Microscopic description of target spin distribution after inelastic scattering to the continuum

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Abstract. Microscopic modeling of inelastic scattering to the continuum is applied to neutron induced reaction on spherical and axially deformed even-even targets. The spin distributions of the residual compound nucleus formed after the fast inelastic process are calculated with two microscopic models and compared to the prescription usually associated to the semi-classical exciton model. As the semi-classical exciton model does not account for angular momentum conservation, it is often assumed that it is the same as the compound nucleus spin distribution, but this forgets the dynamics of the reaction. It is found that microscopic approaches drastically reduce the average spin value in comparison to what was previously assumed. This strongly impacts (n,n'\gamma) as well as isomer production cross sections when high spin levels are involved. New spin cut-off parameters are deduced from the microscopic calculations that can be used as an alternative to previous prescriptions which neglect the reaction dynamics when they are applied in the context of pre-equilibrium emission process.

1 Introduction

An accurate description of medium energy nucleon induced reactions requires the modeling of various reaction mechanisms such as the direct reactions, the pre-equilibrium emission process, and the formation of- and evaporation from the Compound Nucleus (CN). Depending on the energy available and the type of projectile and target, the CN decay is the results of the competition between neutron, gamma or light charged particles emission and fission. Direct reactions design fast collision processes that last the time taken by the projectile to go through the target diameter, that is about \(10^{-22}\) s. for a few MeV neutron scattering off a medium mass target. It includes direct elastic scattering, often referred as shape elastic, as well as direct inelastic scattering.

The direct inelastic scattering includes the excitation of low lying discrete levels and giant resonances that are embedded in the continuum. Beyond the low energy discrete levels, the target spectrum is usually represented by a continuum of excitations. Inelastic scattering to this continuum is usually accounted for within pre-equilibrium models that provide for the high energy component of particle emission spectrum. Pre-equilibrium models should also determine initial conditions of the formed CN, such as distributions in excitation energy, spin and parity.

One of the pre-equilibrium model based on a quantum description of the inelastic process was given by Feshbach, Kermann and Koonin (FKK) who distinguishes multistep direct (MSD) process, where at least one nucleon is in the continuum, and multistep compound (MSC) process, where all the nucleons are bound [1]. It was shown that MSC is a weak process compared to the MSD process [2].

On the contrary, the exciton model uses a semi-classical approach: a master equation describes the evolution of the system step by step in terms of an exciton number, that is the number of particle and hole, and determines at each step the probability to emit a particle in the continuum or to create/destroy one exciton. The particle-hole pair creation and annihilation matrix elements are adjustable parameters which were adjusted considering relevant experimental data (see for instance [3]). Moreover, due to its classical nature, the exciton model does not conserve the spin and parity at each step. As this information is needed to model the CN decay, the exciton model is usually supplemented with an ad-hoc prescription for the spin distribution. The prescription given by Gruppelaar [4] is to our knowledge used by a majority of the nuclear reaction practitioners to model pre-equilibrium emission.

It was previously shown that the spin distribution in the residual nucleus populated after the fast inelastic collision has a strong impact on the description of (n,n'\gamma) reactions [5, 6]. These previous works suggested that, in some specific cases, the spin distribution given by the Gruppelaar’s ad-hoc prescription is insufficient. In contrast, a fully quantum mechanical modeling of the pre-equilibrium process satisfies the conservation laws in physics and provides spin/parity distributions of the residual nucleus [5, 6].

However, those microscopic approaches are not always ideal for applying to nuclear energy and astrophysics because of large computing time. In this regard, the clas-
tical exciton model, which allows a quick determination of the particle emission energy spectrum, seems better suited. We propose an extended semi-classical exciton model, where the spin-parity distributions in the residual CN are constrained by microscopic approaches.

From microscopic pre-equilibrium calculations for neutron scattering up to 30 MeV on a large variety of target nuclei, we deduce systematic formula that can be used in conjunction with the exciton model and be easily implemented in general reaction modeling codes such as TALYS [7], EMPIRE [8], CoH3 [9], and CCCONE [10].

In Section 2 we describe the two quantum approaches to pre-equilibrium emission, that is the DWBA approach with particle hole excitations (DWBA-ph), the DWBA or coupled channel approach with QRPA (Quasi-Particle Random Phase Approximation) one-phonon excitations (JLM/QRPA). Spin distributions calculated with those two quantum mechanics microscopic pre-equilibrium (QMP) models are discussed and compared to the prescription of Gruppelaar in Sec. 3. The impact of these various approaches on (n,n' \gamma) reactions and isomer productions are illustrated in Sec. 4. Then a systematic formulation of the spin cut-off parameters constrained by a sample of QMP calculations is given in Sec. 5. Conclusions and perspectives are finally drawn.

2 Quantum microscopic models for pre-equilibrium emission

In this work, pre-equilibrium emission corresponds to the fast emission of a neutron in the continuum. The continuum is an approximated representation of the target spectrum beyond the discrete excitations at low energies. The pre-equilibrium emission process is modeled either with the classical exciton model or with quantum microscopic approaches. Reviews of the exciton model are available in the literature (see for instance [3]).

Quantum mechanical approach to pre-equilibrium emission can be formulated from the Born development of the inelastic scattering amplitudes to continuum target excitations in term of power of the residual projectile-target interaction. As we are interested in neutron scattering below 30 MeV, a first order truncation of the Born series provides a good approximation: this is the one step direct process. MSC process has been found to be small in comparison to direct process contribution [2], so they are not considered in this work.

2.1 The DWBA-ph model

The first QMP model, labeled DWBA-ph, relies on a description of target excited states given by one-particle one-hole (1p-1h) excitations. The transition amplitude in the one step approximation corresponds to the Distorted Wave Born Approximation (DWBA). The nucleon-nucleon interaction has the Yukawa form and does not include the spin transfer for the sake of simplicity. Averaged DWBA matrix elements are first calculated for each angular momentum and parity transfer and multiplied by an average 1p-1h level density. Single particle levels were obtained from a Nilsson model. This approach to describe the first step of the MSD process is very appealing in term of computing time efficiency. All useful information on the nucleon-nucleon interaction, the single particle scheme and the 1p-1h level density is given by Kawano et al [11].

2.2 The JLM/QRPA model

The second QMP approach is the JLM/QRPA model. It is very similar to the DWBA-ph model for spherical targets as it relies on a first order approximation in term of the residual interaction. However, both the effective interaction and the nuclear structure model are different. Target excitations are now described as one-phonon excitations of a correlated ground state. Those stem from the QRPA nuclear structure method implemented with the Gogny force (see [12, 13]). The residual interaction is taken as to the Jeukenne Lejeune Mauxah complex energy- and density-dependent two body interaction which was previously successfully used to describe nucleon elastic scattering [14] and inelastic scattering to discrete excitations [15–17] for spherical nuclei. Previous successfull applications to deformed targets, for the ground state rotational band levels, were also achieved within the coupled channel framework [18–20].

In this work, the JLM/QRPA model is applied to describe scattering on both spherical and axially deformed targets. One strength of this approach is that it provides a consistent description of direct inelastic, inelastic scattering and the first step of pre-equilibrium emission as the same effective residual interaction and the same nuclear structure model are used to describe those three processes. One limitation is a quite large computing time, which is related to both QRPA nuclear structure and reaction calculations, especially when coupled channels calculations are involved for deformed targets. However with existing and growing computing capabilities, those calculations can be performed for many targets and a large incident energy range.

In the case of spherical nuclei, the inelastic cross section to the continuum is taken as the sum of direct inelastic scattering DWBA cross sections to all one-phonon excitations energetically accessible. A finite energy width, determined empirically, is associated to each phonon excitation energy to account for their finite life regarding the damping towards CN levels and possible particle emission.

Doubly differential cross section then reads

\[
\frac{d^2\sigma(k_f,k_i)}{dEd\Omega_f} = \int dE \sum_N f(E_{k_f} - E_k - E_N) \frac{d\sigma_N(k_f,k)}{d\Omega},
\]

where \(d\sigma_N(k_f,k)/d\Omega\) is the DWBA cross section for one phonon excitation \(N\) (see [15] for details). The sum over \(N\) includes one-phonon excitations with natural parity (with \(\Pi = (-)^J\)) as the JLM folding model does not account for unnatural parity excitations due to its local nature and the absence of two body spin-orbit and tensor terms.

For axially deformed targets, projection techniques are needed to define the target excitations in the laboratory
frame [21]. Axially-symmetric-deformed HFB calculations are first performed imposing time reversal, axial and left-right symmetries. Projection $K$ of the angular momentum $J$ on the symmetry axis and the parity $\Pi$ are thus good quantum numbers. Within the QRPA formalism, a correlated ground states $|0\rangle$ is defined as the phonon vacuum, that is $\Theta_{\sigma K\Omega}|0\rangle=0$. The target’s intrinsc excitations correspond to phonon excitations of this correlated GS. A one phonon excitation reads:

$$\langle \varkappa K^{\Pi} \rangle = \Theta^{\dagger}_{\alpha K\Omega}|0\rangle = \frac{1}{2} \sum_{ij(K^\Pi)} \left( \langle \chi_{\gamma K \Omega} | \eta^i_j | \chi_{\gamma P \Omega} \rangle - \langle -\chi_{\gamma K \Omega} | \eta^i_j | -\chi_{\gamma P \Omega} \rangle \right),$$

where $\Theta_{\sigma K\Omega}|0\rangle = 0$. Projections $\Omega$ and parities $\pi$ of the quasi-particle creation (annihilation) pair operators $\eta^i_j$, $|\eta^{i\dagger}_j\rangle$ are such that $\Omega_{\pi} = K$ and $\eta^i \eta^i_{\pi} = \Pi$. For an even-even nucleus, the GS is such as $K^{\Pi} = 0^+$. Intrinsc states projected over the total angular momentum of states read, for $K = 0$

$$|\varkappa JMK^{\Pi}\rangle = \sqrt{\frac{2J+1}{8\Pi^2}} \int d\Omega D_{J0}^{\dagger}(\Omega)R(\Omega)|\varkappa 0^+\rangle,$$

and for $K \neq 0$

$$|\varkappa JMK^{\Pi}\rangle = \sqrt{\frac{2J+1}{16\Pi^2}} \int d\Omega D_{J^M}^{\dagger}(\Omega)R(\Omega)|\varkappa K^{\Pi}\rangle + (-)^J D_{J}^{\dagger}(\Omega)R(\Omega)|\varkappa K^{\Pi}\rangle,$$

where the $D_{J^M}$ are the Wigner rotation matrices, $R(\Omega)$ the rotation operator, and $|\varkappa K^{\Pi}\rangle$ the time reversed vector $|\varkappa K^{\Pi}\rangle$.

Projected states defined in Eqs. (3) and (4) are identified to a rotational band in the laboratory frame for the GS and for each intrinsic excitations. For even-even nuclei, the spin and parity of levels in these bands satisfy:

$$\Pi^\Pi \geq K^\Pi$$

and $K > 0$,

$$J^\Pi = 0^+, 2^+, 4^+ \cdots \text{ if } K^\Pi = 0^+,$$

$$J^\Pi = 1^-, 3^-, 5^- \cdots \text{ if } K^\Pi = 0^-.$$  

In the present work, the excitation energy in the laboratory frame of a state $|\varkappa JMK^{\Pi}\rangle$ is given by the approximation $E_{\varkappa K\Omega} = E_{\varkappa K\Omega}^{\text{QRPA}} + \frac{\hbar^2 (J+1) K^2}{2I}$, where the energies $E_{\varkappa K\Omega}^{\text{QRPA}}$ are the QRPA eigen-values, and $I$ is approximated by the HFB moment of inertia of the target ground state.

In the intrinsic frame, the GS density $\rho^0_\tau$ and the transition density $\rho^0_\tau$ read

$$\rho^0_\tau = \langle 0 | \sum r^i \Psi^\dagger(\mathbf{r}, \sigma, \tau, \Psi(\mathbf{r}, \sigma, \tau), |0\rangle, \quad (8)$$

and

$$\rho^0_\tau = \langle |\varkappa K^{\Pi}\rangle \sum r^i \Psi^\dagger(\mathbf{r}, \sigma, \tau, \Psi(\mathbf{r}, \sigma, \tau), |0\rangle \rangle.$$  

where $\tau = \pm \frac{1}{2}$ for neutron/proton.

Excitations in the intrinsic frame are represented by all one-phonon QRPA excitations of the correlated ground-state. Then excitations in the laboratory frame are represented by levels defined following Eqs. (3) to (5) for each intrinsic excitation. The MSD emission corresponds to the sum of the direct inelastic scattering to each of these excitations. To determine the direct inelastic scattering cross section for each excitation, coupled channel calculations are performed. They account for couplings between levels of the ground state rotational band and levels from the an excited band. Couplings between levels belonging to two different excited bands are neglected.

The JLM folding model [14, 19] extended to interband coupling is used to generate the optical and transition potentials that enter the definition of the coupled channels equations. Some details of the present JLM/QRPA approach are given in Ref. [22]. Details on the determination of coupling potential and the coupled channel scheme will be given elsewhere [23].

### 3 Spin distribution of populated states

Within QMP approaches, the spin-parity distribution of the populated states in the continuum is readily known as inelastic scattering to target states with given excitation energy $E_x$, a spin $J$ and a parity $\Pi$, are explicitly calculated. For the incident neutron energy $E_n$, the residual nucleus distribution in excitation energy, spin and parity reads

$$R(J, E_n, E_x) = \sum_{\sigma \mu} \langle \sigma \mu | \Psi^\dagger(E_n, E_x) \rangle$$

where $\sigma \mu$ is the inelastic scattering cross section to the $(J, \Pi, E_x)$ state.

As the exciton model do not provide the spin-parity distribution of the residual nucleus, the ad-hoc prescription by Gruppelaar [4] is usually employed. It is based on the level density model

$$R_n(J^\Pi) = f_{\text{II}} \frac{2J+1}{\sqrt{\pi} \sigma^2_n} \exp \left( - \frac{(J+1/2)^2}{4 \sigma_n^2} \right),$$

where $n$ is the exciton number, $f_{\text{II}} = \frac{1}{2}$ the parity distribution, and $\sigma_n^2$ the spin cut-off parameter defined as

$$\sigma_n^2 = 8n A^{2/3}.$$  

Normalization is such as $\sum_{J^\Pi}(2J+1)R_n(J^\Pi) \approx 1$. Note that the $s$-parameter value implemented in the TALYS codes (up to the 1.96 version) is $s = 0.24$, following Gruppelaar prescription [4].

The $R_n(J^\Pi)$ distributions are convoluted with the occupation probabilities for each exciton configurations after emission. With $\sigma_n(E_n, E_x)$ the pre-equilibrium neutron emission component for the exciton number $n$, the spin distribution of the residual nucleus reads

$$R(E_n, E_x, J) = \sum_{J^\Pi} \left( \sum_{n} R_n(J^\Pi) \sigma_n(E_n, E_x) \right).$$

Figure 1 illustrates i) the various $\sum_J R_n(J^\Pi)$ distributions for $n = 3$ to 11 for a target mass $A = 190$ (left panel); ii) the contributions of the exciton model to the continuum emission for various exciton numbers in the residual nucleus for the 14 MeV neutron $^{190}$W reaction (middle panel); iii) the mean spin of the residual nucleus after
Figure 1. For the $^1$H$^2$W reaction, left panel: spin distributions associated to each exciton number from $n=3$ to $n=11$; middle panel: contributions to the neutron emission of each exciton number in the residual nucleus as a function of the excitation energy for $E_{in}=14$ MeV; right panel: mean spin of the residual nucleus for various incident energies as a function of the excitation energy.

Figure 2. For the $n+$ $^{238}$U reaction at $E_{in}$=15 MeV, top panel: average spin of the residual nucleus after pre-equilibrium emission as a function of excitation energy; bottom panel: spin distributions at $E_{out}$=10 MeV. Calculations performed using the exciton model with an empirical spin cut-off parameter $s$-defined in Eq. (12) - value of 0.04 (red dot-dashed curves) or 0.24 (red dashed curves) are compared to calculations performed with the two microscopic approaches JLM/QRPA (full black curves) and DWBA-ph (blue dotted curves).

Spin distributions were calculated for a set of even-even targets within the JLM/QRPA model. The variation of the average spin after integration over excitation energy is illustrated in Fig. 3 for various nuclei in the $A=92$-238 range. On these plots, the average spin grows from $\hbar=2$ at low energy, to $5 \hbar$ at 30 MeV.

4 Impact on (n,n’ γ) cross sections and isomer production

(n,n’ γ) reactions were modeled using the DWBA-ph or JLM/QRPA models, and the exciton model with the Gruppelaar’s spin cut-off prescription. QMP models strongly suppress the γ transitions from levels with high spin which is illustrated in Fig. 4 for E2 transitions inside the ground state rotational band in $^{238}$U: the 210.6-keV ($8^+ \rightarrow 6^+$) transition is strongly reduced while the the 104-keV ($4^+ \rightarrow 2^+$) transition magnitude is almost unaffected. Indeed pre-equilibrium process described by QMP models hardly populates high spin states in the continuum which considerably improves the agreement with experimental data of γ-transition from high-spin excited levels. For the 104-keV transition, small remaining differences are not only related to variations of spin distributions, but also to neutron emission probability that differs between the three models, while for the 210.6 keV transition, the main effect comes from the spin distribution.
The same physical effect can be seen on production cross sections of isomer levels in \((n,n')\) reaction. This is illustrated in Fig. 5 for the production of two isomer levels in \(^{140}\text{Ce}\). The production of the 6\(^+\) level is reduced by 10\% while the production of the 4\(^+\) level is almost unchanged.

5 Systematic formulation

A systematic formulation of the spin cut-off parameter of the form given by Eq. (12) can be inferred from QMP models. Indeed, the functional given by Eq. (11) can be used to fit the JLM/QRPA spin distributions through the adjustment of the parameter \(s\). This is illustrated in Fig. 2 (top panel, compare black full curve to dot-dashed curve).

The linear dependence in \(A^1\), used for the exciton model [see Eq. (12)], is conserved. It can be understood from the classical available angular momentum given by \(L=Rp\), where \(p\) is the classical momentum and is the nuclei radius given by 1.2\(A^{1/3}\).

The chosen functional form for the averaged transferred spin is:

\[
\bar{J} = a(A)E_m^{1/4} + b(A)E_m^{1/4} + c(A)\,.
\]  

\(14\)

with

\[
x(A) = \alpha x A^{1/4} + \beta x, \text{ with } x = a, b, c\,.
\]  

\(15\)

Note that the relation between \(\bar{J}\) and the spin cut-off \(\sigma_n\) is approximately given by the relation

\[
\sigma_n = \frac{\bar{J} + \frac{1}{2}}{\sqrt{8n}}
\]  

\(16\)

This shows the average spin dependence on the exciton number is linear.

Parameters were adjusted to reproduce the spin distributions calculated with the JLM/QRPA model applied to a set of nuclei in the mass range \(A=90-238\) and for neutron energies in the range 0-30 MeV. Both local fits (one per nucleus) and a global fit were performed. They were found to represent quite accurately the microscopic calculation, as illustrated in Fig. 6. The global fit provides the parameters

\[
\alpha_a = -0.680858, \beta_a = 6.37643, \\
\alpha_b = 0.0818127, \beta_b = -0.557189, \\
\alpha_c = 1.14442, \beta_c = -7.1285.
\]  

\(17\)

It represents the overall variations of the average spin with mass and incident energy with a deviation from the microscopic calculations (and local fits) that do not exceed 0.5 \(\hbar\).

6 Conclusion and perspectives

Inelastic scattering to the continuum for neutron induced reactions on even-even targets and in the 0-30 MeV incident energy range was modeled using two microscopic quantum approaches. The first is based on particle-hole excitations of the target while the second describes them as one-phonon QRPA modes. These models were used to predict the spin distribution of the residual nucleus which is formed after the fast inelastic process (as opposed to the slow CN inelastic process). The average spin has been
found to be drastically smaller than the value associated to the semi-classical exciton model. Indeed, the exciton model is complemented with an empirical spin distribution for each exciton number which depends on a spin cut-off parameter. The value of this cut-off implemented in TALYS or Empire codes corresponds to a prescription designed to describe the spin distribution in a CN. However, this prescription does not account for the dynamic of the pre-equilibrium reaction, which favors low angular momentum transfers. As a result, microscopic approaches predict average spin transfers in the range 2-5 $\hbar$, depending of the incident energy and targets, while the spin distribution associated to the exciton model displays an average value larger than 9 $\hbar$, value which grows rapidly with the excitation energy. Comparisons between calculated and experimental ($n,n'\gamma$) cross sections for $\gamma$-decay from high spin ($J>5\hbar$) levels demonstrate that the spin distributions predicted by microscopic models are more realistic than the values previously admitted. The impact on high spin isomer level production cross section is also illustrated.

A new spin cut-off parameterization, given as a function of incident energy and target mass, is extracted from microscopic calculations. It corresponds to the average over excitation energy. This global formula can be easily implemented in nuclear reaction codes to complete the exciton model with spin distributions that we believe to be realistic.

This work is now being extended to include an explicit dependence on both incident and excitation energies for targets in the $A = 16-240$ mass range for both the DWBA- and JLM/QRPA approaches. This work is also being extended to include inelastic scattering of light charged particles. The model needs also to be completed to include unnatural parity excitations, and excitations beyond one particle-hole or one phonon states [24].

References