fits is

$$\varepsilon(E) = A(E)\ P(E; a_1 \ldots a_n)\ F(E; f)\ W(E; b, c)$$

with the parameters $a_1 \ldots a_n$, f, b, and c to be determined. The different factors are discussed below.

1.3 Attenuation factor

$$A(E) = \exp\left[-\sum_{i=1}^{m}\mu_i(E)d_i\right]$$

$A(E)$ stands for the absorption in layers of m different materials placed in front of the detector, μ_i and d_i being the linear attenuation coefficient and the thickness of the ith material, respectively.

The absorber materials that GREMLIN takes into account are C, Al, Si, Fe, Cu, Cd, Sn, Ta, and Pb. The thicknesses (in cm) are given by the user from the keyboard. DATA statements in the code contain the attenuation coefficient of each material for 20 gamma energies ranging from 30 to 4000 keV. Interpolation is done by means of cubic spline curves. Two of the energy meshpoints were chosen to be 67.416 and 88.004 keV, which are the K-edges of Ta and Pb, respectively, and for each of those elements GREMLIN maintains two spline curves, below and above the edge. All other absorption edges for these nine elements lie below 30 keV.

The variables actually used for the spline curves are $\log\frac{E}{E_0}$ and $\log\frac{\mu}{\mu_0}$ ($\mu_0 = 1$ cm^{-1}), since the points are more evenly spaced in the log-log plane.

The attenuation coefficients were calculated from total cross-sections σ given in E. Storm, H.I. Israel, Nuclear Data Tables A7 (1970) 565, according to

$$\mu\ [\mathrm{cm}^{-1}] = \frac{\rho N_A \sigma}{M} = 0.602205\ \frac{\rho\ [\mathrm{g/cm}^3]\ \sigma\ [\mathrm{barn}]}{M\ [\mathrm{g/mol}]}$$

where ρ is the density, N_A Avogadro's number, and M the atomic weight.

1.4 Polynomial factor

The polynomial factor, degree $n \leq 3$,

$$P(E; a_1 \ldots a_n) = \exp\left[\sum_{k=0}^{n} a_k \left(\log \frac{E}{E_0}\right)^k\right] = \frac{\varepsilon}{\varepsilon_0}$$

is a simple representation of the basic decrease of the efficiency with increasing γ energy. The word "polynomial" refers, of course, to $\log \varepsilon$ as function of $\log E$.

The degree n is chosen by the user. GREMLIN finds good initial values for the parameters a_k by fitting a pure nth-degree polynomial in the region above 250 keV, where $P(E)$ can be expected to dominate.

1.5 Functions describing low-energy slope

An inverse-power factor, with arbitrary $N > 0$, and $f < 0$,

$$F(E; f) = \exp\left[f\left(\log \frac{E}{E_0}\right)^{-N}\right]$$

and a "Woods-Saxon"-type factor, with b and $c > 0$.

$$W(E; b, c) = \frac{1}{1 - \exp\frac{b-E}{c}}$$

are optional, and are unlikely to be used simultaneously, although the code allows that. Each represents the low-energy slope of the efficiency curve. Whereas F is just an *ad hoc* mathematical function, W attempts to model the effect of a discriminator threshold in the pulse-handling electronics.

When F was used, good results were obtained with e.g. $N = 5$, but the value of N does not seem to be very crucial. An initial value for the parameter f is found by simply sampling the value of χ^2 throughout a range of f. The range and stepsize are given by the user, but if the code finds the optimum value at an endpoint of the range, it requests a new range and tries again.

Initial values (in keV) for the parameters b and c, in the "Woods-Saxon" case, are given by the user. They are easy to estimate, b being the threshold and c a measure of the "rise time" of this step function.

1.6 Normalization between data sets

In case of more than one data set, initial normalization factors are cho en in the following way: A linear function

$$y^{(j)} = a_0^{(j)} - a_1^{(j)} x$$

is fitted to every data set in the region $E > 250$ keV (j labels the data sets). The efficiency values in data set $\#j$ are then rescaled by replacing y with $y + a_0^{(1)} - a_0^{(j)}$. This is done before determining initial values for the other parameters.

During the main fit, each normalization parameter is corrected after every iteration by a simple χ^2 scan throughout a range of its value. The scan does not have to be iterated, since there is no correlation between the normalization factors.

1.7 The main fit

When all parameters have been given starting values, the full function is fitted to the calibration points by an iterative matrix inversion method (the same that is used for peak-shape fitting in SILVIA). After every iteration (and renormalization, in case of more than one data set) the program displays the χ^2 and the new parameter values and the user decides whether to continue or stop. Convergence is usually rapid thanks to good initial values — often only 2 or 3 iterations of the main fit are necessary.

When the fit is stopped, GREMLIN reports the best (not necessarily the latest) χ^2, the corresponding fitted parameters with errors and correlation matrix, and a table showing values of the fitted function in comparison with the measured efficiencies. Three optional output files can be written on disk at this moment:

1) A text file showing the results of the fit in the same way as on the screen.

2) An input file for TOPDRAWER that can generate a log-log plot of the calibration points and the fitted curve on the laser printer. The user can specify a header text and a different point plot symbols for each data set.

3) A storage file containing the fitted parameter values, information about the functional form used, and absorber thicknesses. This file is read by GREMLIN's Option 2 to calculate γ-ray intensities.

Option 2: INTENSITY CALCULATION

In this option, the program reads a storage file written by Option 1, and can then re-crea the fitted function $\varepsilon(E)$. It also asks the user to specify the kinematics of the experime (masses of projectile and target; bombarding energy; mass and direction θ, ϕ of radiati ejectile) as well as the angular position $\theta_\gamma, \phi_\gamma$ of the γ detector, so that efficiencies can b calculated for the actually detected (Doppler-shifted) γ energies.

The shifted energy is

$$E' = \frac{E}{1 - \frac{v}{c}\cos\alpha}$$

where the velocity v is calculated from the kinematics and α is the angle between the γ-ra and the radiating nucleus.

$$\cos\alpha = \sin\theta \sin\theta_\gamma \cos(\phi - \phi_\gamma) + \cos\theta\cos\theta_\gamma$$

The user now types a series of transition energies E and peak areas $A \pm \Delta A$, and GREMLIN returns the corresponding relative intensities

$$I = \frac{A}{\varepsilon(E')}$$

and errors ΔI. The errors are calculated from

$$\left(\frac{\Delta I}{I}\right)^2 = \left(\frac{\Delta A}{A}\right)^2 + \left(\frac{\Delta\varepsilon}{\varepsilon}\right)^2$$

where the efficiency error is estimated using the correlation matrix C that results from the fit:

$$(\Delta\varepsilon)^2 = \sum_{j=1}^{p}\sum_{k=1}^{p} \frac{\partial\varepsilon}{\partial\alpha_j}\frac{\partial\varepsilon}{\partial\alpha_k} C_{ij}$$

$\alpha_j (j = 1 \ldots p)$ represents all the parameters of the fit.

The derivatives with respect to the parameters have simple analytical expressions:

$$\frac{\partial\varepsilon}{\partial a_j} = \varepsilon(E')\left(\log\frac{E'}{E_0}\right)^j \qquad \frac{\partial\varepsilon}{\partial f} = \varepsilon(E')\left(\log\frac{E'}{E_0}\right)^{-N}$$

$$\frac{\partial\varepsilon}{\partial b} = -\frac{\varepsilon(E')}{c\left(1 + \exp\frac{E'-b}{c}\right)} \qquad \frac{\partial\varepsilon}{\partial c} = \frac{E'-b}{c}\frac{\partial\varepsilon}{\partial b}$$

REFERENCES

ABR53 A. Abragam, R.V. Pound - Phys. Rev. 92:943 (1953)

ABR72 M. Abramowitz, I. Stegun (eds.) - Handbook of Mathematical Functions, National Bureau of Standards, Washington (1972)

ALD56 K. Alder, A. Bohr, T. Huus, B. Mottelson, A. Winther - Rev. Mod. Phys. 28:432 (1956)

ALD66 K. Alder, A. Winther - Coulomb Excitation, Academic, New York, (1966)

ALD75 K. Alder, A. Winther - Electromagnetic Excitation, Theory of Coulomb Excitation with Heavy Ions, North Holland, Amsterdam, (1975)

BOH69 A. Bohr, B. Mottelson - Nuclear Structure, Benjamin, New York, (1969)

BOS77 F. Bosch, H. Spehl - Z. Phys. A280:329 (1977)

BRE77 R. Brenn, H. Spehl, A. Weckherlin, H. Doubt, G. Van Middelkoop - Z. Phys. A281:219 (1977)

CLI69 D. Cline - Bull. Am. Phys. Soc. 14:726 (1969)

CLI72 D. Cline, C. Flaum - Proc. Int. Conf. on Nucl. Struct. Studies using Electron Scatt. and Photoreaction, Sendai 1972, K. Shoda and H. Ui (eds.), Tohoku Univ. (1972)

CLI86 D. Cline - Ann. Rev. Nucl. Part. Sci. 36:683 (1986)

CZ083 T. Czosnyka, D. Cline, C.Y. Wu - Bull. Am. Phys. Soc. 28:745 (1983)

FRA65 H. Frauenfelder, R. Steffen - in Alpha-, Beta and Gamma Spectroscopy, K. Siegbahn (ed), North Holland, Amsterdam, (1965)

GRE84 H. Grein, H. Emling, J. Stachel - GSI Rep. GSI-84-1 (1984)

KRA70 K. Krane, R. Steffen - Phys. Rev. C2:724 (1970)

KRA72 K. Krane - Nucl. Instr. Meth. 98:205 (1972)

LES71 P.M.S. Lesser - PhD Thesis, Univ. of Rochester (1971)

NIK68 V.S. Nikolayev, I.S. Dmitriev - Phys. Lett. 28A:277 (1968)

ROT59 M. Rotenberg, R. Bivins, N. Metropolis, J. Wooten - The 3j and 6j Symbols, The Technology Press, Cambridge, Mass. (1959)

VAR86 B. Varnestig, A. Backlin, C. Fahlander, A. Kavka, T. Lenke, L.E. Svensson - Nucl. Instr. Meth. A248:419 (1986)

GOSIA UPDATE - MAY 1996

OP, THEO

Generates matrix elements according to the geometrical model following Bohr-Mottelson prescription (General Structure of Matrix Elements, paragraph 4-3d in Nuclear Structure). OP, THEO generates only the matrix specified in ME input and writes them on the REST file. It should therefore be used after OP, COUL or OP, GOSI, but before OP, REST command is executed. Fixing, coupling and releasing of the matrix elements is controlled by ME and CONT commands, the only function of OP,THEO being to create numerical values and write them to the restart file. This allows to make model-dependent analyses by specifying the coupling scheme, generating a set of matrix elements and, keeping the values coupled, performing the minimization, thus effectively fitting only geometrical intrinsic moments. To define OP,THEO input the user must divide the levels specified in LEVE input into bands of definite values of K quantum number. First entry under OP, THEO is a number of bands, which, as an input-saver feature, can be given as a negative integer, in which case the remainder of the input to OP, THEO will be ignored and the contents of the restart file not affected. This is helpful if some matrix elements are added or removed using ME option - OP, THEO can then easily be reactivated.
OP,THEO input is divided into two loops. First one is the definition of bands and the levels ascribed to be their members. As usual, LEVE-defined state indices are used to identify the levels. The second loop is the multipolarity loop, which should exhaust all couplings defined in the ME input. Here for each band-to-band coupling (band indices being either identical for inband matrix elements or different for interband matrix elements) one should specify relevant intrinsic moments for a given multipolarity. In general there are three intrisic moments which could be involved. For in-band or equal-K interband transitions only one of them, marked Q1 is relevant. For non-equal K's generally two moments with the projections equal to the sum and difference of K's are required (Q1 and Q2), unless one of the K's is zero, when again only Q1 is needed. For the K-forbidden transitions three parameter Mikhailov formula is used. Thus, in general, three Q-values are to be input for each band-to-band coupling. Note that Q3 - a decoupling parameter - is irrelevant always if none of the K-values assumes the value of 1/2 and Q2 is irrelevant for in-band transitions and for K-allowed, one K=0 interband couplings. Nevertheless, three numbers are required for each band-to-band coupling.
The specification of multipolarities follows the general convention of GOSIA - E1 through E6 are labeled just by 1 through 6, while M1 is labeled as 7 and M2 as 8. Definition of bands and multipolarities should exhaust all couplings included in ME scheme. It is important that calculated matrix elements fit within the user-specified limits.

The structure of the input to OP, THEO is:

NBANDS	Number of user-defined bands. If negative OP,THEO is ignored
K, NLEV	Band definition - K of a band, number of levels in band #1
$N_1, N_2 \ldots\ldots, N_{NLEV}$	Indices of levels forming band #1
.	
.	**The above two records should be repeated NBANDS times to**
.	**define all bands**
.	
λ_1	Start of multipolarity loop - first multipolarity
$NB_i NB_j$	Band indices

Q1,Q2,Q3	Intrinsic moments
NB_i, NB_j	Band indices
Q1,Q2,Q3	Intrinsic moments
.	
.	**The above sequence should be repeated until all possible in- and interband couplings for the first multipolarity are exhausted**
.	
.	
0,0	Ends first multipolarity definition
λ_2	Second multipolarity
NB_i, NB_j	
Q1,Q2,Q3	
NB_i, NB_j	
Q1,Q2,Q3	
.	
.	
0,0	Ends second multipolarity definition
.	
.	
.	
0	Ends multipolarity loop and the input to OP, THEO

Example:

Assume an even-even nucleus X with two bands - a ground state band and a gamma-vibrational band. LEVE and ME setup is as follows:

LEVE
1,1,0,0
2,1,.2,.2 Levels 1,2,3 form the ground-state band, while 4,5,6 form the gamma band
3,1,4,.5
4,1,2,.7
5,1,3,1.1
6,1,4,1.5
0,0,0,0
ME
2,0,0,0,0
1,2,1,-2,2
1,4,1,-2,2
2,2,1,-2,2
2,3,1,-2,2
2,5,1,-2,2
2,6,1,-2,2
3,3,1,-2,2
3,5,1,-2,2
3,6,1,-2,2
4,4,1,-2,2
4,5,1,-2,2
4,6,1,-2,2

5,6,1,-2,2
6,6,1,-2,2
7,0,0,0,0
2,4,1,-2,2
2,5,1,-2,2
3,5,1,-2,2
3,6,1,-2,2

Matrix elements on the restart file can be generated by OP, THEO using the following sequence:

OP, THEO	
2	Two bands
0,3	K of the gsb, # of levels
1,2,3	Level list for the gsb
2,3	K of the gamma band, # of levels
4,5,6	Level list for the gamma band
2	Multipolarity E2
1,1	In-band, gsb
1,0,0	Q1, two zeros irrelevant
1,2	Interband E2
1,1,0	Q1,Q2- Mikhailov formula, none of the K's=1/2, so Q3 irrelevant
2,2	In-band, gamma band
1,0,0	In-band Q1, Q2 and Q3 irrelevant
0,0	Ends E2 loop
7	M1 loop
1,2	Interband M1
1,1,0	Q1 and Q2 for Mikhailov formula
2,2	In-band M1
1,0,0	Q1 for in-band transitions
0,0	Ends M1 loop
0	Ends multipolarity loop and OP, THEO input

As a result, the restart file will be created overriding the values of matrix elements as given in ME input. If the first entry, NBANDS, is changed to -2 OP, THEO will become inactive.