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MONTECARLO CALCULATION OF THE ISOMERIC CROSS SECTIONS RATIO FOR THE REACTION $^{237}Np(n,2n)^{236}Np$

Fabrizio CLERI

E.N.E.A. – Dipartimento Reattori Veloci – C.R.E. Casaccia
P.O. BOX 2400 – I-00100 Roma A.D. (Italy)

Abstract: A Montecarlo calculation of the isomeric cross section ratio for the (n,2n) reaction on ^{237}Np has been carried out based on the Hauser-Feshbach formulation. A standard energy-dependent optical model potential was used, with zero deformation parameters and no spin-orbit coupling. Investigation was made about the role of the energy cut-off value, of the higher multipole (E2) transition, of the gamma-ray versus second neutron emission, of the value of the spin cut-off parameter. The results give the correct qualitative energy dependence of the branching ratio, with the assumption that the 1^- level is the ground state. The spin cut-off value obtained indicates a less pronounced deviation of the nuclear moment of inertia from the rigid-body value, with respect to older evaluations for high-mass nuclei.

(Montecarlo method, coupled-channel statistical model, (n,2n) reactions, isomeric ratios, ^{237}Np)

Introduction

In this work a Montecarlo method is used to calculate the isomeric cross-section ratio of a nuclear reaction involving the heavy nucleus ^{237}Np. When statistical model calculation are carried out, averaged quantities are used as level spacing, gamma-widhts and neutron strenght functions, mean neutron energy spectra, mean angular momentum distributions and so on. Our method makes use of probability distributions derived from the exact coupled-channel cross section formulation in a random walk process which, starting from a certain incident particle energy, leads the compound nucleus to emit particles and decay to low-lying levels in successive stages, and finally to jump to one of the available isomeric states, giving a certain value for the isomeric ratio.

Actually, we do not carry out a true dynamical simulation of the collision and decay processes: the Montecarlo method is here used in a more abstract way, sampling and scoring the value of the ratio of two integrals (the so-called "target game"), rather than tracking the particle path in the phase space, as for example the Intranuclear Cascade Model does.

The (n,2n) reaction on the ^{237}Np nucleus was chosen as a tool for this program due to the fact that, besides the relatively great number of experimental results, it is impossible at present to decide if whether the ground state of the final product ^{236}Np is the long-lived or the short-lived one.

Statistical Model Formulation

Generally speaking, the relative probability of forming one of the final states in a neutron induced reaction depends on the spin difference between the compound states at each stage and the spin of the final states themselves; the distribution of the spins of the intermediate states is more and more broadened with increasing number of steps in the deexcitation process, but a certain connection between the initial compound spin and the formation probability of the isomers persists, which is shown in the energy-dependence of the isomeric ratios.

The basic result of the so-called Hauser-Feshbach model of the evaporation theory (1) for the cross section $\sigma(a,a')$ from a channel with quantum numbers a to a channel a' can be stated as

$$\sigma(a,a') = \pi/k^2 \cdot \Sigma_{J\pi} \frac{(2J+1)}{(2I+1)(2i+1)} \cdot \Sigma_{s\ell}\, T_{s\ell}(a) \frac{\Sigma_{s'\ell'}\, T_{s'\ell'}(a')}{\Sigma_{a''}\, \Sigma_{s''\ell''}\, T_{s''\ell''}(a'')} \quad [1]$$

where the unprimed quantities are referred to incoming channels, the primed quantities to outcoming channels and the sum in the denominator is carried on the whole set of available decay channels a''. Here J is the compound nucleus total angular momentum, I and i are the intrinsic spins of the target nucleus and of the incident particle.

For a (n,2n) reaction, the complete expression reads

$$\sigma(a:b,c) = \pi/k^2 \cdot \Sigma_{J\pi} \frac{(2J+1)}{(2I+1)(2i+1)} \cdot \Gamma_a \cdot \frac{\Gamma_b}{\Sigma_{b'}\, \Gamma_{b'}}\, G_c \quad [2]$$

where the Γ_i are the level widhts and $G_c = \Gamma_c / \Sigma_{c'} \Gamma_{c'}$ is the second neutron emission factor.

In this work the transmission functions have been analithycally defined as functions of the complex factor f_ℓ, whose expression is related to the real and imaginary parts of the optical model potential used (2):

$$T_\ell(a) = \frac{4 \cdot P_\ell \cdot Im(f_\ell)}{[\,1 + P_\ell \cdot Im(f_\ell)\,]^2 + [\,P_\ell \cdot Re(f_\ell)\,]^2} \quad [3]$$

In the formula [3] the P_ℓ are the penetrabilities of classical nuclear reaction studies, multiplied by a conventional reflection factor comprised between 2. and 3. to account for the higher penetrability of a diffused-edge potential with respect to a square well potential, which jumps to zero at the nuclear surface.

The Montecarlo game

The first step of the method is to express the basic elements of the calculation in a form suitable to perform the random sampling. We start with the probability distribution function (PDF) of the angular momentum of the compound nucleus J_c, given by [3]

$$p(J_c,E) = \pi/k^2 \sum_{S=|I-1/2|}^{I+1/2} \sum_{\ell=|J_c-S|}^{J_c+S} \frac{(2J_c+1)}{(2I+1)(2i+1)} T_\ell(a) \qquad [4]$$

where S is the total intrinsic spin of the nucleon–nucleus system.

Summing up the $p(J_c,E)$ over the J_c values will give the following, discrete cumulative distribution function (CDF)

$$P(J_c,E) = \sum_{J_i=0}^{J_c} p(J_i,E) \qquad [5]$$

After unitary normalization, a random number between 0 and 1 can be selected to give a certain compound nucleus angular momentum value.

The second basic element is the following joint distribution function, from which the final angular momentum J_f of the residual nucleus, as well as the orbital angular momentum ℓ and parity $(-1)^\ell$ carried off by the neutron, are selected [4]

$$p(J_f;J_c,E) \propto \rho(J_f) \sum_{S=|J_f-1/2|}^{J_f+1/2} \sum_{\ell=|J_c-S|}^{J_c+S} T_\ell(a) \qquad [6]$$

which is again a discrete PDF like the [4] but depends on the random variable J_c too, and gives the probability for a compound nucleus with angular momentum J_c to emit a neutron with orbital momentum ℓ giving a final state with angular momentum J_f ; the factor $\rho(J_f)$is given by the equation [5]

$$\rho'(E,I) = \rho(E)\,(2I+1)\,e^{-(I+1/2)^2/2\sigma^2} \qquad [7]$$

where σ is the spin cut-off factor.

Practically, a matrix with indices J_c and J_f is constructed and then a sum over J_c like in [5] is carried off, so as to obtain a discrete CDF for each initial compound nucleus angular momentum value J_c, to be randomly sampled to obtain the next step angular momentum J_f

$$P(J_f;J_c,E) = \sum_{J_i=0}^{J_f} p(J_i;J_c,E) \qquad [8]$$

In our sample calculation, gamma-ray emission competition was accounted for between the first and second neutron emission, by an exponential probability distribution starting from the value 1. at the thresold energy and rapidly going to zero after some hundreds of keVs: after the first neutron emission this distribution is sampled to allow an E1 gamma ray emission, with energy [6]

$$E_\gamma = 4(E/a-5/a^2)^{1/2} \qquad [9]$$

where a is the level density parameter in units of MeV^{-1}, that can be expressed as a linear function of the mass number A.

The algorithm thus starts with a certain incident neutron energy and angolar momentum; then, the compound nucleus total momentum is sampled from eq.[5]. At this point, intermediate gamma-ray emission eventually takes place. If the excitation energy of the compound system is above the (n,2n) threshold, a second neutron is evaporated and the final total angular momentum of the residual system is sampled from eq. [8], as well as the orbital angular momentum of the neutron, to adjust the parity of the residual nucleus. Finally, the gamma-ray deexcitation cascade is followed starting from the last value of J_f and E. Successive gamma-ray energies are calculated from the formula [9]; the angular momentum of the residual nucleus is calculated according to a random sampling of the normalized probability distribution function

$$P(J) = (2J+1)\,e^{-(J+1/2)^2/2\sigma^2} \qquad [10]$$

for the available angular momentum values, ranging from $|J-\ell|$ to $J+\ell$ for an angular momentum ℓ of the photon.

The cascade is followed until some cut-off energy is reached: then, decay into one of the two isomeric states is chosen, according to the smaller spin change.

The described procedure implies the statistical independence of the two successive particle emissions, whose probability is simply the product of the single-process probabilities. However, the distribution [8] is conditioned by the preceding step angular momentum J_c and excitation energy E (which, in turn, depends on the selected neutron evaporation energy), which acts as an upper limit of integration.

It is easy to recognize that the designed algorithm samples the ratio

$$R = \frac{\sigma(a,m)}{\sigma(a,g)}$$

the $\sigma(a,m)$, $\sigma(a,g)$ being the cross section for (n,2n) reactions ending to the metastable and ground final states, given by expressions of the type [2]: with this model, the discrete level modelling is extended up to the continuum region and the levels are ordered according to the electromagnetic selection rules, with energies distributed according to some known evaporation spectrum.

The $^{237}Np(n,2n)^{236}Np$ reaction

The reaction

$$^{237}Np + n \rightarrow {}^{236}Np + 2n \qquad [11]$$

with thresold at about 6.8 MeV, leads to the formation of two ^{236}Np isomers, one with half-life of 22.5 hours, with quantum numbers 1^-, and the other with half-life of over $1x10^5$ years, with quantum numbers 6^- [7]. Informations about the branching ratio of the (n,2n) reaction can be obtained either from α-counting of the daughter product of the decay chain ^{236}Pu, or from β-rays counting of irradiated ^{237}Np samples. In spite of the relatively large number of experiments, at present it cannot be decided if the ground state of ^{236}Np should be the short-lived 1^- or the long-lived 6^- one. In ref.[8] it was shown that, depending on the ground state isomer chosen, the branching ratio should be qualitatively represented either by a curve starting from 0. at the thresold energy and monotonically raising towards the measured value of about R=0.65 at 10. MeVs, or by a complementary curve starting from 1. at the threshold, slowly descending towards the same values.

Calculations with the method described in the preceding section were performed, with the approximations reported below, starting from the fundamental state $5/2^+$ of ^{237}Np and considering s-wave incoming neutrons only. According to the level scheme of ref.(7) for ^{236}Np, a small amount (between 10 and 20 %) of E2 decay is allowed.

The transmission functions $T_\ell(E)$ have been computed with the help of the optical model potential of ref.(9), excluding the spin-orbit interaction and in the assumption that the Np isotopes behave as spherical nuclei (i.e. setting the β_i deformation parameters to zero). The same transmission functions have been used for ^{236}Np, ^{237}Np and ^{238}Np isotopes. Partial waves

TAB.1 - OPTICAL MODEL POTENTIAL PARAMETERS

V = 46.2 − 0.3 E	MeV
W = 3.6 + 0.4 E	MeV
r = 1.26	fm
a = 0.615	fm^{-1}

up to ℓ=5 can be included in the calculation, that was performed between 0. and 16. MeVs; in this energy range the probability of a third neutron emission is negligible. No competition from reactions other than (n,γ) was considered. The transmission functions obtained (fig.1) show that the even waves, altough initially of lower importance due to the zero-energy dominance of the odd neutron strenght functions in this mass region, play a dominant role at higher energies, notably above the (n,2n) thresold: around the value E=6.8 MeV an evident crossing appears, which is probably responsible for the opening of the chance for second neutron emission.

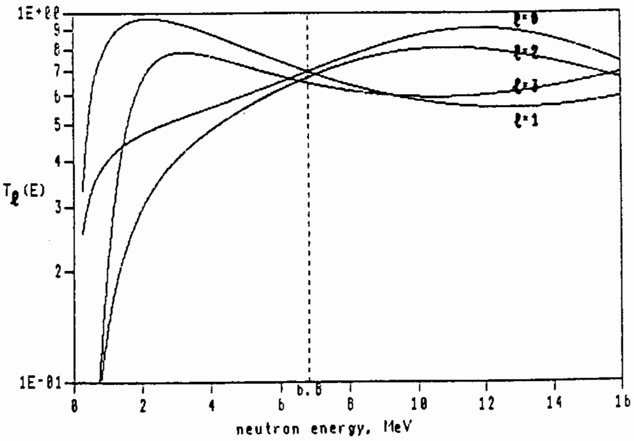

FIG.1 - Transmission functions $T_\ell(E)$ for the first four partial waves.

The spectrum of the evaporated neutrons is taken to be of the form (3)

$$n(E)dE = \sigma_c E^{\ell-1} \cdot \exp(-E/t_m)dE/t_m^{\ell} \qquad [12]$$

where σ_c is the cross section for the inverse reaction, with the following values of the parameters

$$\ell = 16/11 \ , \ t_m = (11/12)E\mathcal{t}/(1+2\mathcal{t}) \qquad [13]$$

The nuclear temperature $\mathcal{t}$ was expressed as a smooth function of the excitation energy E so as to reproduce values ranging from 0.6 to 0.8 with increasing energy, with corresponding greater mean energy for the emitted neutrons.

The level density parameter was taken to be

$$a = 0.142 \cdot A \ MeV^{-1}$$

The spin cut-off parameter was made energy dependent (10)

$$\sigma^2 = 0.0888 \cdot (a \cdot E)^{1/2} \cdot A^{2/3} \qquad [14]$$

and it varies from 6 $\hbar$ to 7 $\hbar$ for excitation energies of the final residual nucleus between 3 and 6 MeV, which are the most probable values before the start of the gamma-ray deexcitation.

The results of a sample Montecarlo run of 50,000 histories for ten incident neutron energy are represented in fig.2, together with the available experimental data. The CPU time was about 10sec/point on a CRAY X-MP/48.

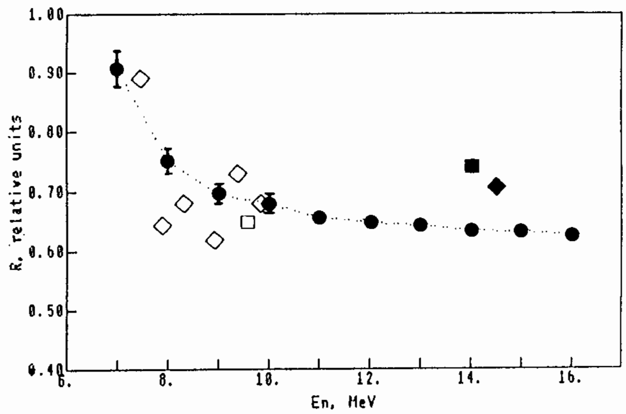

FIG.2 - Results of a Montecarlo run with the 1^- level as the ground state, compared with the available experimental data (◇ ref.(11), ◆ ref.(12), ■ ref.(13), □ ref.(14)).

In these calculations the ground state was assumed to be the short-lived 1^-; this assumption is the same of Kornilov (11), and is in contrast with that of refs.(15) and (16). The feature of correctly reproducing the low-energy dependence of the branching ratio must be noted. At higher energies the results tend to saturate towards a 50/50 sharing of the isomeric ratio, indicating the crudeness of some of the approximations made. The statistical error near the thresold reaches its higher values, about 5 %; in the middle and high energy range the error is negligible (about 1 %).

Influence of the model parameters

Some parametric tests were made on the influence of the model parameters, i.e. the spin cut-off value (see below), the E2 multipole emission percentage, the number of partial waves in the sums [1], and the problem-cut off energy. It is seen that the branching ratio is almost linearly dependent on these parameters, and their influence is broadly constant in energy.

A final consideration can be made about the long-lasting discussion about the values of the spin-cut off parameter σ, that governs the distribution of the spins I of the nuclear levels.

In ref.([17]) a statistical model calculation with the Huizenga-Vandenbosch method was applied to all the experimental available isomeric cross-section ratios, not finding any particular mass dependence of the σ-values: all the data were approximatively about 3 ħ and 4 ħ. This was explained with a progressive reduction of the moment of inertia from the rigid body value by up to 70 % in the heavy mass region, due to the strong residual interactions between nucleons.

In these calculations the σ-value was optimized firstly by performing some trial calculations with an energy independent σ, and then with the formulation [14], that gives the fitted smooth variation with $E^{1/4}$ and is in accord with the indication of ref.([10]). The value obtained of 6-7 ħ is in line with other recent results of statistical model calculations on actinide nuclei (E.Fort ([18]) has derived the value of 6.5 ħ in very refined calculations of the inelastic reactions on ^{241}Am). The deviation of the moment of inertia from the rigid body value turns out to be less pronounced in actinide nuclei with respect to the trend observed in ref.([17]) for the high-A region.

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