Microscopic description of the two-step direct pre-equilibrium process with non-local potentials and collective states

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Abstract
We present our calculation of contributions to the pre-equilibrium emission cross section coming from two-step direct processes, using a fully microscopic approach based on the nuclear matter method, and treating explicitly the non locality in the potentials. Collective states are included using the Random Phase Approximation (RPA) nuclear structure model. Collective excitations enhanced the two-step cross section when compared to a calculation performed with uncorrelated particle-hole excitations. This results, as well as possible improvements of our modeling, are discussed.

1 Introduction

The preequilibrium stage of a nucleon induced nuclear reaction corresponds to the situation in which the projectile shares enough of its kinetic energy and angular momentum with a few nucleons of the target, and excitation lying in the continuum can be reached. This stage can be observed in the experimental energy spectrum of particles emitted, that present a continuous behavior. A quantum-mechanical treatment of the first part of the preequilibrium nuclear reactions, that are associated with Multistep Direct processes (MSD) is a complicated task that requires an accurate description of the target's excited states even in the continuum, along with an appropriate effective interaction. Moreover, in order to reach a usable form of the transition amplitude for practical calculations, a number of approximations have to be made. The three well-known statistical MSD theories are form Tamura-Udagawa-Lenske (TUL) [1], Nishioka-Weidenmüller-Yoshida (NWY) [2] and Feshbach-Kerman-Koonin (FKK) [3]. A review and thorough comparison of the assumptions and approximations in each of these models is given in [4] and references therein and in [5].

There has been some practical calculations made with MSD models [6,7], which use uncorrelated particle-hole (p-h) excitations for the target. Recently, Dupuis achieved a microscopic calculation of the contribution coming from one-step processes [8] using RPA states for the target (implemented with the Gogny D1S force [9]) and the Melbourne G matrix [10] as effective interaction between the nucleon projectile and the target nucleons. In this calculation, non-natural parity transition are taken into account explicitly and the knock-out exchange term is also accounted for without any localization procedure. The results of this study show a good agreement with experimental data where one-step processes are believed to contribute the most, namely at low excitation energy and forward angles; but the analysis of the calculated preequilibrium angular distribution and energy spectrum of the emitted particle shows that at backward emission angles and for excitation energies above approximately 20 MeV, contributions are missing.

The present work is to be seen as a first stage towards the inclusion of two-step direct processes using the same ingredients as in [8], namely an RPA description of the target's states corresponding to two-step processes, the Melbourne G matrix as effective interaction and a modified version of the NWY model. We compare calculations using RPA states, represented by phonons, to calculations with uncorrelated p-h states and investigate interference effects. In section 2, we briefly remind the approximations we use in our MSD model and we present the microscopic ingredients we use for this calculation. In section 3 we display our results and give some comments, and we draw a conclusion and give some perspectives in section 4.

2 MSD model and microscopic ingredients

2.1 Hypotheses for the MSD calculation

The quantum mechanics description of the MSD process starts from the Born expansion of the transition amplitude for an inelastic process leading to the excitation of a target in its ground state (GS) ψ_i to a final target states $|\psi_f\rangle$, namely

$$T^{i\to f} = \langle \chi^-_{\overrightarrow{k_f}}, \psi_f |\; V \;+\; VGV \;+\; VGVGV \;+\; \cdots \; |\chi^+_{\overrightarrow{k_i}}, \psi_i\rangle \;, \tag{1}$$

where V is a residual interaction acting between the the nucleon projectile and the target nucleons. The state $\chi^+_{\overrightarrow{k_i}}/\chi^-_{\overrightarrow{k_f}}$ is the distorted wave in the entrance/exit channel, k_i/k_f and E_{k_i}/E_{k_f} are the associated wave number and kinetic energy. The system Hamiltonian reads $H = H_A + t + V$, where H_A is the target Hamiltonian, t is the kinetic energy operator for the relative motion. The distorted waves in eq. (1) are solution of the Schrödinger equation $(t + U - E_k)\,\chi^{\pm}_{\overrightarrow{k}} = 0$, where U is the optical potential defined as $U = \langle\psi_i|V|\psi_i\rangle$. The many-body propagator G in eq. (1) is $G = \frac{1}{E_{k_i} - U - t - H_A + i\epsilon}$, and its spectral decomposition on eigenstates of H_A and $t + U$ or $t + U^\dagger$ reads

$$G = \sum_N \int \frac{d\overrightarrow{k}}{(2\pi)^{\frac{3}{2}}} \frac{|\tilde{\chi}^+_k, \psi_N\rangle\langle\chi^+_k, \psi_N|}{E_{k_i} - E_k - E^*_N + i\epsilon} \;, \tag{2}$$

where E^*_N is the target excitation energy, namely $H_A|\psi_N\rangle = (E_0 + E^*_N)|\psi_N\rangle$ if E_0 is the GS energy, and $\tilde{\chi}^+_k$ solves $\left(U^\dagger + t - E_k\right)\tilde{\chi}^+_k = 0$.

The doubly differential cross section for a nucleon emitted at given outgoing angle and energy is:

$$\frac{d^2\sigma(\overrightarrow{k_i}, \overrightarrow{k_f})}{d\Omega_f dE_{k_f}} = \frac{\mu^2}{(2\pi\hbar^2)^2}\frac{k_f}{k_i}\sum_f \delta(E_{k_i} - E_{k_f} - E^*_f)|T^{i\to f}|^2 \;. \tag{3}$$

The n-step direct process corresponds to the n$^{\text{th}}$ order of the series (1). Second order involves the excitation of two particle-hole (2p-2h) states, or two phonon states. Such a process is schematically described on Fig. 1. Since we use the Melbourne g-matrix to represent the effective interaction V, contributions to elastic scattering that comes from the coupling of excited states to the GS are already accounted for in the effective interaction, so in our calculation we must not keep them. We also apply the never-come-back approximation, which assumes that at each step of the reaction the process leading to the creation of a new pair p-h is dominant over the processes of scattering and annihilation. Consequently, the coupling terms that are not included in our calculation are displayed in Fig. 1 by dash, thin arrows while the terms we explicitly calculate are embodied by full thick arrows. Considering these assumptions, one-step and two-step processes lead to distinct final states, thus interferences between the first and the second order of the transition amplitude (1) vanish when the cross section is calculated.

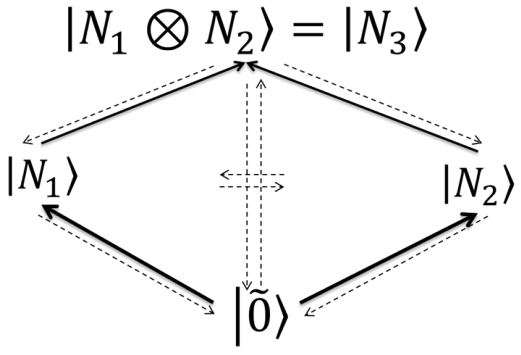

Fig. 1: Schematic representation of the coupling potentials involved in the calculation of a 2-step process. The GS is labeled $|\widetilde{0}\rangle$, target states excited after one-step processes are labeled $|N_1\rangle$ and $|N_2\rangle$, and $|N_3\rangle$ is the target state excited after the second step. Here, we describe the situation where the final state is a 2p-2h (or two-phonon) states made of the N_1 and N_2 1p-1h (or 1-phonon) components. The arrows are defined in the text body.

In our modeling, we consider the two cases in which the target's real states $|\psi_N\rangle$ are a linear combination of either p-h states or RPA states. Moreover, we make use of the sudden approximation used in the NWY model that assumes that configuration mixing is slower than the projectile-target interaction processes. In our approach, this implies that the real intermediate states N_1 and N_2 are shrunk from a linear combination of 1p-1h, 2p-2h, ... (resp. 1-phonon, 2-phonons, ...) states to simply 1p-1h (resp. 1-phonon) states. Consequently of this assumption associated to our use of a 2-body interaction is that the only matrix elements connecting the intermediate state to 2p-2h (reps. 2-phonon) component of the final state remain. Note that we account for the finite life time of the target final states. This leads to replace the delta functions in eq. (3) by the Lorentz distribution $\rho_N(E) = \frac{1}{\pi}\frac{\Gamma_N}{(E-E_N)^2+\left(\frac{\Gamma_N}{2}\right)^2}$ where Γ_N represents the sum of the escape and damping widths. In the present work, we make use of the on-shell approximation which means that we neglect the principal part in eq. (2). Finally, the second order double differential cross section we calculate reads:

$$\frac{d^2\sigma(\overrightarrow{k_i},\overrightarrow{k_f})}{d\Omega_f dE_{k_f}} = \frac{\pi^2\mu^2}{(2\pi\hbar^2)^2}\frac{k_f}{k_i}\sum_f \rho_f(E_{k_i}-E_{k_f})\left|\sum_\beta \langle \chi^-_{\overrightarrow{k_f}},\psi_f|V|\tilde{\chi}^+_{\overrightarrow{k}},\psi_\beta\rangle\langle\chi^+_{\overrightarrow{k}},\psi_\beta|V|\chi^+_{\overrightarrow{k_i}},\psi_i\rangle\right|^2 . \quad (4)$$

Final states f are 2p-2h (resp. 2-phonon) states, β labels 1p-1h (resp. 1-phonon) states, and ρ_f is the density of 2p-2h (resp. 2-phonon) states. This formula includes interference terms between various intermediate β states. The effect of these interferences is shown in section 3.

2.2 Microscopic ingredients

In our calculation, the use the Melbourne G matrix as residual two-body interaction, which is the solution of Bruckner-Bethe-Goldstone equation in all spin and isospin channels for a mapping of nuclear matter densities ρ. The Melbourne G matrix is a local finite range interaction parameterized as a sum of Yukawa form factors:

$$G(\overrightarrow{r},\overrightarrow{r}',\rho,E) = \sum_j G_j(\rho,E)\frac{e^{-\frac{|\overrightarrow{r}-\overrightarrow{r}'|}{\mu_j}}}{|\overrightarrow{r}-\overrightarrow{r}'|} , \quad (5)$$

with μ_j denoting the range of the interaction, and where the energy and density dependent amplitudes $G_j(\rho,E)$ are complex. This interaction is made of a central, a spin-orbit and a tensor terms. Since the Melbourne G matrix is calculated in infinite nuclear matter, we use a local density approximation to make calculations in finite nuclei, following the prescription used in the DWBA98 code [11]. As we earlier mentioned, the potentials obtained from the nuclear matter approach and with a finite-range 2-body effective interaction are non local in the space coordinate basis.

As for the nuclear structure input of our calculation, we first describe uncorrelated states. A 1-body potential between an initial state i and a final state f can be written:

$$U^{i\to f} = \langle f|V|i\rangle = \sum_{\alpha,\beta,k,k'} \langle k',\alpha|V|\widetilde{k,\beta}\rangle \rho^{i\to f}_{\alpha,\beta} a^\dagger_{k'} a_k , \quad (6)$$

with α labeling single particle states, and $|\widetilde{k,\beta}\rangle = |k,\beta\rangle - |\beta,k\rangle$. The term $-|\beta,k\rangle$ generates the knock-out exchange potential which is non-local if V has a finite range. The quantity $\rho^{i\to f}_{\alpha,\beta}$ is a one-body transition density matrix element between initial and final state defined by:

$$\rho^{i\to f}_{\alpha,\beta} = \langle f|a^\dagger_\alpha a_\beta|i\rangle \quad (7)$$

In our study, we calculate the target's GS with the Hartree-Fock (HF) theory implemented with the Gogny D1S force. Details on this implementation can be found in [12]. In the HF theory, the GS is a Slater

determinant written as:

$$|\psi_{HF}\rangle = \prod_{h=1}^{h_{Fermi}} a_h^\dagger |-\rangle \ , \tag{8}$$

with h_{Fermi} labeling the Fermi level and $|-\rangle$ the void of particles. A 1p-1h excited state can be built on this GS using the angular momentum coupled creation and annihilation operator:

$$|1p1h\rangle = \left[a_p^\dagger \otimes a_{\widetilde{h}}\right]_M^J |\psi_{HF}\rangle = \sum_{m_p m_h} (-)^{j_h - m_h} \langle j_p m_p j_h - m_h | JM\rangle \, a_p^\dagger a_h |\psi_{HF}\rangle \ , \tag{9}$$

with $a_{\widetilde{h}}$ the time reversed annihilation operator of a hole state, J the total spin of the excitation and M its projection on the quantization axis, and j_i the intrinsic total angular momentum of the particle i. A 2p-2h state is built by coupling two 1p-1h states to the correct total spin and parity (of the 2p-2h state):

$$|N_3\rangle = n|N_2 \otimes N_1\rangle = n \left[\left[a_{p_2}^\dagger \otimes a_{\widetilde{h_2}}\right]^{J_2} \otimes \left[a_{p_1}^\dagger \otimes a_{\widetilde{h_1}}\right]^{J_1}\right]_{M_3}^{J_3} |\psi_{HF}\rangle \tag{10}$$

with N_3 the 2p-2h state, N_2 and N_1 the two 1p-1h states, n a normalization factor. We can use similar definitions for the RPA cases, considering first the definition of a 1-phonon creation and annihilation operators. Let $|\psi_{\widetilde{0}}\rangle$ denote the void of phonon, describing the GS of the nucleus. We define $\Theta_N^\dagger$ the operator that creates a phonon labeled $|\psi_N\rangle$. We associate to the creation operator its adjoint operator Θ_N that annihilates the vibrational mode N. Formally, these definitions read:

$$|\psi_N\rangle = \Theta_N^\dagger |\psi_{\widetilde{0}}\rangle \quad , \quad \langle\psi_N|\Theta_N = \langle\psi_{\widetilde{0}}| \quad , \quad \langle\psi_{\widetilde{0}}|\Theta_N^\dagger = 0 \quad , \quad \Theta_N|\psi_{\widetilde{0}}\rangle = 0 \tag{11}$$

We use the same definition for the angular momentum coupled operators that we introduced for uncorrelated p-h states, and also for 2-phonon states which reads:

$$|\psi_{N_3}\rangle = n \left[\Theta_{N2}^\dagger \otimes \Theta_{N1}^\dagger\right]_{M_3}^{J_3} |\psi_{\widetilde{0}}\rangle \ , \tag{12}$$

with n a normalization factor.

2.3 The ECANOL and MINOLOP codes

From the definitions previously given, we have written a code called MINOLOP that computes the non local coupling potentials using the Melbourne G matrix and nuclear structure input. In the present work, our practical applications were done using only the central part of these potentials, for the spin-orbit and tensor parts still require some validations. Furthermore, we developed the ECANOL code that solves coupled-channel equations with non local potentials. This code uses a numerical method developed by Arellano and successfully applied to the description of charge exchange reactions [13]. We extended this method to take into account other excitations and be able to make calculations for inelastic scattering, and use the results in our preequilibrium calculations.

3 Results

In equation (4), we mentioned that interference effects are expected to occur. In order to evaluate the effect of these interferences, we made the calculation in the same spirit of that made by Kawano *et al.* [6] of a few random cases with and without interferences. We display on the left panel of Fig. 3 the results for the following case: the GS of ^{90}Zr is 0^+, the states corresponding to one-step processes are a 3^- and a 5^-, and we display the results for the 2^+ and 4^+ 2-phonon states. On the right panel, we display a similar calculation but in the case of uncorrelated p-h excitations, and only in for the 2^+ final state.

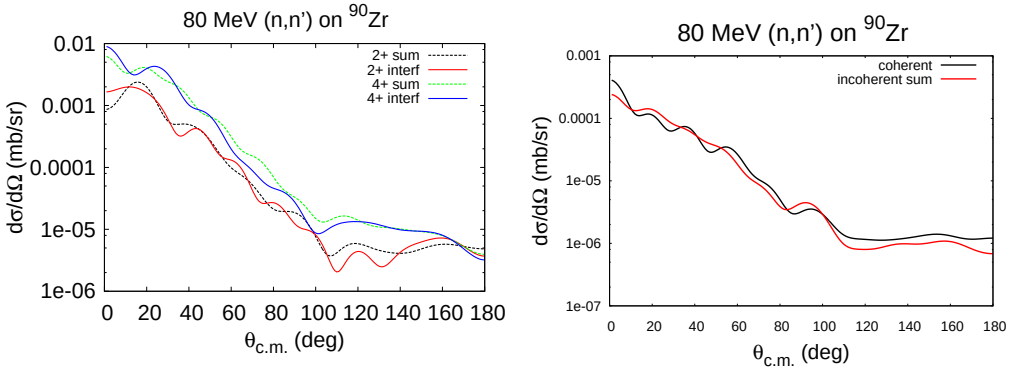

Fig. 2: Angular distribution to 2-phonon (left) and 2p-2h (right) states built by coupling the first, 1-phonon (left) and 1p-1h (right) 3^- and 5^- states in ^{90}Zr for an incident neutron.

We notice that interferences modify the shape of the angular distribution but not the magnitude, and the positions of the relative minima and maxima between coherent and incoherent calculation present a random nature. Also, the relative difference of the integrated cross section is below 10%. This calculation indicates that interference effects should average out provided we include in the preequilibrium calculation a very large number of states. In ^{90}Zr, there are about 10,000 2-phonon states with an excitation energy below 22 MeV, and such a number should be significant enough so that we can make a calculation without interferences (the situation is similar in the case of p-h excitations).

So, we have made a calculation of the contribution to the preequilibrium cross section that comes from 2-step processes, considering a incident neutron with 80 MeV of kinetic energy on ^{90}Zr. We have done two separate calculations: one in which we consider uncorrelated p-h excitations of the target, and one in which we use RPA states. We have included all states with an excitation energy below 16 MeV. As the excitation energy increases, the number of states that correspond to 2-step processes becomes larger and larger than the number of states for one-step processes. Therefore, we expect that the tendencies we observe in the excitation energy range of our calculation will be more pronounced at higher excitation energies. The results are displayed on Fig. 3.

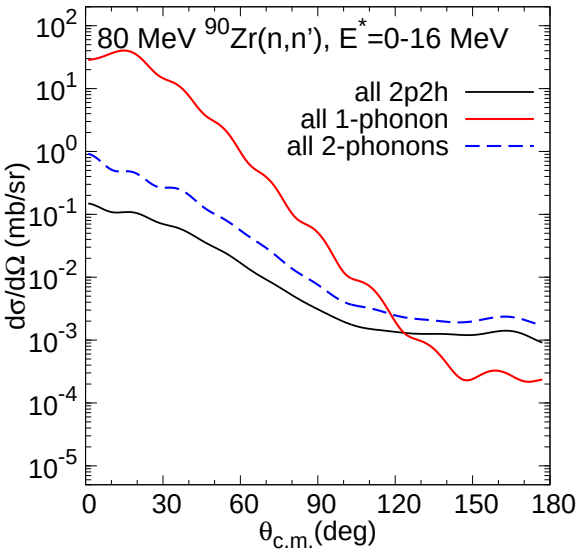

Fig. 3: Comparison between the angular distribution obtained with RPA states for 1 (red curve) and 2-phonon states (blue curve), and with uncorrelated 2p-2h (black curve) state. The excitation energies considered in this calculation range from 0 to 16 MeV.

The contribution that comes from 2-step processes is bigger than the contribution of one-step processes for emission angles above approximately 100°. This can be understood by the larger transfer

of angular momentum in the case of 2-step processes, which leads to emitted particles at higher angles. The contribution that comes from 2-phonon states is bigger than the contribution from 2p-2h states. Two reasons explain this difference: 2-phonon states are collective states, and here the impact of this collectivity is to increase the cross section. The other reason is that in our RPA calculations, we used the Quasi-Boson Approximation (QBA)which can cause a strong violation of the Pauli principle and may artificially enhance the cross section. In the present calculation, it is not possible to distinguish the separate contributions of collectivity and of the QBA.

4 Conclusion

This work is a first step towards the extension of the microscopic calculation of MSD emissions carried out by Dupuis [8] to 2-step processes. Our results indicate that with the present modified version of the NWY model, interference effects should average out with a sufficient number of states. Also, our calculations show the enhancement of the angular distribution at backward emission angles when 2-step processes are accounted for, even at low excitation energies. Finally, we observe the effect due to both collectivity and the use of the QBA in RPA calculations. Possible improvements for this work are the inclusion of all components of the effective interaction so that states with non-natural parity can also be included, lifting the on-shell approximation and check if our observations on interferences are modified, and make a larger calculation that includes states with a higher excitation energy. With the MINOLOP and ECANOL codes that we have developed, such study should be feasible in the near future.

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