OAK RIDGE NATIONAL LABORATORY
operated by
UNION CARBIDE CORPORATION
NUCLEAR DIVISION
for the
U.S. ATOMIC ENERGY COMMISSION

ORNL - TM - 1867

COPY NO. - 67

DATE - June 9, 1967

Neutron Physics Division

A FORMALISM FOR THE CALCULATION OF NEUTRON-CAPTURE GAMMA-RAY SPECTRA*

K. J. Yost

A methodology for the calculation of neutron-capture gamma-ray spectra in light ($A < 70$), magic, and near-magic nuclei has been developed. Nuclear spin and parity effects relative to radiative transition probabilities are explicitly accounted for. Means are provided for allowing electric and magnetic dipole and quadrupole transitions, as well as spin-dependent spin-branching ratios.

DISCLAIMER

OAK RIDGE NATIONAL LABORATORY
OPERATED BY
UNION CARBIDE CORPORATION
NUCLEAR DIVISION
UNION CARBIDE
POST OFFICE BOX X
OAK RIDGE, TENNESSEE 37830

rec'd. 7-13-67 JMR

ERRATA - ORNL-TM-1867

A Formalism for the Calculation of Neutron Capture Gamma Ray Spectra

K. J. Yost

Please add the following sentence to the abstract of subject report:

"The method is intended as a first step in an effort to develop a general capability for the approximation of gamma-ray spectra accompanying neutron capture into well defined nuclear states."

Add the following footnote to cover page:

* An abbreviated and preliminary version of an article to be submitted for journal publication.

THIS PAGE

WAS INTENTIONALLY

LEFT BLANK

Table of Contents

I. Introduction

A substantial amount of effort is necessarily being devoted to the perfecting of means for describing particle and photon transport phenomena to the point that, for instance, meaningful shield optimization studies are possible. It is in general true, however, that the results generated by any calculational method, no matter how sophisticated, are only as valid as the information upon which the calculation is based, be it in the form of boundary conditions in the analytical context, or correspondingly, "input" in the numerical sense.

For gamma-ray transport purposes, part of the problem of providing suitable input information for shield calculations rests with an adequate description of secondary gamma-ray spectra, i.e., spectra resulting from neutron capture by shield materials. Perhaps the principal source of error in representations of neutron-capture gamma-ray spectra lies in the assumption that has to date been virtually inescapable owing to lack of information: that neutron-capture gamma-ray spectra are invariant to incident neutron energy, or, more specifically, that thermal-neutron capture spectra are valid for epithermal-neutron capture spectra. In point of fact, this assumption is warranted only under rather well-defined circumstances: specifically, in materials for which the epithermal-neutron-capture cross section is negligible, or in cases in which neutron capture excites the compound nucleus to its continuum energy range where, by definition, the nearest neighbor mean level spacing is so small and consequent overlap of states so pronounced that incident neutrons of virtually all feasible energies and angular momenta find a variety of capture channels open to them. It then follows that the incident energy of a neutron absorbed into the compound continuum does not define a unique or even significantly probable capture state spin and parity which, in conjunction with spins and parities of lower lying states, would define radiative transition rates and in turn a characteristic gamma-ray spectrum. Continuum capture is expected to be predominant for nuclei whose mass numbers (A) are above 70, with the exception of those whose number of protons (Z) and/or number of neutrons (N) are magic or near-magic.

Several methods have been advanced for the calculation of neutron-capture gamma-ray spectra resulting from capture into the compound nucleus continuum. The first, proposed by E. S. Troubetzkoy,[1] incorporates dipole transition probabilities [the relative probability for the excitation of a state of energy E_f, given a dipole transition from a state of energy E_i, varies as $(E_i - E_f)^3$] and the unmodified nuclear evaporation model expression for nuclear level density. The compound nucleus' level spectrum is divided into continuum and resolved energy ranges, the latter obtaining from the compound nucleus ground state to an arbitrarily defined energy above its highest known (resolved) state.

The second method, proposed by Lundberg and Starfelt,[2] is similar in nature to the Troubetzkoy method except that radiative transition probabilities are derived from an approximation to the so-called giant dipole resonance by way of the well-known theorem of detailed balance. The theorem in this instance relates the photon absorption cross section to the ground-state radiative transition rate. An assumption is then made to the effect that the energy dependence of the ground-state transition probability from an excited state of energy E_i obtains between any two states in the nuclear level spectrum separated by the energy E_i.

It should be emphasized that radiative transition probabilities employed in the foregoing two methods are functions of energy only. Thus, neither of the methods is capable of describing capture gamma-ray spectra where transition probabilities are functions not only of energy but also of spin and parity as prescribed by the nuclear selection rules. This

---

[1]E. S. Troubetzkoy, "Statistical Theory of Gamma-Ray Spectra Following Nuclear Reactions," Phys. Rev. 122, 212 (1961).

[2]B. Lundberg and N. Starfelt, "Gamma Rays from the Capture in Ta and Au of Neutrons from 1 to 4 MeV," Nucl. Phys. 67, 321 (1965).

will generally be true for nuclei with mass numbers less than 70 and/or for those with N and/or Z sufficiently proximate to the magic numbers. In contradistinction to the continuum situation, mean level spacings are of such magnitude that neutron capture is for the most part effected into states well defined with respect to incident neutron energy. The change in shape of neutron-capture gamma-ray spectra with neutron energy is then a consequence of the capture of neutrons of various angular momenta, generally s wave (zero angular momentum) and p wave (one unit of angular momentum). A striking example of this is given by Gibbons et al. in an investigation of epithermal-neutron-capture gamma-ray spectra in 2s-1d shell nuclei.[3]

This paper is devoted to the development of a methodology for the calculation of neutron-capture gamma-ray spectra which accounts explicitly for spin and parity effects in the determination of radiative transition probabilities. The nature of the problem is such that both the analytical and subsequent numerical formulations of the methodology are thought to be of sufficient interest to merit rather detailed exposition.

II. Cascade Dynamics

Discrete State Formulation

In the formulation of nuclear gamma-ray cascade dynamics it is useful to introduce the concepts of nuclear level population, $W(E_i)$, and gamma partial width, $\Gamma_\gamma(E_n,E_i)$, where E_i denotes the energy of the ith nuclear level and E_n denotes the energy of the level from which a gamma transition originates. In all cases, of course, $E_n > E_i$. The partial width for a gamma transition from a level E_n to a lower lying level E_i can be thought of as a measure of the frequency with which a nucleus excited to its nth level de-excites by emitting a gamma ray of energy $E_n - E_i$, neglecting nuclear recoil accompanying photon emission. With proper normalization the partial widths correspond to the probabilities for gamma transitions to all statistically (spin, parity) and energetically

[3] I Bergquist, J. A. Biggerstaff, J. H. Gibbons, and W. M. Good, "Neutron Resonance Capture in 2s-1d Shell Nuclei," Phys. Rev. 18, 323 (1965).

accessible levels. Clearly, these probabilities must sum to unity for each step in the gamma cascade. Level populations, when normalized to a single neutron capture, render the expected number of excitations of a given level per gamma cascade.

Let us first consider a gamma cascade in some hypothetical nucleus, all of whose levels are known. Putting aside for the moment the question of level spin and parity and the associated nuclear selection rules, the gamma spectrum would be completely defined by specifications of transition probabilities obtaining between the various known levels, E_i. In this instance the cascade can be formulated in terms of the following relationships:

$$\Gamma(E_n) = \sum_{i=1}^{n-1} \Gamma_\gamma(E_n,E_i) \quad , \tag{1.a}$$

$$\Delta W(E_n,E_i) = \frac{\Gamma_\gamma(E_n,E_i)}{\Gamma_\gamma(E_n)} W(E_n) \tag{1.b}$$

$$\Delta L(E_n,E_i) = \frac{\Gamma_\gamma(E_n,E_i)}{\Gamma_\gamma(E_n)} W(E_n) \quad , \tag{1.c}$$

where $L(E_n,E_i)$, the line frequency, denotes the frequency with which the gamma line $(E_n - E_i)$ occurs in the gamma spectrum per cascade, and the operator Δ denotes an expected increment in the indicated quantities associated with a transition from the level E_n. Equations (1) exemplify, in the order of their occurrence, the following consequences: (a) the total radiation width of a level is the sum of the partial radiation widths to accessible lower lying energy levels, (b) an increment in the level population of the ith level corresponding to a gamma transition originating with the nth level is given by the product of the probability that the ith state be excited in the transition and the level population of the initial state, and (c) the gamma-ray line frequency per cascade corresponding to the energy $E_n - E_i$ is enhanced by the same amount as is the ith level population.

It should perhaps be emphasized that the gamma width has definite physical significance in terms of the mean lifetime, $\tau(E)$, of a state and, when more than one mode of de-excitation is possible, in terms of the relative probability of de-excitation by radiative transition, $B_\gamma(E)$. In particular,

$$\tau(E) = \frac{\hbar}{\Gamma_\gamma(E)} \quad ,$$

where $\hbar$ denotes the ratio Planck's constant, h, divided by 2π, and

$$B_\gamma(E) = \frac{\Gamma_\gamma(E)}{\Gamma(E)} \quad ,$$

where $\Gamma(E)$ denotes the sum over widths corresponding to possible modes of de-excitation of the excited state at energy E. For calculations in which other than the relative magnitudes of partial widths corresponding to gamma transitions to various energy states are desired, widths may be normalized by reference to a transition of known strength. In the calculation of neutron-capture gamma-ray spectra one is generally concerned with ratios of partial to total gamma widths as in Eqs. (1), in which case such normalization cancels out. In this context the absolute magnitude of the gamma width is not of interest unless it is so small as to effect for all practical purposes the end of a cascade.

It follows directly from the above definitions that

$$W(E_i) = \sum_{k=i+1}^{N} \frac{\Gamma_\gamma(E_k,E_i)}{\Gamma_\gamma(E_k)} W(E_k) \qquad (2.a)$$

and

$$L(E_n,E_i) = \sum_{k=1}^{N} \sum_{k'=1}^{k} \frac{\Gamma(E_k,E_{k'})}{\Gamma(E_k)} W(E_k)\, \delta[E_k - E_{k'} - (E_n - E_i)] \quad , \qquad (2.b)$$

with N denoting the number of states in the energy region bounded by the compound nucleus neutron-capture and ground states.

Gamma-ray spectrum calculations typically involve nuclei whose low-lying levels have been identified as to energy and statistics, but whose intermediate- (> 2 MeV) and high-energy states remain undefined. Further, for nuclei with mass numbers greater than, say, 70 (and for which the proximity of Z or N to the magic numbers is negligible), compound nucleus excitation energies following neutron capture are well within the nuclear energy level "continuum" where level spacing is so small and the consequent overlap of states so great as to make impossible the positive identification of a neutron-capture state solely on the basis of a knowledge of the capture energy. Consequently, the formulation of gamma-ray cascade dynamics for virtually all materials requires a "statistical" model of the nucleus. For present purposes, a particularly applicable review of the statistical approach to nuclear structure has been given by Goldstein.[4]

Continuum or Unresolved Level Formulation

For compound nucleus excitation energies for which either the mean level spacing is so small that the level can be said to form a continuum of states, or where the states are reasonably discrete but unresolved as to energy, spin, and parity, it is convenient to formulate gamma cascade dynamics in terms of a level density, $\rho(E)$. Here, the sum over discrete states in Eq. (1.a) becomes an integral of the product of the partial width for the excitation of a group of levels contained in a unit energy interval about some energy E and the level density at E. In particular:

$$\Gamma(E) = \int_{E_c}^{E} \Gamma(E,E') \, \rho(E') \, dE' + \sum_{k=1}^{N} \Gamma(E,E_k) \quad , \qquad (3)$$

the latter term accounting for N resolved levels below the continuum whose lower energy bound is denoted by E_c. In the continuum or unresolved level context, level populations and line frequencies become, respectively, the composite populations of all levels contained in some unit energy interval (population density) and the collective frequency with which gamma transitions involving initial and final states separated by energies common to

[4]H. Goldstein, "Statistical Model Theory of Neutron Reactions and Scattering," in Fast Neutron Physics, Part II, Chapter V.J., Interscience Publishers, 1963.

some unit energy interval (spectral density) occur. Both quantities are presumed normalized to a single gamma cascade.

In what follows it will be convenient to define excitation probabilities, T(E,E'), given by

$$T(E,E') = \frac{\Gamma(E,E')\ \rho(E')}{\Gamma(E)} \quad . \tag{4}$$

The population density obtaining at some energy E following a neutron capture that has resulted in a compound nucleus excitation energy, E_n, has the form

$$W(E) = S(E) + \int_{E}^{E_n} W(E')\ T(E',E)\ dE' \quad , \tag{5}$$

with

$$S(E) \equiv \frac{\Gamma(E_n,E)}{\Gamma(E)} \quad .$$

The function S(E) accounts for level excitation at E resulting from an initial gamma transition originating with the capture state. The integral expression in Eq. (5) then accounts for excitations resulting from secondary transitions initiated from excited levels between E and the capture state at E_n. Discrete level populations in the "resolved" energy region below the continuum ($0 \leq E \leq E_c$) are given by

$$W(E_k) = S(E_k) + \int_{E_c}^{E_n} W(E')\ T(E',E_k)\ dE' + \sum_{k'=k+1}^{N} W(E_{k'})\ T(E_{k'},E_k) \quad , \tag{6}$$

with N again denoting the number of levels with known energies and statistics. The spectral density for this case is as follows:

$$L(E) = \int_{E_c}^{E_n} dE' \int_{E_c}^{E'} dE'' \; W(E') \; T(E',E'') \; h(E,E',E'')$$

$$+ \sum_{k=1}^{N} \int_{E_c}^{E_n} W(E') \; T(E',E_k) \; h(E,E',E_k) \; dE'$$

$$+ \sum_{k=1}^{N} \sum_{k'=1}^{k} W(E_k) \; T(E_k,E_{k'}) \; h(E,E_k,E_{k'}) \quad , \qquad (7)$$

where $h(E,E',E'')$ is defined to be the product of two Heaviside functions,

$$h(E,E',E'') \equiv H[(E' - E'') - (E - \tfrac{1}{2})] \; H[(E + \tfrac{1}{2}) - E' - E'')] \quad ,$$

with

$$H(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases} .$$

Finally, the normalization specified in Eq. (4) assures that

$$\int_{0}^{E_n} L(E') \; dE'' = E_n \quad ;$$

i.e., energy has been "conserved" in the formulation of the gamma cascade process.

Nuclear Spin and Parity

It was pointed out in an earlier portion of this paper that the primary motivation for developing the subject methodology had to do with the inclusion of level spin and parity in the determination of radiative transition probabilities. Radiative transitions between states of an excited nucleus are governed by the nuclear selection rules relative to allowed or (more or less) probable changes in nuclear spin and parity

accompanying the transitions. These selection rules are in turn a direct function of the multipolarity and type (electric or magnetic) of the emitted radiation.

While it is not the purpose of this paper to delve into the physics of nuclear radiative transitions in any detail, some cursory consideration of the essentials of the theory would be appropriate at this point.[4] Gamma rays emitted in radiative transitions between nuclear states can be categorized in terms of an index, ℓ, which determines their angular momentum relative to the emitting nucleus. The index ℓ, together with the designation of the radiation as either electric or magnetic, determines its parity. Assuming conservation of angular momentum and parity in the residual nucleus-photon system, one can deduce the spin and parity of the post-transition state from the knowledge of the respective pre-transition state and emitted photon angular momenta and parities. Or, considering the process from a slightly different standpoint, given a state of known statistics (spin and parity) from which a radiative transition is to take place, one may determine the photon angular momentum and parity which will yield a certain set of residual nuclear level statistics. Energy considerations aside then, the probability for exciting a particular post-transition state is proportional to the probability for the emission of a photon of appropriate description.

In the context of this paper only dipole and quadrupole radiative transitions will be of interest. Table 1 gives the nuclear selection

Table 1. Nuclear Selection Rules for Dipole and Quadrupole Radiative Transitions

Transition Type	Allowed Spin Change*	Parity Change
Electric dipole	0, $\pm$1	Yes
Magnetic dipole	0, $\pm$1	No
Electric quadrupole	0, $\pm$1, $\pm$2	No
Magnetic quadrupole	0, $\pm$1, $\pm$2	Yes

*0 → 0 transitions are forbidden.

[4]H. Goldstein "Statistical Model Theory of Neutron Reactions and Scattering," in Fast Neutron Physics, Part II, Chapter V.J., Interscience Publishers, 1963.

rules pertinent to gamma radiation of this description. In the formulation of gamma cascade dynamics one must be concerned not only with the totality of "allowed" transitions, but more particularly with the relative probabilities of spin and parity changes within the set of possible transitions. In addition to the statistical aspects of radiative transition probabilities there are, of course, energy considerations. The relative probability for excitation of a level of energy E_f in a transition originating with a level of energy E_i is given by $(E_i - E_f)^3$ for dipole transitions and $(E_i - E_f)^5$ for quadrupole transitions. Thus, other considerations aside, quadrupole transitions result in a "harder" gamma-ray spectrum than do dipole transitions.

With nuclear selection rules and the energy dependence of dipole and quadrupole transition probabilities in hand, it is possible to define mathematically the spin- and parity-dependent gamma cascade process. The following definitions will be found useful:

$\rho_{J,\pi}(E)$ = density of spin J parity π states at energy E.

$W_{J,\pi}(E)$ = population density of spin J parity π states at energy E.

$$\Gamma_{\ell,J,\pi}(E) = \int_{E_c}^{E} (E-E)^{2\ell+1}\, \rho_{J,\pi}(E')\, dE' + \sum_{k'=1}^{N} (E-E_{k'})^{2\ell+1}\, \delta(\pi-\pi_{k'})\, \delta(J-J_{k'}).$$

$$T_{\ell,J,\pi}(E,E') = (E-E')^{2\ell+1}\, \rho_{J,\pi}(E')\, \Gamma_{\ell,J,\pi}(E).$$

$b(e/m)\ell\ (J\text{-}J',E)$ = probability for nuclear spin increment (J-J'), given an electric/magnetic radiative transition of polarity, ℓ, originating from an intial spin J state at E. The selection rules require that:

$$b(e/m)\ell\ (J\text{-}J',E) = 0, \quad \begin{matrix} J=J'=0 \\ J' < 0 \end{matrix}, \quad \ell = 1,2,$$

$$b(e/m)1\ (J\text{-}J',E) = 0, \quad |J\text{-}J'| > 1,$$

$$b(e/m)2\ (J\text{-}J',E) = 0, \quad |J\text{-}J'| > 2;$$

$p(e/m)\ \ell(J,E) \equiv$ probability that a radiative transition from spin state J at E will be electric/magnetic of polarity ℓ.

A final bit of notation: $(-\pi)^{\ell}$ will denote a change of parity relative to π if ℓ is odd, and no change if ℓ is even.

It follows directly from the foregoing definitions that

$$W_{J,\pi}(E) = \sum_{J'} \sum_{\ell} \int_{E}^{E_n} dE' \left\{ pe\ell(J',E')\ be\ell(J'\text{-}J,E')\ T_{\ell,J'(-\pi)^{\ell}}(E',E) \right.$$

$$\left. + pm\ell(J',E')\ bm\ell(J'\text{-}J,E')\ T_{\ell,J'(-\pi)^{\ell+1}}(E',E) \right\} \qquad (8.a)$$

$$L(E) = \sum_{J,\pi} \sum_{J'} \sum_{\ell} \int_{E_c}^{E_n} dE' \int_{E_c}^{E'} dE''\ W_{J,\pi}(E')\ h(E,E',E'') \left\{ pe\ell(J,E') \right.$$

$$\cdot be\ell(J\text{-}J',E')\ T_{\ell,J'(-\pi)^{\ell}}(E',E'')$$

$$\left. + pm\ell(J,E')\ bm\ell(J\text{-}J',E')\ T_{\ell,J'(-\pi)^{\ell+1}}(E',E'') \right\} \qquad (8.b)$$

The sum over ℓ implies that dipole and quadrupole radiation has been taken into account.

A resume of the physics of neutron-capture gamma radiation as it pertains to the phenomenological approach of this paper must necessarily include a brief discussion of the quantum mechanics of a neutron interaction with the nucleus. This is, to a point, the simplest of two-body problems to treat in that the system potential vanishes outside the (arbitrarily defined) nuclear boundary. The Hamiltonian is then just that of the kinetic energies of the neutron and nucleus in the center-of-mass coordinate system. The solution of the wave equation under these circumstances is a plane wave of the form e^{ikz}, where z denotes the distance between the nucleus and the incident neutron. The latter can be expanded into spherical harmonics, or so-called partial waves, of order ℓ, where ℓ is an integer defining the angular momentum associated with

the partial waves. Further analysis results in a decomposition of the neutron-capture cross section into various ℓ components corresponding to the relative probabilities of the capture of neutrons with associated angular momenta. In addition to bringing to a reaction differing angular momenta, the partial waves determine, in conjunction with the ground-state parity of the target nucleus, the parity of the compound nucleus capture state. In particular, odd-ℓ angular momenta result in a capture state parity change relative to the target nucleus ground state, whereas even-integer momenta preserve the target nucleus ground-state parity in the compound nucleus capture state. Here, of course, the incident neutron is presumed to interact with the target nucleus in its ground state.

The foregoing discussion has, under certain circumstances, profound implications for the shape of neutron-capture gamma-ray spectra. The nuclear energy level spectrum is composed of the superposition of spectra of various angular momenta and parity. An excited state de-excites, usually to lower lying levels accessible through the application of the selection rules of Table 1. For example, consider neutron capture by and subsequent de-excitation of a target nucleus with ground-state spin and parity $J^\pi = \frac{1}{2}^+$. Consider first the capture of an s-wave ($\ell = 0$) neutron. The neutron brings to the reaction an intrinsic spin angular momentum, 1/2. According to the vector addition rules, compound capture states of the following description are accessible: $J^\pi = 0^+, 1^+$. If a 0^+ state is formed, a ground-state transition ($0 \rightarrow 0$) is strictly forbidden. If, on the other hand, a 1^+ state is formed, a ground-state transition is still relatively improbable since such a transition would be either magnetic dipole or electric quadrupole in nature. As discussed in a subsequent portion of this paper, these are generally, though by no means always, improbable relative to electric dipole transitions.

Assume next that the target nucleus described above captures a p-wave ($\ell = 1$) neutron. The accessible compound capture states are: $J^\pi = 0^-, 1^-, 2^-$. The 0^- capture state cannot result in a ground-state transition ($0 \rightarrow 0$). However, the $J^\pi = 1^-$ state can de-excite by way of a ground-state transition by either an electric dipole or a magnetic quadrupole transition. The latter is expected to be several orders of magnitude less

likely than the former. In summation, then, an s-wave capture would result in a capture gamma spectrum essentially devoid of a ground-state transition, whereas a p-wave capture spectrum might exhibit a rather strong ground-state line. Of course, this sort of an argument is relevant to any compound nucleus state and the consequent enhancement or suppression of the gamma line corresponding to an initial capture state transition to it.

The effect of spin and parity on the relative probability of high-energy gamma transitions can be appreciable in a slightly less obvious way. Assume for the moment that the relative probabilities for spin changes consistent with the selection rules (hereinafter to be referenced as spin branching probabilities) are equal for dipole and quadrupole transitions for all spin states. In this simple context the probability for a gamma transition from some initial state to one of a group of accessible final states is primarily a function of two quantities: (1) the energy difference between the two states, and (2) the number of accessible final states. In general, the more numerous the possible transitions, the less the probability for any particular one. The density of nuclear spin states is expected to be spin dependent. In particular,

$$D_J(E) = D_0(E)\ f(E,J), \quad f(E,J) < 1, \quad J > 0$$

and

$$f(E,J') \leq f(E,J), \quad J' \geq J \ ,$$

where $D_0(E)$ and $D_J(E)$ are, respectively, the mean level spacings for spin zero and spin J states, and $f(E,J)$ is an as yet undefined function of spin and energy relating the two. Thus, for the stated conditions on the spin branching parameters, the higher the spin of an excited state, the lower the probability for a radiative transition to a given statistically accessible state.

III. Numerical Formulation

Equations (8) formally define the spin- and parity-dependent gamma cascade process. The problem of a tractable numerical formulation of the methodology, however, still remains. The approach taken in the calculations exhibited in this paper is embodied in a digital computer code, DUCAL, written in the FORTRAN-63 and FORTRAN-IV languages for use on the CDC-1604 and IBM-7090 and -360 machines, respectively. It can perhaps be best described in terms of FORTRAN-like variables actually used in the code. Their definition, in some cases, will closely resemble variables defined in the analytical formulation just discussed. One main difference between the analytical and numerical approaches rests with the fact that in the latter it will be necessary to index many variables with respect to the gamma cascade transition number.

As in the analytical formulation, the index ℓ may take on values of one and two corresponding to dipole and quadrupole transitions, respectively. The following variables will be useful in the discussion:

T(E/M) ℓ(I,J) ≡ spin branching probability, the probability that an electric/magnetic radiative transition of polarity ℓ originating with a spin I state excites a spin J state. The angular momentum selection rules are taken into account in the calculation of the probability of the various spin changes.

P(E/M)ℓ^r ≡ relative probability for an electric/magnetic radiative transition of polarity ℓ to a resolved energy level.

P(E/M) ℓ^u(I) ≡ relative probability for an electric/magnetic radiative transition of polarity ℓ to an unresolved level for the Ith cascade transition. [Note that the cascade transition index appears in the unresolved level transition probabilities but not in their resolved counterparts. The relationship between the two types of probabilities is discussed in conjunction with Eq. (13).]

PPL(I,J) ≡ probability that the Ith cascade transition originates with an even parity, spin J state.

PMI(I,J) ≡ probability that the Ith cascade transition originates with an odd parity, spin J state.

For compound nuclei with integral spins, the first indexed state corresponds to a spin zero state, while for odd half integral spin nuclei the index "1" denotes a spin 1/2 state.

From the foregoing definitions it follows that

$$PPL(I,J) = \sum_{J'=JD}^{J+1} \left\{ PE1^{r} \cdot TE1(J',J) \cdot PMI(I-1,J') + PM1^{r} \cdot TM1(J',J) \cdot PPL(I-1,J') \right\} + \sum_{J'=JQ}^{N+2} \left\{ PE2^{r} \cdot TE2(J',J) \cdot PPL(I-1,J') + PM2^{r} \cdot TM2(J',J) \cdot PMI(I-1,J') \right\} \qquad (9.a)$$

and

$$PMI(I,J) = \sum_{J'=JD}^{J+1} \left\{ PE1^{r} \cdot TE1(J',J) \cdot PPL(I-1,J') + PM1^{r} \cdot TM1(J',J) \cdot PMI(I-1,J') \right\} + \sum_{J'=JQ}^{J+2} \left\{ PE2^{r} \cdot TE2(J',J) \cdot PMI(I-1,J') + PM2^{r} \cdot TM2(J',J) \cdot PPL(I-1,J') \right\} , \qquad (9.b)$$

Note that no energy dependence is associated with PPL(I,J) and PMI(I,J). Equations (9) and Table 2 are presented in the rather detailed form for illustrative purposes only. Henceforth, an attempt will be made to keep the notation somewhat more compact. Equation (9.2), for instance, may be written as

Table 2. Sum Limits as a Function of Nuclear Spin

Spin State (J)	JD	JQ
0	2	2
$\frac{1}{2}$	1	1
1	1	1
$\frac{3}{2}$	1	1
≥ 2	J-1	J-2
$\geq \frac{5}{2}$	J-1	J-2

$$PPL(I,J) = \sum_{J'} \sum_{\ell} \left\{ PE\ell^{r}\ TE\ell(J',J)\ [PMI(I-1,J')\ \delta(\ell-1) + PPL(I-1,J')\ \delta(\ell-2)] \right.$$

$$\left. + PM\ell^{r}\ TM\ell(J',J)\ [PMI(I-1,J')\ \delta(\ell-2) + PPL(I-1,J')\ \delta(\ell-1)] \right\} , \quad (10)$$

where the J' summation extends over all spins of interest. Limits on the J' summation are redundant in view of the fact that angular momentum selection rules have, by definition, been incorporated into the spin branching probabilities.

Let E_n and E_c define, as previously, the neutron-capture state excitation energy and the (arbitrary) energy separating the resolved and unresolved portions of the compound nucleus level spectrum, respectively. This interval is divided into an arbitrary number of energy subintervals or bins. Each bin is assigned a population, W(I,J), indexed according to cascade transition number and relative position (top to bottom) within the (E_n,E_c) energy interval. The transition index, I, denotes the step in the gamma cascade during which the energy levels contained within bin I are excited W(I,J) "times." Thus, W(I,J) is in fact the total increment in the bin J bounded level populations associated with Ith gamma transitions from all higher energy bins [see Eq. (18)]. It is perhaps worth

emphasizing here that Ith transition photons can be emitted from all bins, where $J \leq I$, and from all resolved levels. For instance, the first transition from the compound capture state will scatter W(I,J)'s among all energy bins and resolved levels. Each bin and level then becomes a source for second transition photons.

For the energy range $E_c \leq E \leq E_n$ some assumption must be made about the level spectrum. The actual energy level spectrum of a nucleus is a composite of sets of levels characterized by various combinations of spin and parity. Level spacings of each spin parity set are assumed to be distributed statistically in energy about some spin- and energy-dependent mean level spacing. The latter were defined for the calculations exhibited in this paper by an expression suggested by Newton[6] for the mean level spacings of spin zero states, D_0. The Newton formulation for D_0 takes into account pairing energies (even-odd nucleon effects) and the effect of proximity to the magic numbers and the attendant marked increase in mean level spacing. The mean level spacing is expected to vary with spin, J, roughly as $(2J + 1)^{-1}$. Bloch[7] has proposed a somewhat more realistic expression to account for the spin dependence of level spacing as follows:

$$f(J,E) \sim e^{-J^2/2\sigma^2} - e^{-(J+1)^2/2\sigma^2}, \qquad (11)$$

σ being a slowly varying empirical function of energy. When the parameter σ is available, Eq. (10) spin dependence is used in spectrum calculations.

For each gamma transition from either the capture state or the energy bins in the compound nucleus excitation interval, $E_c \leq E \leq E_n$, a nuclear level spectrum is constructed based upon a composite mean level spacing which is dependent upon energy and transition number and is defined by the relation

---

[6]T. D. Newton, "Shell Effects on the Spacing of Nuclear Levels," Canadian J. Phys. 34, 804 (1956).

[7]C. Bloch, Phys. Rev. 93, 1094 (1954).

$$D(I,E) = \sum_{J'=1}^{NJ} \left\{ PPL(I,J') + PMI(I,J') \right\} D_o(E)\ f(E,J) \quad , \qquad (12)$$

where NJ denotes the number of spin states to be considered and I and J' are, respectively, the transition number and spin. The result, by way of emphasis, is a weighted average of the mean level spacings of accessible spin and parity states for the Ith gamma cascade transition.

As indicated previously, the superscripts r and u on the symbols denoting multipole transition probabilities define the probabilities for the indicated types of transitions to states in the resolved and unresolved energy ranges, respectively. The $P(E/M)^r_\ell$ are the probabilities that are predicted theoretically, without regard for the availability of lower lying states of appropriate statistics to which such transitions are "allowed." They are not always applicable within the context of the composite level spectrum formulation embodied in Eq. (12). Specifically, compound mean level spacings rendered by Eq. (13) are predicated upon the assumption that the mean level spacings of states of spin J (even and odd parity) defined in Eq. (12) obtain over the entire unresolved energy range of the compound nucleus. It may well be, however, that for certain energy bands within the unresolved region, mean level spacings of states of particular spin and parity may differ significantly from their expected values. Such an eventuality may substantially influence the shape of capture gamma-ray spectra when the energy band composes, say, the lowest 10 percent of the unresolved range, and in addition the spins and parities of the affected states render them accessible through capture state transitions.

Excitation of unresolved states near the resolved-unresolved energy boundary is heavily favored over the excitation of higher energy states due to the energy dependence of the radiative transition probabilities. Thus the total contribution of unresolved states to a particular cascade transition rests almost exclusively with accessibility of states in the lower portion of the unresolved level spectrum. In order to account for the effect of significant local irregularities in mean level spacing in this region, spin- and parity-dependent mean level spacing functions,

$\rho_\pi^{\pm}(J)$, are defined. The superscripts + and - refer, as usual, to states of even and odd parity, respectively. The functions are intended to represent ratios of mean level spacings expected on theoretical or experimental grounds to those predicted in Eq. (12). The relationship between resolved and unresolved electric dipole transition probabilities has the form

$$PE1^u(I) \equiv \sum_J \sum_{J'} [PPL(I,J)\ \rho_\pi^-(J') + PMI(I,J)\ \rho_\pi^+(J')]\cdot TE1(J,J')\cdot PE1^r \quad .$$

Similar expressions hold for the other unresolved transition probabilities.

With the composite mean level spacing in hand, an actual nuclear level spectrum is constructed by a Monte Carlo technique by which consecutive level spacings are determined by repeatedly sampling from a Porter-Thomas or chi-square distribution with "four degrees of freedom."[8] This probability density function has the form

$$P(x)\ dx = 4x\ e^{-2x}\ dx \quad , \tag{13}$$

where

$$x = S/D(I,E) \quad ,$$

S being the variable level spacing. The maximum of the distribution (13) occurs at $x = 1/2$. The mean value of x is unity, which in turn yields a mean level spacing equal to D(I,E) for the constructed spectrum. In practice the distribution (13) is repeatedly sampled until an energy below E_c is reached at which point the last level is discarded and the process terminated. Since the sampling equation

$$\int_0^x P(x')\ dx' = \rho \quad ,$$

---

[8]C. E. Porter and R. G. Thomas, Phys. Rev. 104, 483 (1956).

where ρ is a random number ≤ 1, is transcendental in x, the actual sampling is effected by means of a rejection technique.[9]

Finally, a level density is formed by imposing a probability density function in the form of a chi-square distribution with two degrees of freedome about each statistically determined level energy. This distribution function is a simple exponential, i.e.,

$$P(x)\ dx = \frac{1}{2}\, e^{-x}\ dx \quad , \tag{14}$$

with x defined relative to the statistically determined level energy, E_o, as

$$x \equiv |E - E_o| \ / \ D(I,E) \quad .$$

The normalization factor 1/2 ensures that

$$\int_{-\infty}^{\infty} P(x')\ dx' = 2 \int_{o}^{\infty} P(x')\ dx' = 1 \quad .$$

The net result is thus a set of probability density functions of the form (14) distributed about statistically distributed midpoints.

Let E_{k-1}, E_k, E_{k+1}, and E_{k+2} be four consecutive level probability density function midpoints generated by random sampling as per Eq. (14). The resulting "level density" function for the Ith transition, $E_k \geq E \geq E_{k+1}$, has the form

$$\rho(E) = \frac{F(\infty)}{D(I,E_{k-1})}\, e^{X_{k-1}} + \frac{e^{X_k}}{D(I,E_k)} + \frac{e^{-X_{k+1}}}{D(I,E_{k+1})} + \frac{F(N)}{D(I,E_{k+2})}\, e^{-X_{k+2}} \quad , \tag{15}$$

with

$$X_k \equiv (E - E_k)/D(I,E_k) \quad ,$$

---

[9]Herman Kahn, Applications of Monte Carlo, Rand Corporation Report AECU-3259 (April 19, 1954).

and

$$F(m) = \sum_{\ell=0}^{m} e^{-\ell} \quad ,$$

where N denotes the number of statistically generated energy levels in the interval $E_c \leq E \leq E_{k+2}$. The functions F(n) represent the contributions of levels above and below the energy interval of interest.

Let E_{Jm} define the midpoint energy of energy bin J, i.e.,

$$E_{Jm} = \frac{1}{2} \left[E_{J-1} + E_J\right] \quad .$$

Then, define

$$G\ell(I,J) \equiv \sum_{\ell} \left[PE\ell^{u}(I) + PM\ell^{u}(I)\right] \cdot \int_{E_c}^{E_{Jm}} (E_{Jm} - E')^{2\ell+1} \rho(I,E')\, dE'$$

$$+ \sum_{K=1}^{N} \sum_{L=1}^{NJ} \cdot \left[E_{Jm} - E(K)\right]^{2\ell+1} \left[PPL(I-1,L) + PMI(I-1,L)\right]$$

$$\left\{ PE\ell^{r} \cdot TE\ell\left[L,J(K)\right] \left[\delta(\ell - 1)\, \delta[1 + \pi(K)] + \delta(\ell - 2)\, \delta[1 - \pi(K)]\right] \right.$$

$$+ PM\ell^{r}(L) \cdot TM\ell\left[L,J(K)\right] \left[\delta(\ell - 1)\, \delta[1 - \pi(K)]\right.$$

$$\left. \left. + \delta(\ell - 2)\, \delta[1 - \pi(K)]\right]\right\} \qquad (16)$$

where $\pi(K) = +1$ with Kth energy level of even/odd parity. Further, let

$$K_{\ell}[(I,J',J)] = \int_{E_c}^{E_{Jm}} (E_{Jm} - E')^{2\ell+1} \rho(I,E')\, dE' \;/\; G\ell(I,J) \quad . \qquad (17)$$

In terms of these definitions, the expression for bin populations as a function of transition number (I) and bin index (J) becomes:

$$W(I,J) = \sum_{J'=1}^{J+1} W(I-1,J') \sum_{\ell} \sum_{L=1}^{NJ} \left\{ PE\ell^{u}(I) + PM\ell^{u}(I) \right\} K\ell(I,L,J) \quad , \quad (18)$$

and the transition-dependent level population is given by

$$WL(I,K) = \sum_{J'=1}^{NB} W(I-1,J') \sum_{\ell} \sum_{L=1}^{NJ} \Bigg[[PE\ell^{u}(I) + PM\ell^{u}(I)] \; E_{Jm} - E(K)^{2\ell+1}$$

$$[E_{Jm} - E(K)]^{2\ell+1} \; / \; G\ell(I,J') \Bigg] [PPL(J,L) + PMI(I,L)]$$

$$\Big\{ PE\ell^{r} \; TE\ell[L,J(K)] \; \Big[\delta(\ell - 1) \; \delta[1 + \pi(K)] + \delta(\ell - 2) \; \delta[1 - \pi(K)] \Big]$$

$$+ PM\ell^{r} \; TM\ell[L,J(K)] \; \Big[\delta(\ell - 1) \; \delta[1 - \pi(K)] + \delta(\ell - 2) \; \delta[1 + \pi(K)] \Big] \Big\}$$

$$+ \text{inter-level terms.} \quad (19)$$

Equation (18) for the composite level population of the Jth energy bin is the transition-dependent numerical formulation equivalent of its analytical counterpart given in Eq. (8.a).

THIS PAGE

WAS INTENTIONALLY

LEFT BLANK

Internal Distribution

1-2. L. S. Abbott
3. R. G. Alsmiller, Jr.
4. V. R. Cain
5. H. C. Claiborne
6. C. E. Clifford
7. F. H. Clark
8. J. H. Gibbons
9. F. C. Maienschein
10. R. W. Peelle
11. E. A. Straker
12. D. K. Trubey
13-32. K. J. Yost
33. G. Dessauer (consultant)
34. B. C. Diven (consultant)
35. M. H. Kalos (consultant)
36. L. V. Spencer (consultant)
37-38. Central Research Library
39. Document Reference Section
40-59. Laboratory Records Department
60. Laboratory Records ORNL RC
61. ORNL Patent Office

External Distribution

62. P. B. Hemmig, Division of Reactor Development and Technology, U. S. Atomic Energy Commission, Washington, D. C. 20545
63. I. F. Zartman, Division of Reactor Development, U. S. Atomic Energy Commission, Washington, D. C. 20545
64. H. Goldstein, Columbia University, Mudd Building, New York, New York
65. C. P. McCallum, Jr., Division of Space Nuclear Systems, U. S. Atomic Energy Commission, Washington, D. C.
66. M. B. Wells, Radiation Research Associates, Inc., 1506 West Terrell, Fort Worth, Texas 76104
67-81. Division of Technical Information Extension (DTIE)
82. Division of Research and Development (ORO)