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MECHANISMS OF RADIATIVE NEUTRON CAPTURE REACTION AND CALCULATIONS OF NEUTRON INDUCED PHOTON PRODUCTION DATA

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Abstract: This paper describes the program developed to calculate neutron induced photon production data and the physical fundamentals the program based upon. Special attention has been paid to the mechanisms of radiative neutron capture reaction which mainly account for the production of high energy photon component. The mechanisms are classified and reviewed according to the hierarchy of quasiparticle number in the excited configurations including transitions from one-quasiparticle configurations (potential capture, valence capture, interference between potential and valence capture, radiative capture in compound elastic scattering channel), transitions from three quasiparticles (semidirect capture, annihination of 3Q(2p1h) configurations, inelastic valence capture, radiative capture in compound inelastic scattering channels), and compound nucleus process (statistical model). For each process, the following questions are discussed: physical significance, schematic representation, calculation formula, test of characteristics that distinguish the mechanism, comparison of theory with data, and remaining problems. Based on these analyses, a computer code to calculate neutron-induced photon production data has been developed, including also contributions from cascade decays of residual nuclei via other reactions by statistical model. Some results by using this program are shown and compared with measured data. Due to limitation in space, this paper can only contain headlines of the model and program.

(photon production data, model code, reaction mechanism, (n,γ) reaction, channel capture, doorway mechanism, statistical model)

TRANSITIONS FROM ONE-QUASIPARTICLE CONFIGURATIONS - CHANNEL CAPTURE

CHANNEL WAVE FUNCTION AND CHANNEL CAPTURE CROSS SECTION

A transition from the entrance channel configuration (1Q) is usually called the channel radiative capture. The entrance channel wave function is

$$U^{+J}_{\ell j}(r) = \mathrm{Re}\langle U^{+J}_{\ell j}\rangle + \frac{1}{2}\sum_{\lambda(J)} \frac{\Gamma^{\ell j}_{n\lambda}}{E_\lambda - E - \frac{1}{2}\Gamma_\lambda} \frac{\mathrm{Im}\langle U^{+J}_{\ell j}(r)\rangle}{\mathrm{Im}\langle K^{J}_{\ell j}\rangle} ,$$

which consists of two terms: the potential scattering wave function and resonance scattering wave function, corresponding to the potential capture and valence capture, respectively. The channel capture cross section from a scattering partial wave (l,j) to a final state f is

$$\sigma^{ch}_{\ell j,f} = \frac{4}{3}\frac{k_\gamma^3}{\hbar v}\frac{\pi}{k^2}\sum_J \frac{(2J+1)}{2(2I+1)} \langle \ell j J\|D_I\|\ell_f j_f J_f\rangle$$

$$(2J_f+1)S_f\,\bar{e}^2 \frac{4}{|1-i\,K^J_{\ell j}|^2}\left|\int_R^\infty r\,U^{+J}_{\ell j}(r)\,U_{\ell_f j_f}(r)dr\right|^2$$

Potential capture

Schematic representation: the potential scattering neutron is captured into a low-lying single particle orbit with emission of photon without disturbing the target core.

Calculational formula: use the first term of the channel wave function.

Tests to identify the characteristics of the mechanism:

- Check the final state correlation ($\sigma^{po}_{\ell j,f} \propto S_f$) outside the resonances.
- Check the linear dependence of $\sigma^{po}_{\ell j,f} \propto E_\gamma$
- Compare, quantitatively, the magnitudes of measured and predicted partial capture cross sections.
- Observe the interference effect between potential and valence capture in (γ,n) and (n,γ) reactions.

Points to be cleared up:

- Examine the agreement of the theory with data by using a global optical model potential.
- The controversy on testing the linear dependence.
- Since the major contribution to the cross section comes from the external region, it is difficult to understand why the agreement by using a square well rather than a diffuse-edge well is very good in some cases.

Valence capture

Physical significance: the valence capture model describes a transition related to the change of state from the entrance channel configuration in the resonance wave function by radiative emission in the field of a spectator core.

Calculational formula: by using the second term of the channel wave function, and writing the cross section in a Breit-Wigner form, one gets the valence radiative width of a resonance state, Λ, to a final state f

$$\Gamma^{v}_{\lambda\gamma f} = \frac{4}{3}\frac{k_\gamma^3}{\hbar v}\langle \ell j J|D_I|\ell_f j_f J_f\rangle (2J_f+1)\,S_f\,\bar{e}^2$$

$$\frac{1}{|1-i\langle K^J_{\ell j}\rangle|^2}\left[\frac{\int_R^\infty r\,\mathrm{Im}\langle U^{+J}_{\ell j}(r)\rangle\,U_{\ell_f j_f}(r)dr}{\mathrm{Im}\langle K^J_{\ell j}\rangle}\right]^2 \Gamma^{\ell j}_{\lambda n}$$

Tests to identify the characteristics of the mechanism:

- Check the initial state correlation and final state correlation.
- Compare, quantitatively, the magnitudes of the measured and predicted partial dadiative widths.
- Check the gamma-ray energy dependence of the partial capture cross section
- Observe the interference effect between the valence and potential capture in (γ,n) and (n,γ) reactions.

Remaining problems:

- Some examples for which the valence capture model fails to explain, quantitatively, the data: Mo-100(n,γ), Zr-96(n,γ).
- The valence capture model can account for about 1/2 and 1/10 of the observed partial radiative widths in 3p and 4s size resonance region, respectively.
- Determine, experimentally, whether or not the initial and final state correlations as well as k-effect exist in the 4s region.
- Explain the "Maverick transition" of E1 effective charge.
- Explain the absence of contributions from large body of excited target configurations.
- Identify and explain the alternative correlation phenomena, such E1-M1 and $\Gamma_{\lambda f}$-$\Gamma_{\lambda f'}$ correlations.

Interference effect between potential and valence capture

Two kinds of interference effects

- One is due to superposition of the wave functions.
- the other is due to the relative magnitude of the areas above and below the abscissa enclosed by the radial integrand.

Calculational formula

$$\sigma^{ch}_{0\frac{1}{2},f} = \sigma^{po}_{0\frac{1}{2},f} \left[1 - (a^J - R')k \frac{\int_R^\infty r\, N_{0\frac{1}{2}}(r)\, U_{\ell_f j_f}(r)dr}{\int_R^\infty r\, \mathrm{Re}\langle U^{+J}_{0\frac{1}{2}}(r)\rangle U_{\ell_f j_f}(r)dr}\right]^2$$

where a^J is the coherent scattering length and R' the potential scattering length.

Constructive and destructive interference: For a nucleus above a size resonance of s-wave neutron strength function, nearby strong resonances would be at a negative energy, resulting in $a^J > R'$. In this case destructive interference is expected to occur. In contrast to this, constructive interference most likely occurs for a nucleus below the s-wave size resonance.

Examples

- C-12(n,γ) at thermal energy for destructive interference.
- Ca-40(n,γ) at thermal energy for constructive interference.

Resonance-averaged channel capture cross sections

Calculational formula

$$\langle\sigma^{ch}_f\rangle = \frac{4}{3}\frac{k^3_\gamma}{\hbar v}\frac{\pi}{k^2}\sum_{\ell jJ}\frac{(2J+1)}{2(2I+1)}\langle\ell jJ\|D_I\|\ell_f j_f J_f\rangle \cdot$$

$$(2J_f+1)\, S_f\, \bar{e}^2\, (R^{J(B)}_{\ell j\ell_f j_f} + R^{J(V)}_{\ell j\ell_f j_f} + R^{J(C)}_{\ell j\ell_f j_f}).$$

The first term contains the hard sphere and distant resonance contributions. The second term involves the contribution from the averaged near resonance wave functions. The third one is a fluctuation term, which is proportional to the mean square fluctuation of the S-matrix element.

Physical significance: In the terminology of the optical model, the sum of the first two terms can be regarded as due to the direct capture of the shape elastic scattering wave, and the third as due to the radiative capture in the compound elastic channel.

Some preliminary results:

- The fluctuation term is the dominant one among the three terms at neutron energy less than 1 MeV.
- At some mass and energy regions, e.g. 2p, 3s and 3p size resonance regions, the average channel capture cross sections may account for one third of the total (n,γ) cross sections.
- Even in favourable cases, it is difficult to observe, experimentally, any final correlation for resonance-averaged spectroscopy.

TRANSITIONS FROM THREE QUASIPARTICLE CONFIGURATIONS, DOORWAY MECHANISM

Three quasiparticle configurations (mostly 2p1h state) are usually called doorways states, since they can be regarded as a link between the entrance channel configurations and more complicated states. it is difficult to study the doorway mechanism since:

- There is no direct link between the measurable quantities and those describing the doorway states, in contrast to the single quasiparticle case.
- The number of configuration increase rapidly with the involved quasiparticle number, and we have not sufficient knowledge about the distribution of 3Q state against excitation energy.

Semidirect capture

Schematic representation: an incident neutron excites the giant dipole resonance through two-body isovector interaction, at the same time, the neutron is inelastically scattered into a bound single particle state. Then the giant dipole state may undergo a deexcitation by the emission of a gamma-ray.

Calculational formula: the direct-semidirect capture cross section is

$$\sigma^{nSD}_{lj,f} = \frac{4}{3}\frac{k^3_\gamma}{\hbar v}\frac{\pi}{k^2}\sum_J \frac{2J+1}{2(2I+1)}\langle ljJ\|D_I\|l_f j_f J_f\rangle$$

$$(2J_f+1)\, S_f\, \bar{e}^2\, |T_D+T_{SD}|^2 ,$$

where T_D is the direct capture amplitude, T_{SD} is the semidirect capture amplitude, containing a neutron-phonon coupling factor.

Tests to identify the characteristics of the mechanism:

- Observe the giant resonance structure of gamma-ray yield feeding certain final states.
- Observe the structure in gamma-ray spectrum, which corresponds to the single particle component of final state.
- Systematic comparison of measured and predicted cross sections in a wide range of energy for various projectiles.

Remaining problems:

- Give reasonable explanations for the complex particle-phonon coupling function and the magnitude of its imaginary part.
- Some examples for which the model fails to reproduce the data, e.g. Pb-208(n,γ).
- Observe and identify the giant $E2$ and M1 resonances and extend the DSD model to include

their contributions.

- Look for the link between the DSD model and the pre-equilibrium model.

Annihilation of 3Q (2p1h) configuration

For example,

$$|p_{3/2}\, s_{1/2}^{-1}\, p_{1/2}\, ;\, \frac{1}{2}^{+}) \longrightarrow |p_{1/2}\, ;\, \frac{1}{2}^{-}) \; ,$$

$$|3d\ 3p^{-1}\ 4s\ ;\ \frac{1}{2}^{-}) \longrightarrow |4s\ ;\ \frac{1}{2}^{+}) \quad .$$

Possible candidates

- Observe resonance capture exhibiting modest final state correlation but a low fraction of the valence radiative width.
- Observed possible common doorways for p-wave neutron strength and M1 radiative strength in Pb isotopes.
- The observed correlations between E1 and M1 partial radiative widths in some nuclei such as Cl-35, Fe-56.
- The 5.5 MeV pigmy resonance, whose long standing problem might be interpreted in terms of 2p-1h annihilation.

Open problems

- Study the distribution of the 3Q configuration fragments.
- The effective charge and the influence of GDR state.

Inelastic valence capture

For example,

$$|1\ 2^{+}\ ,\ d_{5/2}\ ;\ \frac{1}{2}^{+}) \xrightarrow{E1} |1\ 2^{+}\ ,\ p_{3/2}\ ;\ \frac{1}{2}^{+})$$

There are few calculations in the context of this kind of transition, however neither the initial nor the final state can be readily connected to experimentally measurable quantities.

Resonance-averaged inelastic channel capture

Physical significance: radiative capture in the compound inelastic scattering channel.

Calculational formula

$$\langle\sigma_{f}^{ich}\rangle = \frac{\pi}{k^{2}} \sum_{\ell j J \ell' j'} \frac{(2J+1)}{2(2I+1)} \frac{T_{\alpha\ell j} T^{J}_{f,\beta\ell' j'}}{T^{J\pi}} W^{J\pi}_{\alpha\ell j\beta\ell' j'}$$

where $T^{J}_{f,\beta\ell' j'}$ can be regarded as the radiative transmission coefficient in the compound inelastic scattering channel (l',j').

Open problems: the problems encountered here are similar to those in optical model: there is no conclusive evidence that the optical potential well for inelastic channel resembles the ground state one, this is also true for the magnitude of the spectroscopic factor in inelastic channel.

Preliminary results: Table 1 shows the fractions of the three contributions (elastic channel capture, inelastic channel capture and compound nucleus capture) to the calculated total (n,γ) cross sections for a number of nuclei at neutron energies of 0.1 MeV, 1.0 MeV and 2.0 MeV, respectively.

TRANSITIONS FROM 5Q AND ABOVE 5Q CONFIGURATIONS, STATISTICAL MODEL

There is practically no acceptable approach to calculate explicitly the fragment distribution and contribution to the (n,γ) reaction cross section from 5Q and above 5Q configurations. In addition, there is no sign that one alone of these configurations would play an important role. Thus all of these decay modes are grouped together and handled by the statistical theory. Here we list only some of the subjects concerned:

- Basic assumptions and calculational formulae of the statistical model.
- Distributions of E1 and M1 strength function.
- Distribution of E1 and M1 partial radiative width, verification of Porter-Thomas rule.
- Brink-Axel postulate and its verification.
- Resonance-averaged spectroscopy.

CALCULATIONS OF NEUTRON INDUCED PHOTON PRODUCTION DATA

Based upon the preceding analyses, a model code to calculate the neutron induced gamma-ray data, including gamma-ray production cross section, photon multiplicity, photon energy spectrum as well as reaction and level cross sections, has been developed. These data are needed in many applications, such as gamma-ray heating calculations for reactors, weapon effect predictions, material damage estimates and shielding design calculations. In addition to multi-step Hauser-Feshbach model, the principal feature of this program is that a special attention has been paid to the calculations of non-statistical processes in radiative neutron capture reaction, which mainly produce higher energy gamma ray. As we know the higher energy component of photon is crucially important for photon transportation and shielding calculations as well as damage estimates.

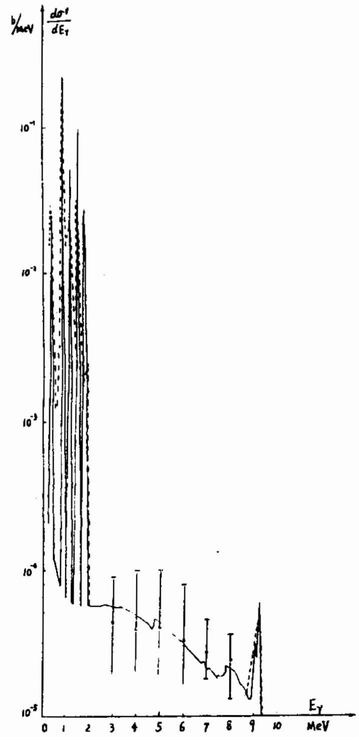
In this code, the full energy range is divided into two regions. At higher energy region, specifically MeV region of neutron incident energy and dense discrete resonance region where average over incident energy is meaningful, the code provides resonance-averaged reaction cross sections and photon production data. Four processes are expected to contribute to the radiative neutron capture cross section in this energy region, namely cascade de-excitations of compound nucleus, radiative capture in the compound elastic and inelastic scattering channel, and direct-semidirect capture. Multistep Hauser-Feshbach model and statistical cascade de-excitation model are used to calculate the initial populations of compound nucleus at each step and de-excitation of residual nucleus other than radiative capture reaction. At lower neutron incident energy, e.g. the region below the first resolved resonance or where an effective resonance average can not be performed, three processes are taken into account in the code to calculate radiative capture cross section, i.e. cascade de-excitation of compound nucleus, potential and valence capture. The interference effect between the last two terms are explicitely included.

Troubetzkoy's formalism are used to calculate cascade de-excitation of compound nucleus by emission of gamma-ray, where the angular momentum and parity effects are taken into account. This code accepts the Becchetti-Greenless's globle optical model to provide particle transmission coefficients and Brink-Axel giant dipole resonance model to calculate gamma ray transmission coefficients. The level densities are those of Gilbert-Cameron with the pairing and shell parameters of Cook.

This code has been used to provide systematic data set. Given here are two examples shown in Fig. 1.

Table 1. Fractions of different processes in the calculated (n,γ) cross sections

	Non-statistical						Statistical		
	Elastic channel capture			Inelastic channel capture			Compound nucleus capture		
	0.1 MeV	1.0 MeV	2.0 MeV	0.1 MeV	1.0 MeV	2.0 MeV	0.1 MeV	1.0 MeV	2.0 MeV
Al-27		0.622	0.466		0.075	0.179		0.303	0.355
Fe-56	0.348	0.176	0.160	0.09	0.174	0.079	0.560	0.650	0.760
Ge-74	0.048	0.017	0.011	0.0	0.016	0.022	0.952	0.967	0.967
Zr-90	0.312	0.114	0.051	0.0	0.0	0.012	0.688	0.886	0.937
Ba-138	0.148	0.060	0.051	0.0	0.0	0.019	0.852	0.94	0.93
Hg-200	0.058	0.015	0.006	0.0	0.023	0.11	0.942	0.962	0.884



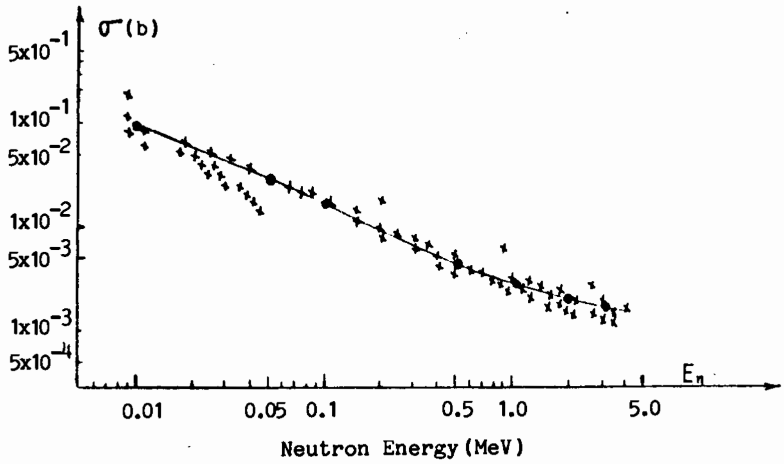


Figure 1 Mn-55(n,γ) cross section and gamma-ray energy spectrum ($\vartheta = 125^\circ$, $E_n = 2$ MeV).

——— Calculated,

------ ϕ x Measured.