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ROLE OF SPIN IN PRE-EQUILIBRIUM CALCULATIONS[1]

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The influence of proper inclusion of the angular-momentum couplings within the master equations approach to the pre-equilibrium exciton model is studied in 14 MeV neutron-induced reactions and compared to the spin-independent calculations. The influence of spin variables is usually small for the neutral ejectiles, but rather significant in the proton channel, so that the use of the simpler spin-independent calculations appears as an oversimplification.

1. Introduction

The pre-equilibrium model combines in a natural way the pre-equilibrium nuclear reaction concept with the equilibrium statistical decay. This is enabled via the master equations approach, that allows one to follow the time evolution of the reaction system up to its complete decay. The great advantage is a *consistent* calculation of multiple particle emission as well as multiple γ emission at all stages of the reaction. The model has been extended to account for angular momenta [1], opening thus also a possibility to calculate also discrete γ ray production. It is important that the nucleon as well as the γ-emission rates of the pre-equilibrium decay automatically take over their correct equilibrium (Hauser-Feshbach) form in the angular-momentum version of the model.

We have used the advantage of a unifying description of a nucleus throughout all the course of a reaction, and studied the influence of spin variables on the resulting particle and γ spectra. To this aim, we have chosen two reactions induced by 14 MeV neutrons, once on a spin 0^+ target of ^{56}Fe, and on ^{93}Nb nucleus of spin $(9/2)^+$ in the second case. The spin-dependent calculation has been complemented by its spin-independent counterpart to highlight the specific features of the role of angular momentum on observable quantities.

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2. Master equations with spin coupling

The set of master equations of the exciton model with explicit treatment of spin variables and all possible couplings and cascades is (see e.g. [2])

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

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 transition rates to neighbouring states, and L is the total integrated emission rate of particles and γ rays.

Here, we assume that we do not deal with the spin mixing (suggested recently by Kun [3]). Spin conservation justifies here the master equations of type (1), where the only way how we can reach different values of angular momentum is via particle (and/or γ) emission.

The angular momentum dependence has been developed for the pre-equilibrium decay by Obložinský *et al.* [1]. Thus, as expected, the nucleon emission rate per energy and time unit is

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

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 [4]. At any stage of the reaction $\mathcal{R}_\nu(n)+\mathcal{R}_\pi(n)=1$; the initial values as well as those at equilibrium depend on the type of reaction and neutron-proton composition of the system.

The particle-hole state density $\omega_n(E,J)$ is given as a product of the energy and the spin parts,

$$\omega(n,E,J) = \frac{g(gE-A_{ph})^n}{p!h!(n-1)!}R_n(J)\ , \quad (3)$$

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

$$R_n(J) = \frac{2J+1}{2\sqrt{2\pi}{\sigma_n}^3}\exp\left(-\frac{(J+1/2)^2}{2{\sigma_n}^2}\right)\ , \quad (4)$$

with σ_n being the spin cut-off parameter.

The transition rates from an n-exciton state to a more complicated one $n\to(n+2)$ are taken factorized [1]

$$\lambda^+(E,J,n) = \frac{2\pi}{\hbar}|M|^2 {Y_n}^{\downarrow} {X_{nJ}}^{\downarrow}\ . \quad (5)$$

In eq. (5), $|M|^2$ 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 the angular momentum part of the squared transition matrix element together with the angular momentum part of the accessible final states. The energy part $Y_n^{\downarrow}$ is just that of the spin-independent case (see e.g. [5]), and the spin part ${X_{nJ}}^{\downarrow}$ is given as [1]

$${X_{nJ}}^{\downarrow} = \frac{1}{R_n(J)}\sum_{j_4 Q} R_1(Q)\tilde{F}(Q)R_{n-1}(j_4)\Delta(Qj_4J)\ , \quad (6)$$

where $\Delta(Qj_4J)$ is 1 for $|Q-j_4|\le J\le Q+j_4$ and 0 otherwise, and

$$\tilde{F}(Q) = \sum_{j_3 j_5}(2j_5+1)R_1(j_5)(2j_3+1)F(j_3)\begin{pmatrix} j_5 & j_3 & Q\\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\ , \quad (7)$$

and the angular momentum density of pair states, where the particle-hole pair (spins j_1 and j_2, respectively) couples to the total pair spin j_3, is

$$F(j_3) = \sum_{j_1 j_2}(2j_1+1)R_1(j_1)(2j_2+1)R_1(j_2)\begin{pmatrix} j_1 & j_2 & j_3\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}^2\ . \quad (8)$$

In eqs. (6) to (8), Q is the spin of a particle (hole) initiating the intranuclear transition, which results in three excitons with spins j_1, j_2 and j_5, respectively; j_4 is the spin of the inert or "spectator" part of the excitons.

We have assumed the single-particle γ radiative transitions and the validity of the Brink-Axel hypothesis [6] in accord with [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 the full angular momentum couplings, the γ emission rate λ_γ from an n-exciton state is [1]

$$\lambda_\gamma([E,J,n]\xrightarrow{\epsilon_\gamma}[U,S,m]) = \frac{\epsilon_\gamma^2\sigma_{\mathrm{GDR}}(\epsilon_\gamma)}{3\pi^2\hbar^3c^2}\frac{b_{mS}^{nJ}\,\omega(m,E-\epsilon_\gamma,S)}{\omega(n,E,J)}\ , \quad (9)$$

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

$$b_{mS}^{nJ} = \frac{y_m^n x_{mS}^{nJ}}{y_m^m x_{mS}^{mJ} + y_m^{m+2} x_{mS}^{m+2J}}\ . \quad (10)$$

In eq. (9), $\sigma_{\mathrm{GDR}}(\epsilon_\gamma)$ is the photo-absorption cross section. The energy terms y's are those appearing in the spin-independent formulation of the model, and the corresponding spin coupling terms are

$$x_{nS}^{nJ} = \frac{3(2J+1)}{R_n(S)}\sum_{j_1j_2j_3}(2j_1+1)R_1(j_1)(2j_2+1)R_1(j_2)R_{n-1}(j_3)\times\begin{pmatrix} j_2 & 1 & j_1\\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}^2\begin{Bmatrix} j_2 & j_3 & S\\ J & 1 & j_1\end{Bmatrix}^2\ , \quad (11)$$

$$x_{nS}^{n+2J} = \frac{2J+1}{2S+1} \sum_{j_1 j_2} (2j_1+1)R_l(j_1)(2j_2+1)R_l(j_2) \begin{pmatrix} j_2 & j_1 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^2 \Delta(S1J) . \quad (12)$$

For the particle (hole) radiative scattering, its angular momentum is j_1 before and j_2 after the γ is emitted, whereas j_1 and j_2 denote the momenta of the annihilating particle-hole pair in the second case [1].

By solving the set of master equations, we get the time integrals of the occupation probabilities,

$$\tau(i,E,J,n) = \int_0^\infty P(i,E,J,n,t)\mathrm{d}t , \quad (13)$$

which are essential in calculations of cross sections of all kinds. Thus, for example, the angle-integrated energy spectrum from the originally created composite system ($i = 0$) at its initial excitation energy E_c is

$$\left(\frac{\mathrm{d}\sigma_x}{\mathrm{d}\epsilon_x}\right)_0 = \sum_{J_c,n} \sigma(E_c,J_c)\tau(0,E_c,J_c,n)\lambda_x([0,E_c,J_c,n] \xrightarrow{\epsilon_x} [\text{anything}]) . \quad (14)$$

Here, $\sigma(E_c, J_c)$ is the cross section of a creation of the composite system. For subsequent emissions, we have to trace $\sigma(i, E_c, J_c, E, J)$, which 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 population cross section incorporates the preceding history of the system by cascade deexcitation and particle emissions before the present emission.

Our approach obviously incorporates the equilibrium (compound nucleus) emission as its natural limit, and — in practice — a significant portion of the emission occurs at or very close to the equilibrium stage.

The initial configuration in the nucleon-induced reactions is taken to be $1p0h$. For nucleon emission, this is a practical equivalent of $2p1h$, but this difference is significant for the γ-emission. The intra-nuclear transition rates (eq. (5)) are fixed by a proper choice of the matrix element. 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 [9], where it depends on the per exciton excitation energy, $e = E/n$. The value of $K' = 100$ MeV^3 has been found to yield reasonable results [10]. The squared matrix element $|M|^2$ for the spin version of the model is established from the condition [1]

$$|M|^2 < X_{nJ}{}^{\downarrow} >= |M_{nonspin}|^2 , \quad (15)$$

where the averaging is performed over J. This procedure ensures the consistency of the nucleon emission spectra obtained in both the spin and the nonspin versions of calculations. The condition (15) has been evaluated at $n = 3$, the most dominant exciton state for the nucleon emission in nucleon-induced reactions. We adopt the same approach of fixing the value of the matrix element for other reactions as well.

In our pilot calculation, a simple equidistant-spacing scheme of states has been used with $g = A/13$; the pairing corrections have not been considered here.

As the aim of our present study was to demonstrate the influence of the proper spin description on the calculated quantities, we did not adjust the parameters as to be able to follow the data more closely, but we simply preferred their global (*a priori*) values.

3. Results and discussion

The first comparison of spin-dependent and spin-independent formulation has been presented in [1]. It was based only on the primary γ contribution to the total γ emission spectrum from the original composite system of ^{56}Fe+n, mainly that from the lowest exciton state. The conclusion therein (and till recently the only pre-equilibrium one) reported only negligible differences between the two calculations for the case studied. Today, spin effects in the pre-equilibrium decay are a topical item (see e.g. the recent paper by Chadwick *et al.* [11]).

We have considered two reactions with projectiles at energies close to 14 MeV, namely those induced by 14 MeV neutrons on ^{56}Fe and ^{93}Nb and by 17 MeV ^{3}He on ^{93}Nb, to perform a comparison of spin-dependent and spin-independent versions of the pre-equilibrium exciton model. They differ mainly by their target spin, which (obviously) influences directly the spin distribution of the composite system. The target spins are 0^+ for ^{56}Fe, and $(9/2)^+$ for ^{93}Nb.

The calculations have been performed using the pre-equilibrium code PEGAS [2] or its updated version PEGAS-D with discrete transitions added. The code PEGAS is a fully pre-equilibrium one based on the master equations approach to the exciton model, where all the emission (even that from the compound nucleus stage) is expressed in the terms of the pre-equilibrium formalism. The particle and the γ emissions can be interspersed as needed.

For a reference spin-independent calculation, we have used the PEQAG code [12], with properly adjusted input parameters, so that both the codes (PEGAS and PEQAG) should yield results very close one to the other. The only difference included is just the presence of spin coupling.

The particle and γ spectra calculated in the spin-independent formulation of the model and those with full inclusion of the angular momentum couplings obviously differ. Generally, this difference is small in the neutron channel in both the reactions, and negligible in ^{56}Fe$(n, x\gamma)$ spectra (fully in accord with Obložinský [1]). The change in the γ spectra from ^{93}Nb+n is more than was seen in the case of zero-spin target of ^{56}Fe; however, the difference is still not essential. What is influenced strongly, is the proton emission, which is amplified in the spin-dependent calculations with respect to the spin-independent ones [13]. This difference may reach even a factor of two or somewhat more, as is the case of ^{93}Nb(n, xp) spectra, and it is somewhat smeared out in the other reaction. The essence of this feature arises from the projection of the spin distribution of the composite system (centered around $4\hbar$ in the ^{56}Fe+n system and a broader distribution nearby $6\hbar$ in the ^{93}Nb+n system) on the angular-momentum dependence of the transition coefficients T_l (T_l's are much supressed for low l values in the proton case, whereas they are ≈ 1 for neutrons there). The hypothesis about the

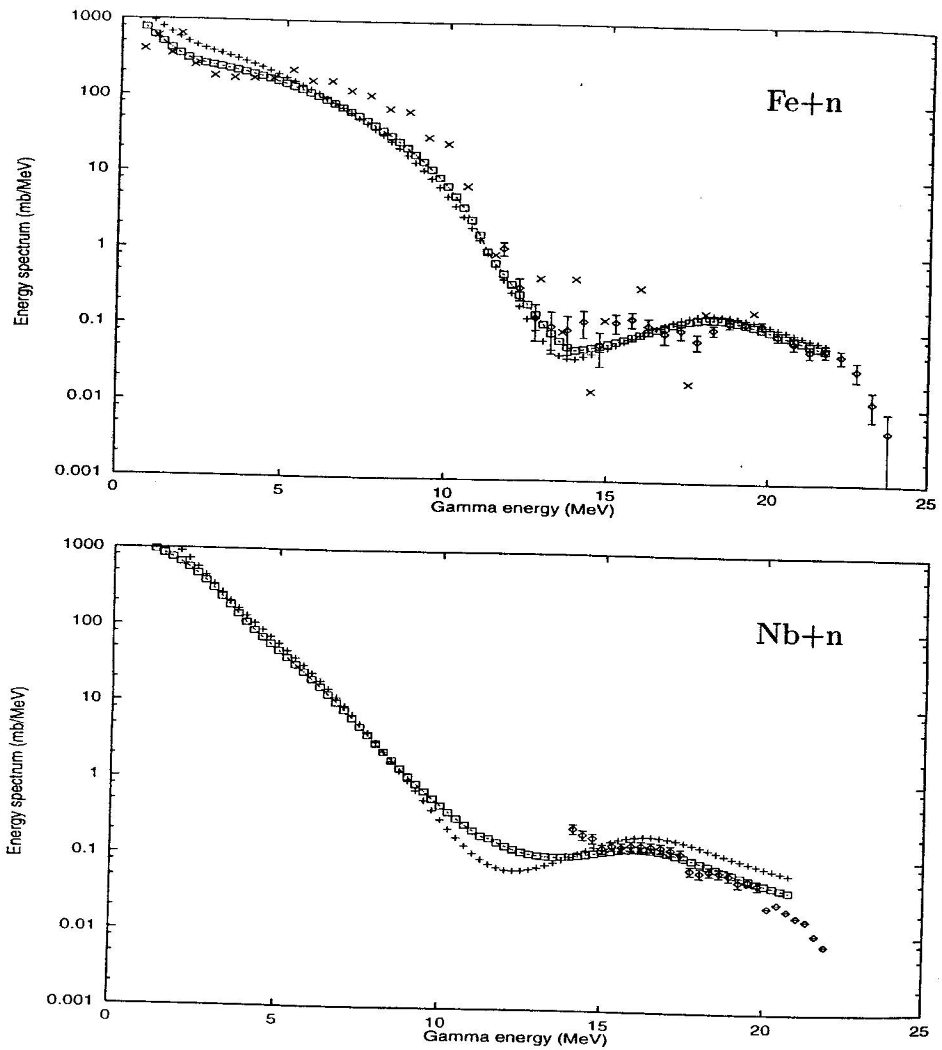

Fig. 1. Gamma spectra from ^{56}Fe+n (upper part) and ^{93}Nb+n (lower part) at 14 MeV. The experimental data are drawn as isolated diamonds with errorbars (Fe+n: Ref. [14]; Nb+n: Ref. [15]) or ×'s (Fe+n, Ref. [16]). The spin-dependent calculations are drawn by squares; the spin-independent ones by +'s.

origin of the neutron-to-proton differences between the spin-dependent and the spin-independent calculations has been verified by a calculation of two "ghost" reactions, which correspond to an incident proton yielding the same composite system as was in the case of the 14 MeV incident neutrons.

The inclusion of discrete levels and the transitions between them is not a less interesting task than was the study of the continuum spectra and their related quantities. Our fully pre-equilibrium code has been applied also to this aim. The reaction studied was ^{93}Nb$(n, n'\gamma)$, where the ground state has a $(9/2)^+$ spin and the isomeric one at 0.03 MeV is $(1/2)^-$. Here, our calculations lead to σ_g = 137 mb and σ_m = 76 mb, and we have got also the information about the relative weights of feeding of each state (whether by the particle emission, by γ-deexcitation of the continuum, or by decay from discrete levels).

Another case has been the ^{39}K$(n, x\gamma)$ reaction, measured recently by Hlaváč *et al.* [17] (and before that by many other authors), where we have calculated several strong γ transitions observed in $(n, n'\gamma)$, $(n, n'p\gamma)$ and $(n, p\gamma)$ reactions (see [18]). The discrepancies between our calculations and the data are comparable in size to the spread of data obtained in various laboratories.

4. Conclusions

We have studied the influence of the spin effects on the particle and γ spectra in two selected reactions at excitation energies of several tens of MeV. Whereas the presence of spin couplings yields no significant effect on the neutron (and γ) spectra for the reactions induced by neutrons at zero-spin target, departures from this condition give rise to significant effects, especially in the case of proton emission, where the effect can reach more than a factor of three in some cases.

Therefore, the further use of spin-independent calculations is a kind of oversimplification which may lead to improper results and it should be taken with extreme caution only. More detailed investigation of the effects is currently in progress.

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References

[1] P. Obložinský: *Phys. Rev. C* **35** (1987) 407 ;
P. Obložinský, M.B. Chadwick: *Phys. Rev. C* **42** (1990) 1652

[2] E. Běták, P. Obložinský: *Code PEGAS*. Report INDC(SLK)-001. IAEA Vienna 1993

[3] S.Yu. Kun: *Phys. Lett. B* **319** (1993) 16 ;
Z. Phys. A **348** (1994) 273

[4] C.K. Cline: *Nucl. Phys. A* **A193** (1973) 417

[5] E. Běták: *Comp. Phys. Comm.* **9** (1975) 92

[6] D.M. Brink: Thesis. Univ. Oxford (1955)

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

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

[9] C. Kalbach: *Z. Phys.* *A* **287** (1978) 319

[10] F. Cvelbar, E. Běták: *Z. Phys.* *A* **332** (1989) 163 ;
F. Cvelbar, E. Běták, J. Merhar: *J. Phys.* *G* **17** (1991) 113

[11] M.B. Chadwick *et al.*: *Phys. Rev.* *C* **49** (1994) R2885

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

[13] E. Běták, P. Obložinský: *in Proc. 7th International Conference on Nuclear Reaction Mechanisms, Varenna 1994 (Ed. E. Gadioli).* Univ. Milano, 1994, p. 186

[14] M. Budnar *et al.*: Report No. INDC(YUG)-6/L. IAEA Vienna 1979

[15] F. Rigaud *et al.*: *Nucl. Phys.* *A* **173** (1971) 551

[16] S. Hlaváč, P. Obložinský: Report No. INDC(CSR)-5/GI. IAEA Vienna 1983

[17] S. Hlaváč, I. Turzo, L. Dostál: *in* Measurement, Calculation and Evaluation of Photon Production Data, *Bologna November 1994 (Ed. P. Obložinský).* Report INDC(NDS)-334. IAEA Vienna 1995, p. 29

[18] E. Běták, S. Hlaváč: Progress Report on IAEA Contract No. 7811/R1/RB (*unpublished,* 1995)