International Atomic Energy Agency

INDC(SLK)-001
Distrib.: G

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PEGAS

Pre-Equilibrium-Equilibrium Gamma-And-Spin Code

(PC version)

E. Beták and P. Oblozinsky
Institute of Physics, Slovak Academy of Sciences,
Dúbravská cesta 9,
84228 Bratislava, Slovak Republic

March 1993

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

Reproduced by the IAEA in Austria
March 1993

INDC(SLK)-001
Distrib.: G

PEGAS

Pre-Equilibrium-Equilibrium Gamma-And-Spin Code

(PC version)

E. Betàk and P. Oblozinsky
Institute of Physics, Slovak Academy of Sciences,
Dúbravská cesta 9,
84228 Bratislava, Slovak Republic

Report of the IAEA Research Contract Nr. 5148/R2/RB

March 1993

PEGAS

Pre-Equilibrium-Equilibrium Gamma-And-Spin Code

(PC version)

E. Běták and P. Obložinský
Institute of Physics, Slovak Academy of Sciences,
Dúbravská cesta 9,
CS-84228 Bratislava, Czechoslovakia *

Bratislava, October 1992

PEGAS is a Pre-Equilibrium-Equilibrium Gamma-And-Spin code, based on the unified model of nuclear reactions. Therein, the equilibrium (compound-nucleus) emission is treated as an organic part of the pre-equilibrium emission. The code has two important novel features: the angular-momentum couplings are correctly taken into account for all processes (equilibration, particle and γ emission), and nucleon as well as γ emissions are calculated with all possible cascades for all possible sequences of the ejectiles. The Master equations of the exciton model serve as a basis for the calculations. All the couplings caused by successive particle and/or γ emissions are fully incorporated. Doing that, up to 150,000 coupled Master equations are to be solved. To enable wide spread and usage of the code, every possible effort has been put to make it as compact as possible, so that the program exe-form fits cca 510 KB of memory and can be therefore run at standard PC's under the operational system DOS. The present version of the code is designed for reactions induced by nucleons (though other projectiles are allowed as well), leading to the composite system with the excitation energy not much exceeding 30 MeV and with nuclear spins limited to $< 15\hbar$.

I. INTRODUCTION

Nuclear reaction models based on pre-equilibrium concepts have become a standard tool in analyses of experimental data, predictions of unknown data as well as in evaluations of many important nuclear data. However, several simplifications are currently used in the existing codes. The main handicap has been the lack of possibilities to trace a complete development of the reaction system including the consistent treatment of cascade emissions. Thus, for example, the pre-equilibrium emission is often limited to the primary particle only. The second handicap is the absence of angular momentum in the formalism used. In several codes a simplified treatment of angular momentum conservation is included, however, no code is available yet where this treatment is made in a full and correct way. All this is overcome by the present PEGAS code. The code PEGAS has been developed within the Research Contract with the International Atomic Energy Agency No. 5148 "Development of Improved Formalism in the Frame of Pre-Equilibrium/Compound Nuclear Reaction Theory and Code for Particle and Gamma Emission Spectra at Medium Excitation Energies".

In the PEGAS code, the equilibrium (compound-nucleus) emission is treated as an organic part of the pre-equilibrium emission. The master equations of the exciton model serve as a basis for the calculations. All the couplings caused by successive particle and/or γ emissions are fully incorporated within the code, what leads typically to several tens of thousands of coupled equations. Dimensions of arrays in the present version are sufficient to handle and to store 10 nuclei $\times$ 50 energies $\times$ 20 exciton states $\times$ 15 values of spin, what corresponds to a maximum of 150,000 coupled master equations. To enable wide spread and usage of the code, every possible effort has been put to make it compact, so that the program exe-form fits cca 510 KB and can be therefore run at standard PC's under the operational system DOS. This has been achieved by minimalizing dimensions of all arrays. The user of better computing facilities may, however, lift these limitations and enlarge the dimensions to the size needed.

The code is based on the master equation approach to preequilibrium nuclear reactions developed over years by one of us [1,2]. We extended this approach by adopting the full angular momentum formalism for intranuclear cascade, particle as well as γ emission developed by another of us [3] (see also [4]). Under the support of the International Atomic Energy Agency we developed further these two ingredients and combined them into one consistent formalism. The result of its fast computational solution is the present code designed for PC computers.

II. MODEL AND FORMALISM

A. Model

The unified model combines in a natural way the pre-equilibrium nuclear reaction concept with the equilibrium statistical decay. This is possible via the master equation approach to the pre-equilibrium exciton model, that allows one to follow the time evolution of the reaction system up to its complete decay. In order to handle properly cascades of γ rays, the ususal set of master equations (tens of equations) has been enlarged to couple also different excitation energies as well as various nuclei. This gives rise to typically tens of thousands of equations, that can, however, be solved pretty fast even on small PC's [1,2]. The great advantage of such a model is a consistent calculation of multiple particle emission as well as multiple γ emission. The model has been quite recently extended to account for angular momenta [3], opening thus a possibility to calculate also discrete γ ray production. It is important that in the angular-momentum version of the unified model, the nucleon as well as the γ emission rates of the pre-equilibrium decay automatically take over their correct equilibrium (Hauser-Feshbach) form.

The system of master equations of the pre-equilibrium decay is often used for one nucleus and one excitation energy; however, in our approach we included all possible feedings caused by the γ de-excitation as well as by particle emissions. These particle and γ couplings are schematically depicted in Fig. 1.

To be fully consistent with the underlying physics, we have further correctly included all couplings by the angular momentum. Below, we put the basic equations of the model and its physical ingredients.

The set of master equations used is

$$\begin{aligned}\frac{\mathrm{d}P(i,E,J,n,t)}{\mathrm{d}t} &= P(i,E,J,n-2,t)\,\lambda^{+}(i,E,J,n-2) \\ &+ P(i,E,J,n+2,t)\,\lambda^{-}(i,E,J,n+2) \\ &- P(i,E,J,n,t)\,[\lambda^{+}(i,E,J,n)+\lambda^{-}(i,E,J,n)+L(i,E,J,n)] \\ &+ \sum_{i',J',n',x} \int P(i',E',J',n',t)\,\lambda_x([i',E',J',n'] \xrightarrow{\epsilon} [i,E,J,n])\mathrm{d}\epsilon, \quad (1)\end{aligned}$$

where $P(i,E,J,n,t)$ is the occupation probability of a nucleus i at the excitation energy E, spin J and the exciton number n, λ^{+} and λ^{-} are the transitional rates to neighbouring states, and L is the total integrated emission rate of particles (protons π and neutrons ν) and γ rays

$$L(i,E,J,n) = \sum_{x=\nu,\pi,\gamma} \int \lambda_x([i,E,J,n] \xrightarrow{\epsilon} [\text{anything}])\mathrm{d}\epsilon\,. \quad (2)$$

The last term in (1) ensures the coupling of different nuclei and various excitation energies.

The nucleon emission rate per energy and time unit is

$$\lambda_{\pi,\nu}([E,J,n] \xrightarrow{\epsilon} [U,S,n-1]) = \frac{1}{h}\frac{\omega(n-1,U,S)}{\omega(n,E,J)}\mathcal{R}_{\pi,\nu}(n)\sum_{j=|S-1/2|}^{S+1/2}\sum_{l=|J-j|}^{J-j} T_l(\epsilon)\ , \quad (3)$$

where $\omega(n,E,J)$ is the particle-hole state density defined below, T_l's are the transmission coefficients of the emitted nucleon and $\mathcal{R}_x(n)$ is the charge factor for a given type of a nucleon [5]. At any stage of the reaction

$$\mathcal{R}_\nu(n) + \mathcal{R}_\pi(n) = 1, \quad (4)$$

whereas the initial values as well as those at equilibrium depend on the type of reaction. Thus, for example, for reactions induced by neutrons

$$\begin{aligned} \mathcal{R}_\nu(1) &= 1, & \mathcal{R}_\nu(\bar{n}) &= N/A, \\ \mathcal{R}_\pi(1) &= 0, & \mathcal{R}_\pi(\bar{n}) &= Z/A. \end{aligned} \quad (5)$$

In eq. (5), $\bar{n}$ is the equilibrium exciton number.

The particle-hole state density $\omega_n(E,J)$ is

$$\omega(n,E,J) = \frac{g(gE-A_{ph})^n}{p!h!(n-1)!}R_n(J), \quad (6)$$

where g is the single-particle level density, the exciton number n is divided into particles p and holes h, $n = p + h$, A_{ph} is the correction term due to the Pauli principle, and the spin part is

$$R_n(J) = \frac{2J+1}{2\sqrt{2\pi}{\sigma_n}^3}\exp\left(-\frac{(J+1/2)^2}{2{\sigma_n}^2}\right), \quad (7)$$

where σ_n is the spin cuf-off parameter.

The intranuclear transition rates are

$$\lambda^{\pm}(E,J,n) = \frac{2\pi}{\hbar}|M|^2 Y_n^{\downarrow} X_{nJ}^{\downarrow}, \quad (8)$$

where $|M|^2$ is the energy part of the average squared transition matrix element of the residual interaction, $Y_n^{\downarrow}$ is the energy part of the accessible final states, and $X_{nJ}^{\downarrow}$ represents angular momentum part of the squared transition matrix element together with the angular momentum part of the accessible final states. The $Y_n^{\downarrow}$ is given as [6]

$$Y_n^{\downarrow} = \frac{g}{2(n+1)} \frac{(gE - A_{p+1,h+1})^{n+1}}{(gE - A_{ph})^{n-1}}, \tag{9}$$

where we did not show the correction term for the finite depth of the nuclear potential well, which is not effective for energies below 40 MeV. The $X_{nJ}{}^{\downarrow}$ is given as [3]

$$X_{nJ}{}^{\downarrow} = \frac{1}{R_n(J)} \sum_{j_4 Q} R_1(Q) \tilde{F}(Q) R_{n-1}(j_4) \Delta(Q j_4 J), \tag{10}$$

where $\Delta(Q j_4 J)$ is 1 for $|Q - j_4| \leq J \leq Q + j_4$ and 0 otherwise, and

$$\tilde{F}(Q) = \sum_{j_3 j_5} (2j_5 + 1) R_1(j_5) (2j_3 + 1) F(j_3) \begin{pmatrix} j_5 & j_3 & Q \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}^2, \tag{11}$$

and the angular momentum density of pair states is

$$F(j_3) = \sum_{j_1 j_2} (2j_1 + 1) R_1(j_1) (2j_2 + 1) R_1(j_2) \begin{pmatrix} j_1 & j_2 & j_3 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^2. \tag{12}$$

In eqs. (10) to (12), the notation of spins is explained in Figure 2.

The γ emission mechanism encoded into the PEGAS code is based on the $E1$ single-particle γ radiative transition, Brink-Axel hypothesis, and it uses the giant dipole resonance γ-ray strength function [7,8]. The γ emission is associated with the change of the energy of a single nucleon (which eventually may fill in the corresponding hole, decreasing thus the exciton number by -2). With full angular momentum couplings, the γ emission rate λ_γ from an n-exciton state is [3]

$$\begin{aligned} \lambda_\gamma([E,J,n] \xrightarrow{\epsilon_\gamma} [U,S,n]) &= \frac{\epsilon_\gamma^2 \sigma_{GDR}(\epsilon_\gamma)}{3\pi^2\hbar^3c^2} \frac{b_{nS}^{nJ}\, \omega(n, E-\epsilon_\gamma, S)}{\omega(n,E,J)}, \\ \lambda_\gamma([E,J,n] \xrightarrow{\epsilon_\gamma} [U,S,n-2]) &= \frac{\epsilon_\gamma^2 \sigma_{GDR}(\epsilon_\gamma)}{3\pi^2\hbar^3c^2} \frac{b_{n-2S}^{nJ}\, \omega(n-2, E-\epsilon_\gamma, S)}{\omega(n,E,J)}, \end{aligned} \tag{13}$$

where $U = E - \epsilon_\gamma$ and the branching ratios are

$$b_{mS}^{nJ} = \frac{y_m^n x_{mS}^{nJ}}{y_m^m x_{mS}^{mJ} + y_m^{m+2} x_{mS}^{m+2J}}. \tag{14}$$

In eq. (13), $\sigma_{GDR}(\epsilon_\gamma)$ is the photo-absorption cross section. The energy terms y's are

$$\begin{aligned} y_n^n &= gn, \\ y_n^{n+2} &= g^2 \epsilon_\gamma, \end{aligned} \tag{15}$$

and the corresponding spin coupling terms

$$x_{nS}^{nJ} = \frac{3(2J+1)}{R_n(S)} \sum_{j_1 j_2 j_3} (2j_1+1)R_1(j_1)(2j_2+1)R_1(j_2)R_{n-1}(j_3) \times \begin{pmatrix} j_2 & 1 & j_1 \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix}^2 \begin{Bmatrix} j_2 & j_3 & S \\ J & 1 & j_1 \end{Bmatrix}^2 \quad (16)$$

and

$$x_{nS}^{n+2J} = \frac{2J+1}{2S+1} \sum_{j_1 j_2} (2j_1+1)R_1(j_1)(2j_2+1)R_1(j_2) \begin{pmatrix} j_2 & j_1 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^2 \Delta(S1J). \quad (17)$$

The notation of spins involved is depicted in Fig. 3.

By solving the set of master equations, one arrives to time integrals of the occupation probabilities,

$$\tau(i,E,J,n) = \int_0^\infty P(i,E,J,n,t)\mathrm{d}t, \quad (18)$$

which are essential in calculations of spectra, cross sections, and other interesting quantities. Thus, the angle-integrated energy spectrum of a particle or a γ quantum emitted from the originally created composite system ($i = 0$) at the full initial excitation energy E_c is

$$\left(\frac{\mathrm{d}\sigma_x}{\mathrm{d}\epsilon_x}\right)_0 = \sum_{J_c,n} \sigma(E_c,J_c)\tau(0,E_c,J_c,n)\lambda_x([0,E_c,J_c,n] \xrightarrow{\epsilon_x} [\text{anything}]). \quad (19)$$

The cross section of a creation of the composite system by a projectile with the incident energy ϵ_{proj} is

$$\sigma(E_c,J_c) = \pi\lambda^2 \frac{2J_c+1}{(2s_a+1)(2I+1)} \sum_{S=|I-s_a|}^{I+s_a} \sum_{l=|J_c-S|}^{J_c+S} T_l(\epsilon_{proj}). \quad (20)$$

The full particle and/or γ production spectrum is obtained by the summation over all nuclei within the reaction chain and an integral over all possible excitation energies E

$$\frac{\mathrm{d}\sigma_x}{\mathrm{d}\epsilon_x} = \sum\!\!\!\!\!\!\int_{E,J,J_c,n,i} \sigma(i,E_c,J_c,E,J)\tau(i,E,J,n)\lambda_x([i,E,J,n] \xrightarrow{\epsilon_x} [\text{anything}]). \quad (21)$$

Here, $\sigma(i,E_c,J_c,E,J)$ represents the population cross section of a nucleus with the excitation energy E and spin J, when the original composite system was created

with the cross section $\sigma(E_c, J_c)$. The polulation cross section incorporates the preceding history of the system by cascade deexcitation and particle emissions before the present emission.

The computer code PEGAS enables one to calculate arbitrarily complicated cross sections, even for coincident quantities, like the exclusive spectra, differential γ multiplicities, γ spectra from a selected type of multiparticle reaction like $(a, bc\gamma)$ etc. All of them can be written in a similar manner as eq. (21), however, their structure might be not so transparent as the above, because it depends on whether one needs all possible permutations and combinations of ejectiles or not.

B. Algorithm

Fig. 4 brings the basic flowchart of the code PEGAS. The huge system of master equations can be solved using the very happy fact that the emissions from later stages (and lower energies) cannot influence the earlier one which proceeds from former stages within the reaction chain and/or higher excitation energy. So, in practice, the huge system of master equations is splitted, similarly as in the preceding codes (see Refs. [1,2]), into subsets each just for one nucleus, one excitation energy and one value of the spin. Each subset of master equations is then solved by the fast algorithm developed by Chatterjee and Gupta [9].

C. Parameters

The initial configuration to be used for the γ emission calculations in nucleon-induced reactions is generally accepted to be $n_0 = 1$.

The second quantity to be fixed is the intensity of intranuclear transition rates ($\lambda^{\pm}$ in eqs. (8)). To do that we have used the average squared matrix element of the residual interaction $|M_{nonspin}|^2$ of spin-independent calculations according to the parametrization of Kalbach [10], where it depends on the per exciton excitation energy, $e = E/n$. If e is between 7 and 15 MeV, the matrix element takes the form

$$|M_{nonspin}|^2 = K' A^{-1/3} e^{-1}; \tag{22}$$

and more complicated dependence is outside the interval quoted. The constant K' is taken from the systematics; a value of $K' = 100$ or 110 MeV^3 has been found to yield reasonable results [11]. The squared matrix element $|M|^2$ for the spin version of the unified model encoded into PEGAS is established from the condition [3]

$$|M|^2 < X_{nJ}{}^{\downarrow} >= |M_{nonspin}|^2, \tag{23}$$

where the averaging is performed over J. This procedure ensures consistency of nucleon emission spectra obtained in both the spin and the nonspin versions of

calculations. This renormalization of the matrix element is fixed at $n = 3$, the most dominant exciton state for the nucleon emission.

The code assumes individual single-particle level densities for each nucleus in the sequence. The default option of the code is the simple value of $g = A/13$ for all included nuclei. The pairing corrections are not included in the PC version of PEGAS. Their introduction needs more effort. Technically, it can be easily done, but the user must be well aware of all possible consequences of the way in which he has introduced the pairing. Especially, the pairing can enter effectively binding energies or the densities of states to influence particle emission, then the intranuclear transition rates as well as the γ de-excitation process itself.

The spin cut-off parameter has been taken in the form of Herman and Reffo [12]

$$\sigma_n{}^2 = (0.24 + 0.0038E)nA^{2/3}. \tag{24}$$

The particle trasmission coefficients were approximated by the use of formulae by Murthy et al. [13]. However, their replacing by other types of transmission coefficients, taken e.g. from the full optical model calculation, is a trivial task and can be achieved by replacing the command `CALL TRANS` in the main program just by the input of the transmission coefficients or by calling another, more sophisticated procedure.

Similarly, the γ photoabsorption cross section is used in the Lorentzian form

$$\sigma_{GDR}(\epsilon_\gamma) = 53.2\text{mb}\frac{NZ}{A}\frac{\Gamma^2}{(\epsilon_\gamma{}^2 - E_{GDR}{}^2)^2 + \epsilon_\gamma{}^2\Gamma^2}, \tag{25}$$

with $\Gamma = 5$ MeV and

$$E_{GDR} = 29\sqrt{(1 + 2/A^{1/3})/A^{1/3}} \tag{26}$$

[14]. Replacing these global recipe (the command `SG(IE)=CHAGUG(ENGY)`) by the values from tables (e.g. [15]) supplied on the input or by calculation of individual formula (e.g. double-peaked Lorentzian) for the GDR cross section (in mb) is easily possible.

III. CODE DESCRIPTION

A. Basic features

The computer code PEGAS is based on codes PEQAG and PEQGM reported earlier [1,2]. To be able to handle spin variables, the angular momentum couplings as in [3] have been incorporated so that the resulting code is significantly larger. The present version of the PEGAS source is about 40 KB, what is nearly twice the

size of that of PEQAG. The code is available from the International Atomic Energy Agency as well as from the authors.

The computer code PEGAS is developed to run on standard PC's under DOS, currently still the most common operational system. DOS is developed to operate on 640 KB memory, and it leaves just about 520 KB for an embedded code. This has been a severe restriction in writing the code PEGAS. The current version needs about 510 KB core memory plus about 3.5 MB scratch space on a disc, which is freed after the code has finished. The user with a more powerful computing facility, such as a mainframe, a workstation, or the operational system UNIX that overcomes the DOS memory restriction, is advised to enlarge dimensions and to change the code into a more powerful instrument. The present version is limited to not more than 50 energy steps (i.e. the excitation energy divided by the energy step cannot exceede 50), 20 different exciton states (e.g., $n = 1, 3, 5, ..., 41$ in the composite nucleus), 15 different values of spin for each nucleus (either integer or half-integer, starting with 0 or 0.5), and at most 10 calculated nuclei within the reaction chain (this means up to 4 nucleon emissions interspaced by gammas as needed). Each of these limitations is easy to lift at any time; however, the enlarged version of the code will not fit any more 520 KB memory window left by DOS.

To increase the allowed number of energy steps one has simply to change dimensions of all arrays, which are 50 in the present version of the code, to the amount required and to change correspondingly the condition, which checks the number of energy steps and which is located between the labels `518` and `519` of the main program.

Similarly, increase of the possible number of exciton states means lifting those dimensions of arrays, which are now equal to 20, to the desired higher value. In conjunction with that, this limit is also in the line `3450 alps(20,ij)=0.`, and should be modified accordingly.

Increase of the allowed upper limit for spin can be done by changing dimensions from present 15 to another value and simultaneously replacing the condition ... `.LE. 14.5` ..., which appears at many places of the present code, by the new limit. However, the spin-coupling coefficients functions `CLEBSH` and `SIXJ` have been tested only for the values of angular momenta, which are used throughout our version of the code. The user is warned to be very careful when doing this step, because these routines are very sensitive to the machine precision when used for higher values of angular momenta. Our general advice is to put them to still higher precision than is the double precision used presently.

The last possible modification suggested here is enlarging the size of the reaction chain of nuclei, which is to be calculated. It means lifting the present value of 10 to

selected higher values, further defining the charge factor $\mathcal{R}$ for the later stage of the reaction; and increasing the number of files (currently T1 to T9) to be scratched on a disc. Doing that, a possible conflict with the DOS or FORTRAN options might appear.

Even though the inclusion of angular momentum is a necessary condition for incorporation of discrete γ transitions, the present PEGAS code includes only the transitions between continuum (quasicontinuum) states. A possible extension of the code in this direction cannot be handled straightforwardly on a PC computer since modifications are needed in the particle-hole state densities, the energy loops, and an extra procedure is needed for a decay of discrete states.

In order to make the code as compact as possible, every possible effort has been put to save the memory needed. Thus, just for example, only the carefully selected variables remain in the double precision, and all the rest was given to the single precision to minimize the memory requirements.

The time needed for the test run (14 MeV n on ^{93}Nb with the energy step of 0.5 MeV) took about 45 minutes at PC-386.

B. Input and output

The program is designed to excitation energies not much exceeding 30 MeV. This limit is closely related to not more than 15 allowed values of angular momentum. The projectile is coded using its key-number (1-n, 2-p, 3-d, 4-t, 5-^{3}He, 6-α). However, only nucleon transmission coefficients T_l are provided by the code, approximated by formulae from ref. [13]. For other projectiles (and also for the case the user needs a more sophisticated approach), the transition coefficients have to be supplied on the input.

The **input** file consists of the following lines:

LINE	*FORMAT*	*INPUT QUANTITIES*
1	1X,79H	Title card of the calculation.
2	3I4	N of the composite nucleus, Z of the composite nucleus, projectile key number.
3	6F8.	Excitation energy of the composite nucleus (MeV), energy step (MeV), matrix element constant K' (MeV^3), ground-state spin of the target, ground-state spin of the composite nucleus, projectile binding energy (if not n or p) in composite nucleus

4	10F6.	Neutron binding energies (MeV) in nuclei according their keys ($i = 0$ means initial composite nucleus: CN; $i = 1$ is CN after emission of 1 neutron: CN$-n$; similarly 2: CN$-p$; 3: CN$-2n$; 4: CN$-(n+p)$; 5: CN$-2p$; 6: CN$-3n$; 7: CN$-(2n+p)$; 8: CN$-(n+2p)$; 9: CN$-3p$). *NOTE: If the excitation energy of the system is not sufficient to emit all considered particles, the later part of the set of binding energies are just dummy variables.*
5		The same for protons (MeV).
6	10F6.	Single-particle level densities (MeV^{-1}) in the same order as were the binding energies (*a blank line implies* $g = A/13$ *to be used for all nuclei*).
7	10F6.	Projectile transmission coefficients at their incident energy for $l = 0, 1, ..., 9$ (*if needed by the user*).
8		As above, for $l = 10, 11, ..., 14$.

The output is directed into the output file. However, an information about how the program proceeds (not the physically relevant information itself) appears also on the screen. The program asks for the input and the output files, repeats the title of the calculation on the screen, and afterwards informs by printing the appropriate nuclear key number about each cycle over the nucleus calculated within the reaction chain and it types the current excitation energy calculated.

The **output** file starts with the program head and the title of the calculation, afterwards it repeats the most important input data (nuclear mass, initial excitation energy, binding energies, etc.). Next is the table of the intranuclear transition rates, particle and gamma emission rates for the highest energy calculated and the spin with maximal contribution to the reaction cross section. The first column is the number of holes h (note that the exciton number $n = 2h+1$ for the nucleus with the key $i = 0$), transition rates λ^+, λ^-, emission rate $L_{\pi+\nu}$, energy integrated γ emission rate rate (all in sec^{-1}). The next table printed is that of master equations solution (to save the space, only its part for the maximally contributing spin is printed; however, all spins are calculated). It contains the excitation energy, the spin, part of the cross section exhausted (from the current energy E and spin J) by particle emission and by γ's, total cross section of the population of the current energy and spin, and the product $\sigma(i, E_c, J_c, E, J)\tau(i, E, J, n)$ as obtained from the master equations for three lowest exciton states. Next, we arrive to spectra (in mb/MeV) from the nucleus given, which already includes all γ de-excitations. Therefore, due to the γ multiplicity, the sum of cross sections is somewhat higher than the initial population

cross section of a given nucleus. All this procedure is repeated for all nuclei within the reaction chain. Finally, the full production cross section of neutrons, protons and gammas (summed over all nuclei) is printed.

In order to bring a better illustration, we present in Fig. 5 the calculated γ spectra from 14 MeV $n+^{93}$Nb. The test run input file, a copy of the output appearing on the screen, and a representative part of the output file are given in the Appendices.

ACKNOWLEDGMENTS

This work was supported in part by the International Atomic Energy Agency under the Contract No. 5148/RB. We are grateful to the IAEA Nuclear Data Section, notably to Prof. V.A. Konshin and Dr. A.B. Pashchenko, for constant interest. Partial support of this work by the Slovak Academy of Sciences grant No. 042/92 is also acknowledged.

* E-mail (EUNET) address: **betak@savba.cs**.

[1] E. Běták and J. Dobeš, *Code PEQGM*, Report IP EPRC SAS 43/1983 (Inst. Phys., Bratislava, 1983).

[2] E. Běták, *Code PEQAG*, Report INDC(CSR)-016/LJ (IAEA, Vienna, 1989).

[3] P. Obložinský, Phys. Rev. **C35**, 407 (1987).

[4] P. Obložinský and M.B. Chadwick, Phys. Rev. **C41**, 1652 (1990).

[5] C.K. Cline, Nucl. Phys. **A193**, 417 (1973).

[6] E. Běták, Comp. Phys. Comm. **9**, 92 (1975).

[7] E. Běták and J. Dobeš, Phys. Lett. **84B**, 368 (1979).

[8] J.M. Akkermans and H. Gruppelaar, Phys. Lett. **157B**, 95 (1985).

[9] A. Chatterjee and S.K. Gupta, Z. Phys. **A301** (1981) 271.

[10] C. Kalbach, Z. Phys. **A287** (1978) 319.

[11] F. Cvelbar and E. Běták, Z. Phys. **A332**, 163 (1989);
F. Cvelbar, E. Běták, and J. Merhar, J. Phys. **G17**, 113 (1991).

[12] M. Herman and G. Reffo, in Nuclear Level Densities Bologna 1989 (World Scientific, Singapore 1992). p. 103.

[13] K.H.N. Murthy, S.K. Gupta, and A. Chatterjee, Z. Phys. **A305** (1982) 73;
E **A307** (1982) 374.

[14] S.A. Fayans, lecture (1982).

[15]S.S. Dietrich and B.L. Berman, At. Data Nucl. Data Tbl. **38**, 199 (1988).

APPENDIX A: INPUT FILE

```
SPIN-test Nb+n, 14 MeV              Data October 1992
 53  41    1
 21.100     0.50     100.    4.5     0.0      100.
 7.23  8.83  6.73  7.88  8.64  6.57 12.05  7.19  7.93  5.79
 6.54  6.04  9.56  5.85  9.39  8.47  5.16  8.69  7.69 11.60
```

APPENDIX B: COPY OF TEXT FROM THE DISPLAY

```
Input data file ?    nb.dat
Output list file ?   nb.out
SPIN-test Nb+n, 14 MeV                Data October 1992
PEGAS                cycle = 0          (maximum = 9)
21.1 20.6 20.1 19.6 19.1 18.6 18.1 17.6 17.1 16.6
16.1 15.6 15.1 14.6 14.1 13.6 13.1 12.6 12.1 11.6
11.1 10.6 10.1  9.6  9.1  8.6  8.1  7.6  7.1  6.6
 6.1  5.6  5.1  4.6  4.1  3.6  3.1  2.6  2.1  1.6
 1.1   .6
PEGAS                cycle = 1          (maximum = 9)
13.9 13.4 12.9 12.4 11.9 11.4 10.9 10.4  9.9  9.4
 8.9  8.4  7.9  7.4  6.9  6.4  5.9  5.4  4.9  4.4
 3.9  3.4  2.9  2.4  1.9  1.4   .9
PEGAS                cycle = 2          (maximum = 9)
14.6 14.1 13.6 13.1 12.6 12.1 11.6 11.1 10.6 10.1
 9.6  9.1  8.6  8.1  7.6  7.1  6.6  6.1  5.6  5.1
 4.6  4.1  3.6  3.1  2.6  2.1  1.6  1.1   .6
PEGAS                cycle = 3          (maximum = 9)
 5.0  4.5  4.0  3.5  3.0  2.5  2.0  1.5  1.0   .5

PEGAS                cycle = 4          (maximum = 9)
 7.8  7.3  6.8  6.3  5.8  5.3  4.8  4.3  3.8  3.3
 2.8  2.3  1.8  1.3   .8
PEGAS                cycle = 5          (maximum = 9)
 5.0  4.5  4.0  3.5  3.0  2.5  2.0  1.5  1.0   .5

PEGAS                cycle = 6          (maximum = 9)
PEGAS                cycle = 7          (maximum = 9)
PEGAS                cycle = 8          (maximum = 9)
PEGAS                cycle = 9          (maximum = 9)
Stop - Program terminated.
```

APPENDIX C: PART OF THE OUTPUT FILE

PEGAS - Pre-Equilibrium-Equilibrium Gamma And Spin Code
(by E. Betak and P. Oblozinsky)
== version October, 1992 ==

SPIN-test Nb+n, 14 MeV Data October 1992

A = 94 Eexc = 21.10 MeV energy step = .50 MeV
Reaction c.s. = 1591.0 mb K' = 100. MeV**3
GDR param: E = 16.3 MeV width = 5.00 MeV peak c.s. = 246. mb
Single-particle level dens. (1/MeV) and binding energies (MeV) :

KEY	0	1	2	3	4	5	6	7	8	9
g	7.23	7.15	7.15	7.08	7.08	7.08	7.00	7.00	7.00	7.00
B(N)	7.23	8.83	6.73	7.88	8.64	6.57	12.05	7.19	7.93	5.79
B(P)	6.54	6.04	9.56	5.85	9.39	8.47	5.16	8.69	7.69	11.60

holes	lambda(+)	lambda(-)	particle rate	gamma rate
0	.1560E+22	.0000E+00	.0000E+00	.6942E+18
1	.3466E+22	.3291E+18	.5665E+21	.2979E+18
2	.2761E+22	.1818E+20	.1570E+21	.9859E+17
3	.2149E+22	.7138E+20	.5050E+20	.3665E+17
4	.1631E+22	.1822E+21	.1689E+20	.1616E+17
5	.1167E+22	.3768E+21	.4928E+19	.8706E+16
6	.7433E+21	.6703E+21	.1481E+19	.5576E+16
7	.4468E+21	.1024E+22	.3792E+18	.4066E+16
8	.2470E+21	.1484E+22	.7546E+17	.3274E+16
9	.1212E+21	.2062E+22	.1014E+17	.2877E+16
10	.5012E+20	.2773E+22	.8788E+12	.2769E+16
11	.0000E+00	.3631E+22	.0000E+00	.2937E+16

Master equations for nucleus of key 0

E	J	particle	gamma	population c.s.	time integrals		
21.1	5.0	240.8	.5663	241.4	.15E-18	.60E-19	.80E-19
20.6	5.0	.5297E-04	.1220E-06	.5309E-04	.18E-28	.28E-28	.27E-26

SPECTRA (in mb/MeV) from nucleus of key 0

Energy	neutrons	protons	gammas	
.500	391.00	.18896	.97207	
1.000	402.65	.73136	.86045	
1.500	372.62	1.5882	.73786	
2.000	322.59	2.7388	.64728	
4.000	133.71	7.9030	.46314	
6.000	65.794	11.618	.39454	
8.000	35.663	9.0744	.29792	
10.000	21.302	6.9924	.20505	
12.000	10.026	4.6071	.20886	
14.000	.00000	1.1543	.36022	
16.000	.00000	.00000	.70557	
18.000	.00000	.00000	.55370	
20.000	.00000	.00000	.30850	
Integrals	1499.8	87.341	8.9445	mb

Master equations for nucleus of key 1

E	J	particle	gamma	population c.s.	t i m e	i n t e g r a l s	
13.4	4.5	8.017	.2155	8.233	.00E+00	.52E-21	.11E-18
12.9	4.5	9.670	.3200	9.990	.00E+00	.12E-20	.25E-18

SPECTRA (in mb/MeV) from nucleus of key 1

Energy	neutrons	protons	gammas	
.500	768.62	27.001	406.75	
1.000	480.53	67.898	345.50	
1.500	263.88	94.668	299.63	
2.000	131.66	104.02	256.63	
4.000	2.7677	48.148	96.086	
6.000	.00000	5.1173	21.222	
8.000	.00000	.00000	2.9678	
10.000	.00000	.00000	.31543	
12.000	.00000	.00000	.19368E-01	
Integrals	870.37	329.75	1059.9	mb

SUMMED SPECTRA (in mb/MeV)

Energy	neutrons	protons	gammas	
.500	1206.8	27.190	2061.3	
1.000	907.55	68.629	1301.7	
1.500	648.54	96.256	957.94	
2.000	459.91	106.76	705.46	
4.000	136.65	56.051	113.83	
6.000	65.795	16.735	22.136	
8.000	35.663	9.0744	3.2681	
10.000	21.302	6.9924	.52064	
12.000	10.026	4.6071	.22823	
14.000	.00000	1.1543	.36022	
16.000	.00000	.00000	.70557	
18.000	.00000	.00000	.55370	
20.000	.00000	.00000	.30850	
Integrals	2417.0	417.09	3171.0	mb

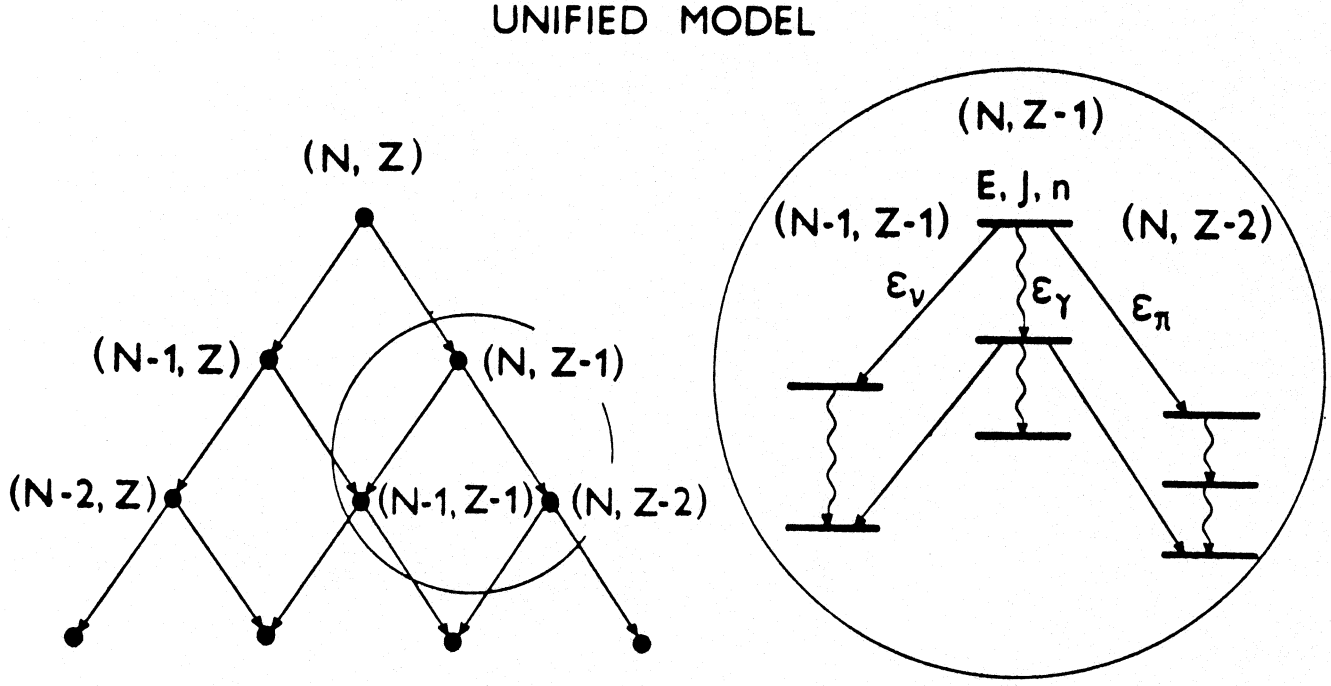

FIG. 1. Schematical view of a chain of nuclei in the unified model. In a given nucleus one considers different excitation energies, spins as well as exciton numbers so that also complicated γ cascades can be calculated.

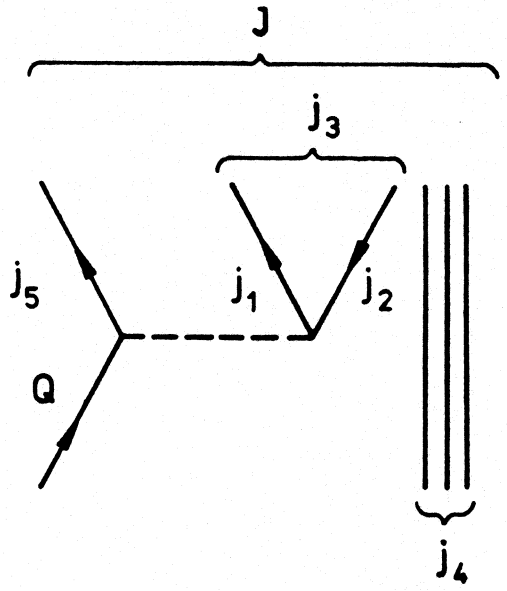

FIG. 2. Diagram of the $X_{nJ}{}^{l}$ function for intranuclear transitions.

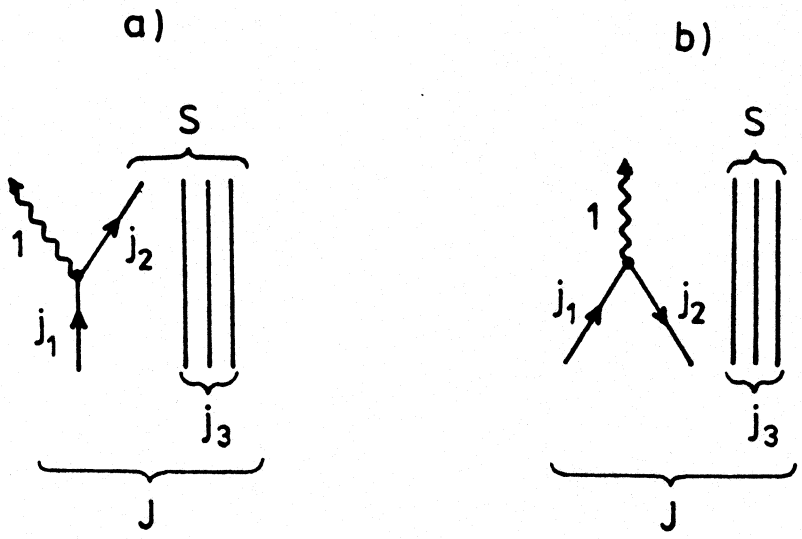

FIG. 3. Diagram of *a*) x_{nS}^{nJ} and *b*) $x_{nS}^{n\pm 2J}$ functions for the γ emission.

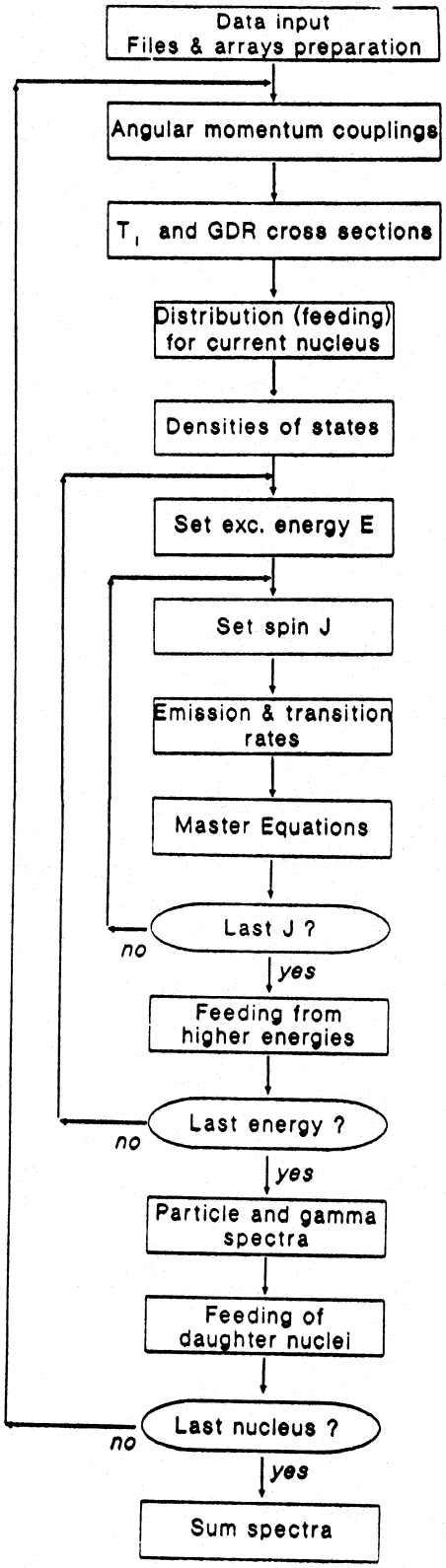

FIG. 4. Flowchart of the PEGAS code.

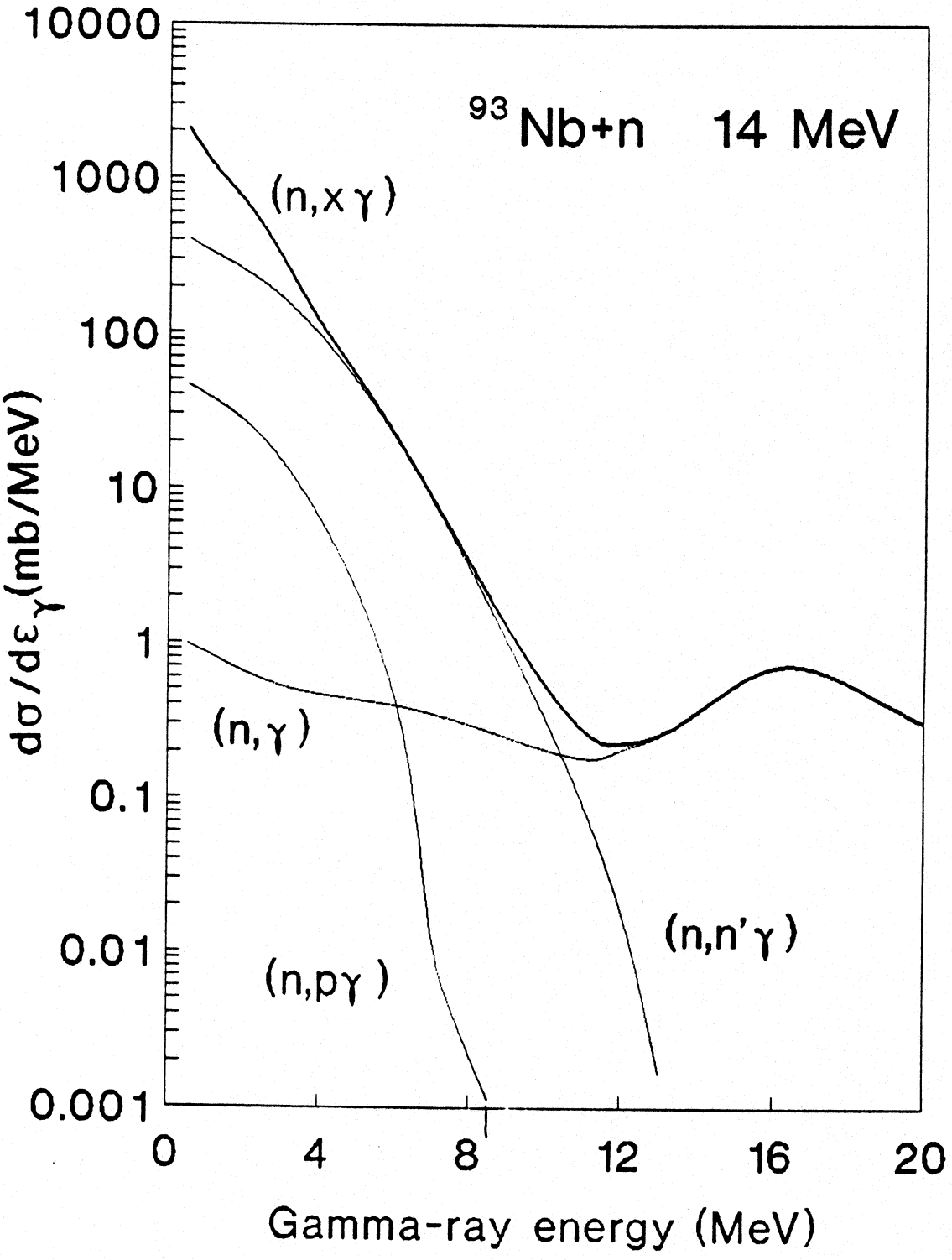

FIG. 5. The γ production spectrum from $^{93}Nb + n$ at 14 MeV calculated by the PEGAS code.