

RESEARCH REPORT

- Contract nr.:** 194/2017 (PN-III-P4-ID-PCE-2016-0649)
- Project:** Parallel theoretical study of the two components of the prompt fission neutrons: dynamically released at scission and evaporated from fully accelerated fragments
- Project director:** Dr. Nicolae Carjan
- Phase nr. 1/2017:** The shape of the energy spectrum of neutrons emitted during scission

1 Phase objective

The evolution of the impulse distribution and of the energy spectrum of the scission neutrons during their separation from the fissionable nucleus.

2 Activities

The Fourier transform calculation of single particle wave functions in spherical and deformed nuclei. The deduction of corresponding impulse distributions.

3 Abstract

The Fourier transform of single particle wave functions in cylindrical coordinates is applied to the study of neutrons released during scission. We propagate the neutron wave packets in time through the bi-dimensional time dependent Schrödinger equation with time dependent potential. We separate the parts of these wave packets that are in the continuum and calculate their Fourier transforms at different times: immediately after scission ($T = 1 \times 10^{-22}$ sec) and at several intervals afterwards (until $T = 50 \times 10^{-22}$ sec). The momentum distributions corresponding to these Fourier transforms are then estimated. The evolution of these distributions in time provides an insight into the separation of the neutron from the fissioning system and asymptotically gives the kinetic energy spectrum of that particular neutron.

4 Phase report

4.1 Introduction

The goal of the project is to provide elements for answering the important question of the nature and relative abundance of the two components of prompt fission neutrons (PFN): released at scission and evaporated from fully accelerated fragments.

We have used a dynamical scission model to estimate the main properties of the scission neutrons (SN), based on the solution of the time-dependent Schrödinger equation [1], [2]. When the calculated data have been compared with measurements of PFN during $^{235}\text{U}(\text{n}_{\text{th}},\text{f})$ the experimental trends are well reproduced. Based on this evidence, one cannot decide anymore which is the main source of PFN. It is therefore necessary to extend the application of our model to other observables and other fissioning systems to see how far this agreement holds. Also, the same quantities will be calculated with both models (scission and evaporation) to decide which is more realistic.

In the present phase we will determine the energy spectrum of the SN. For this we need to calculate the Fourier transforms (FT) of the unbound parts of the wave packets that describe the SN immediately after scission. These will provide the SN momentum distribution from which one can derive the kinetic energy distribution. It is expected that at low and high kinetic energies the SN spectrum differs from the evaporation spectrum leading to an opportunity to distinguish between the two components of the PFN.

To make possible the treatment of both spherical and deformed nuclei, we have developed adequate numerical procedures to calculate the FT of a WF in cylindrical coordinates [3]. After a short description of the numerical methods used, we apply them to the scission neutrons and present some relevant results.

4.2 Formalism

4.2.1 Continuous case

The standard form of the Fourier transform of a function $\Psi(\vec{r})$ in three dimensions is:

$$\Phi(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} \Psi(\vec{r}) e^{-i\vec{k}\vec{r}} d^3\vec{r}, \quad \vec{k} = \vec{p}/\hbar. \quad (1)$$

It gives the probability in the momentum space i.e., the probability that the nucleon has its momentum \vec{p} in the volume element $d^3\vec{p}$.

In our applications we consider nuclear forms with axial symmetry so that we use the cylindrical coordinates (ρ, z) and omit the dependence on the angle θ . It can be shown that the Fourier transform in this case has the form:

$$F(R, Z) = 2\pi \int_{-\infty}^{\infty} \left[\int_0^{\infty} f(\rho, z) J_0(2\pi\rho R) \rho d\rho \right] e^{-2\pi izZ} dz \quad (2)$$

where J_0 is the zero-order Bessel function of the first kind. The transform with respect to the variables ρ, R is called the zero-order Hankel transform. Thus, the Fourier transform in cylindrical coordinates implies a combination of Hankel and one-dimensional Fourier transforms. The form used in quantum mechanics is based to the relations $R = k_\rho/(2\pi)$ and $Z = k_z/(2\pi)$. The variables ρ, z belong to the position space, while k_ρ, k_z belong to the momentum space. The factor $1/2\pi$ is introduced as a phase convention.

4.2.2 Discrete grid

Suppose now that the function $f(\rho, z)$ is known only on the nodes of a discrete grid. Then, the Fourier transform will be also a discrete function, approximation of the continuous transform. Let $\rho_j = \rho_0 + j\Delta\rho$, $j = 0, 1, \dots, M - 1$ and $z_k = z_0 + k\Delta z$, $k = 0, 1, \dots, N - 1$ be the points (uniformly spaced) defining the grid for which $f(\rho_j, z_k)$ are given. The function $f(\rho, z)$ is supposed to be zero or negligible for $\rho > \rho_{M-1}$, $z < z_0$ and $z > z_{N-1}$. The Fourier transform will be also calculated on a grid with the mesh points R_m, Z_n . For any R_m from the discrete grid, let us consider the integral:

$$H(R_m, z) = 2\pi \int_0^\infty f(\rho, z) J_0(2\pi\rho R_m) \rho d\rho \quad (3)$$

For a position $z = z_k$, since f is negligible beyond ρ_{M-1} , one has

$$H(R_m, z) \approx 2\pi \int_{\rho_0}^{\rho_{M-1}} f(\rho, z) J_0(2\pi\rho R_m) \rho d\rho.$$

The integral on the interval $[\rho_0, \rho_{M-1}]$ is represented as a sum of integrals on subintervals of the size $2\Delta\rho$. To approximate these partial integrals we have deduced a quadrature formula (see [3]) whose coefficients are expressed in terms of Bessel and Struve functions [4] of order 0 and 1.

Let us now consider the integral:

$$F(R_m, Z) = \int_{-\infty}^\infty H(R_m, z) e^{-2\pi izZ} dz. \quad (4)$$

The variable Z takes a set of N values defined as

$$Z_n = \frac{n - N/2}{N\Delta z}, \quad n = 0, 1, \dots, N - 1.$$

The value of $F(R_m, Z_n)$ is approximated by using the Fast Fourier Transform - FFT [5]. In conclusion, the values $F(R_m, Z_n)$, representing the Discrete Fourier Transform in cylindrical coordinates, are obtained by the discrete Hankel (ρ -axis) and Fourier transforms (z -axis).

4.3 Application to the scission neutrons

We apply the Fourier transform of single particle wave functions in cylindrical coordinates to the study of neutrons released during scission. The neutron wave packets are

propagated through the bi-dimensional time dependent Schrödinger equation (TDSE) with time dependent potential (TDP):

$$i\hbar\frac{\partial\Psi(\rho, z, t)}{\partial t} = \mathcal{H}(\rho, z, t)\Psi(\rho, z, t), \quad (5)$$

$$\mathcal{H}\Psi = \begin{bmatrix} O_1 - CS_c & -CS_a \\ -CS_b & O_2 - CS_d \end{bmatrix} \begin{bmatrix} f^{(1)} \\ f^{(2)} \end{bmatrix}, \quad O_{1,2} = -\frac{\hbar^2}{2\mu}\left(\Delta - \frac{\Lambda_{1,2}^2}{\rho^2}\right) + V(\rho, z, t). \quad (6)$$

Δ is the Laplacean, V is the potential, C is a constant and the operators S_a, \dots, S_d represent the spin-orbit coupling. We use a realistic mean field potential of Woods-Saxon type adapted to nuclear shapes described by generalized Cassini ovals [6]. The wave functions have two components corresponding to spin “up” and spin “down”. For a given projection Ω of the total angular momentum on the symmetry axis they assume the form:

$$|\Psi\rangle = f^{(1)}(\rho, z)e^{i\Lambda_1\theta}|\uparrow\rangle + f^{(2)}(\rho, z)e^{i\Lambda_2\theta}|\downarrow\rangle, \quad \Lambda_1 = \Omega - \frac{1}{2}, \quad \Lambda_2 = \Omega + \frac{1}{2}. \quad (7)$$

Due to the axial symmetry, only the coordinates ρ and z remain.

4.3.1 Dynamical Scission Model

According to the Dynamical Scission Model [1], [2], we separate the calculation in two stages:

1)The scission process itself, i.e., the neck rupture and its absorption by the fragments. The corresponding nuclear configurations are defined by two sets of deformations: $\{\alpha^i\}$ (just before scission) and $\{\alpha^f\}$ (immediately after scission). The duration of this stage is relatively short ($\Delta T \approx 10^{-22}$ sec) and therefore the potential in which the neutrons move changes rapidly.

2)The detachment from the fragments of the fraction of the neutrons that are left unbound at the end of the previous stage. Since, at this stage, their motion is much faster than that of the just separated fragments we maintain the fragments at the configuration $\{\alpha^f\}$ and therefore keep the potential constant during the subsequent propagation in time.

In the 1st stage we follow the time evolution of the wave functions corresponding to each neutron state that is occupied at $\{\alpha^i\}$. At each time step the nuclear shape and the potential is changing as the deformation parameter set varies uniformly from $\{\alpha^i\}$ to $\{\alpha^f\}$. The initial wavefunctions (at $t = 0$) are taken as eigensolutions of the eigenvalue problem: $\mathcal{H}\Psi = E\Psi$. To solve it, the infinite physical domain is replaced by a finite one, which is discretized on a grid with the mesh points ρ_j and z_k . At each point the partial derivatives in \mathcal{H} are approximated by finite difference formulas [7]. The eigenvalue problem is transformed into an algebraic eigenvalue problem with a large sparse matrix, which is solved by an appropriate method (Arnoldi) [8]. The propagation

in time is performed by a numerical scheme of Crank-Nicolson type [9]. At the end of this stage we calculate quantities like:

- The probability that a neutron occupying the state $|\Psi^i\rangle$ before scission populates a state $|\Psi^f\rangle$:

$$a_{if} = \langle \Psi^i(\Delta T) | \Psi^f \rangle = 2\pi \int \int \rho \Psi^i(\Delta T) \Psi^f d\rho dz.$$

- The probability that the neutron is emitted, given by:

$$P_{em}^i = v_i^2 \left(\sum_{unbound} |a_{if}|^2 \right) = v_i^2 \left(1 - \sum_{bound} |a_{if}|^2 \right)$$

where v_i^2 are the occupation probabilities of the initial eigenstates.

- The emitted part of the wave packet:

$$|\Psi_{em}^i\rangle = |\Psi^i(\Delta T)\rangle - \sum_{bound} a_{if} |\Psi^f\rangle.$$

In the 2nd stage we follow these wave packets (that describe the unbound neutrons) in time (by TDSE with the potential fixed for the set $\{\alpha^f\}$) and calculate their FT at certain time intervals T .

4.3.2 The evolution of the emitted wave functions and of the momentum distributions; the energy spectrum

We have investigated the reaction $^{235}\text{U}(n_{th}, f)$ with the light fragment mass $A_L = 96$ (which is the most probable experimental mass asymmetry). Two parameters of the Cassini representation have been considered: α (elongation) and α_1 (mass asymmetry). We have chosen: $\alpha = 0.985$ (before scission) and $\alpha = 1.001$ (after scission). The parameter α_1 results from the condition of fixed ratio of the fragment volumes that corresponds to $A_L=96$. We have performed the Fourier transform for several wavefunctions corresponding to $\Omega = 1/2$. At each point in the (k_ρ, k_z) plane are associated an absolute value $K = \sqrt{k_\rho^2 + k_z^2}$ and a probability $P = |F(k_\rho, k_z)|^2 k_\rho \Delta k_\rho \Delta k_z$. To represent the K -distributions as histograms, we divide the domain of K -values in equal intervals and group the points according to the interval to which they belong. Summing up the probabilities of the points in each group one obtains the probability $P(K)$ that a neutron has its K -value in the respective interval. In the figures 1 and 2 are shown the emitted wavefunctions with the indices 30 and 33 (as sum of square moduli of the two components) aside with the momentum histograms at different times T . The time-dependent wavefunctions are represented relative to the function at $T = 20$, while the values on the ordinates of the histograms are the $P(K)$ probabilities multiplied by 10^2 .

As one can see, at increasing time intervals the wavefunction values are diminishing, showing that the neutron is leaving the nucleus. At the same time, the K -distributions are shrunked to lower values, reflecting the fact that the neutrons are less and less present in the potential well. At large times they tend to a gaussian shape.

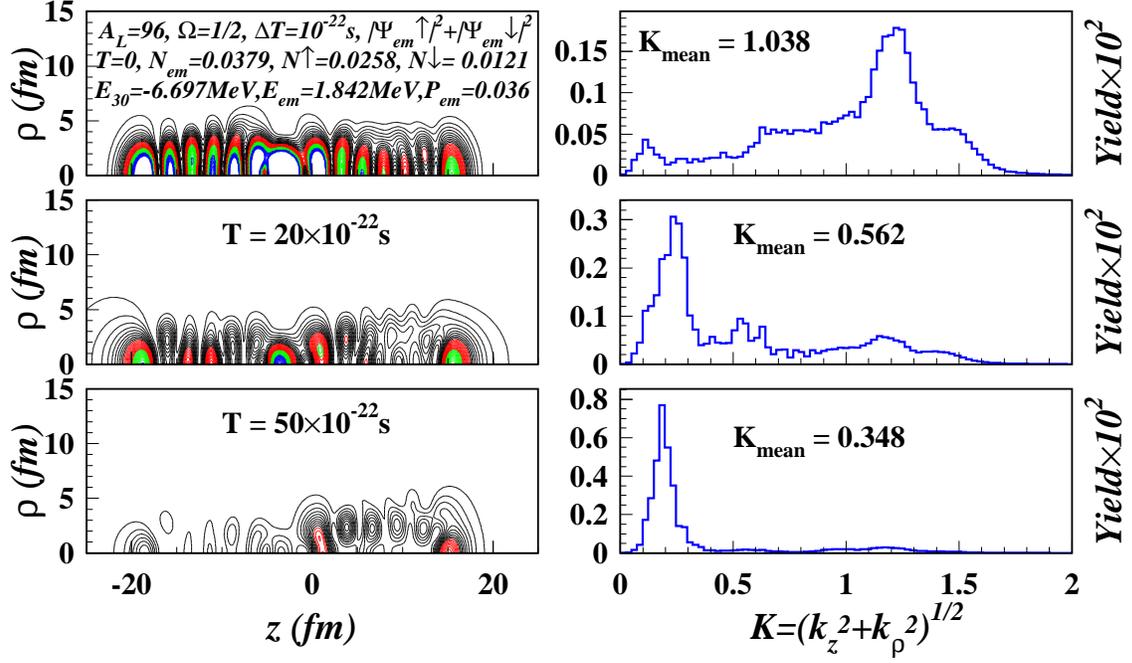


Figure 1: Square modulus of the emitted WF₃₀ and momentum distribution at different times T. N_{em} is the norm of the emitted function, N_\uparrow , N_\downarrow are the norms of the two components and $K_{\text{mean}} = \frac{\sum_{m,n} K P}{\sum_{m,n} P}$, $P = k_\rho |F|^2 dk_\rho dk_z$.

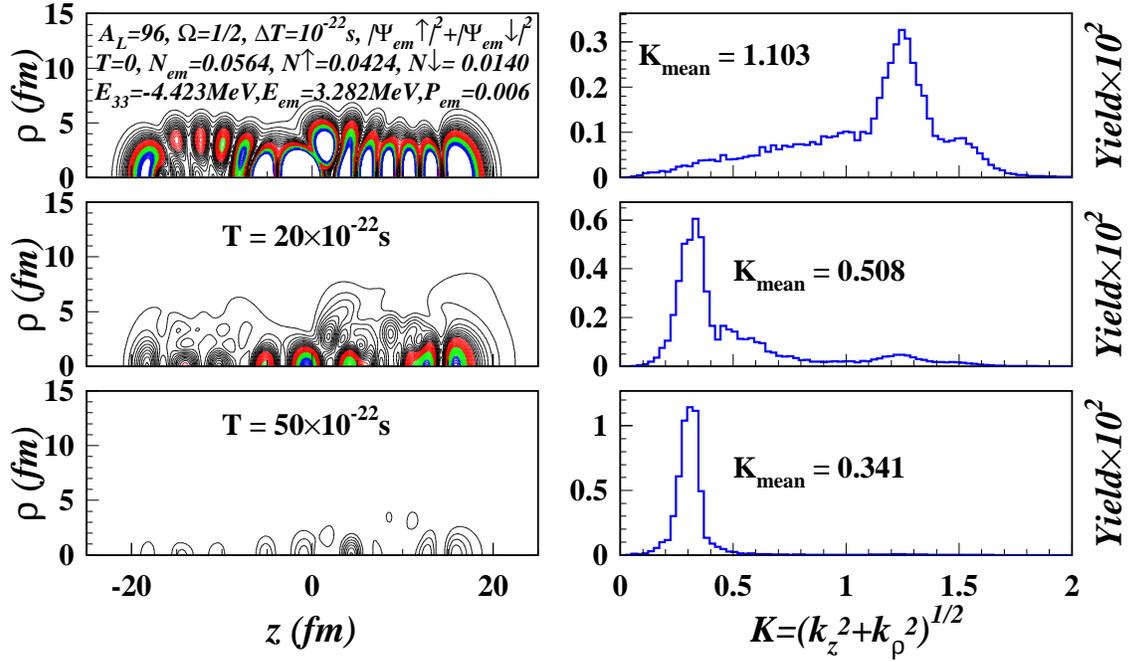


Figure 2: The same as in Fig.1 but for the emitted WF₃₃.

From the momentum distribution one can deduce the kinetic energy distribution (according to $E = \frac{\hbar^2}{2\mu} K^2$). To obtain the whole kinetic energy spectrum one has to repeat such calculations for all the states at each Ω value. Here we present results only for $\Omega=1/2$ states and from WF_{11} to WF_{41} . The states lying at the bottom of the well (WF_1 to WF_{10}) have negligible P_{em} values. Note however that $\Omega = 1/2$ gives the dominant contribution (65%).

Fig. 3 shows kinetic energy spectra for two individual states (30 and 33) around the Fermi level and the sum for all $\Omega=1/2$ states with the index above 10 (having energies greater than -23 MeV). The total spectrum presents a maximum around 0.7 MeV and an exponentially decreasing tail till 5 MeV in qualitative agreement with the measured spectrum [10] of all prompt fission neutrons (PFN). For a quantitative comparison with experimental data, states with higher Ω values ($3/2$ to $9/2$) has to be included in the calculations.

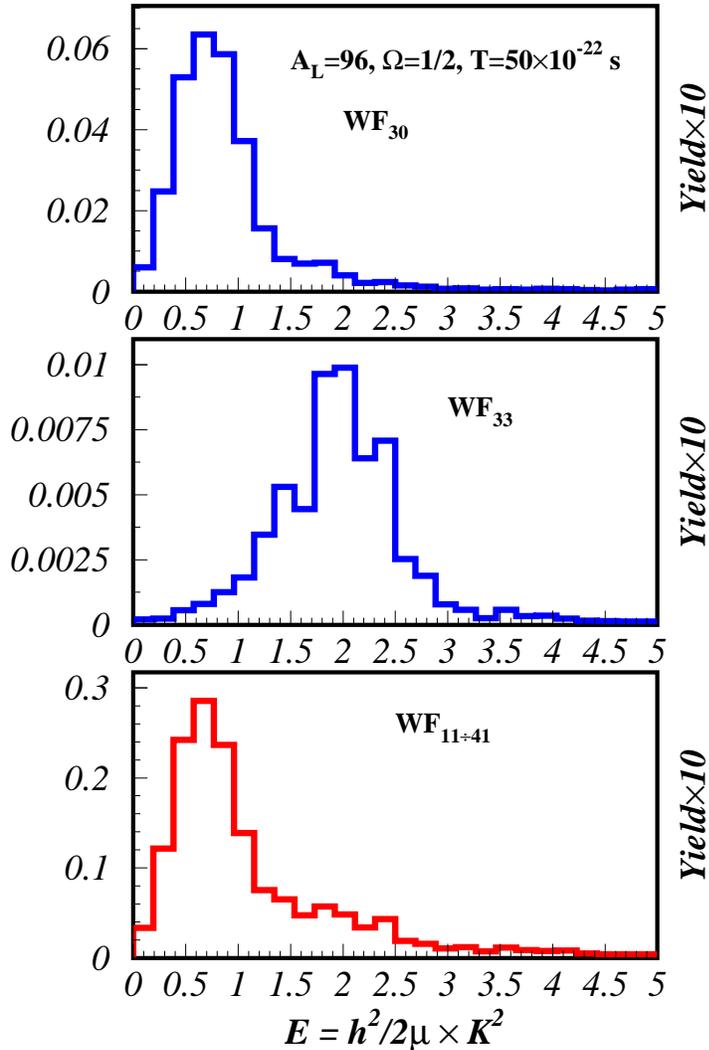


Figure 3: Energy distribution at $T = 50 \times 10^{-22}$ sec ($Yield = P(K) \times v_i^2$).

4.4 Conclusions

In this work we have presented numerical procedures to calculate the Fourier transform on wave functions given in cylindrical coordinates and applications to the study of scission neutrons. As initial functions for our procedure we have taken single-particle states in extremely deformed nuclei associated with the wave packets of the neutrons released during scission. We propagate the neutron wave packets in time through the bi-dimensional TDSE with TDP. We select $\Omega=1/2$ states and calculate their Fourier transforms at different times T and the momentum distributions corresponding to these transforms. From such distributions one can follow the separation of the neutron from the fissioning system and obtain the kinetic energy spectrum of each emitted neutron. The shape of the energy spectrum obtained summing over all emitted neutrons resembles the measured PFN spectrum. For a more accurate comparison the effect of reabsorption of the unbound neutrons by the imaginary potential has to be taken into account.

References

- [1] M. Rizea, N. Carjan, *Nuc. Phys. A* **909**, 50–68 (2013)
- [2] N. Carjan, M. Rizea, *Phys. Lett. B* **747**, 178–181 (2015)
- [3] M. Rizea, N. Carjan, *Eur. Phys. J. A* **52**, 368 (2016)
- [4] M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions*, (8th ed., Dover, New York, 1972) 358, 496
- [5] W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling, *Numerical Recipes* (Cambridge Univ. Press, 1996) 451–453
- [6] V.V. Pashkevich, *Nucl. Phys. A* **169**, 275–293 (1971)
- [7] M. Rizea, V. Ledoux, M. Van Daele, G. Vanden Berghe, N. Carjan, *Comp. Phys. Commun.* **179**, 466–478 (2008)
- [8] R. B. Lehoucq, D. C. Sorensen, C. Yang, *ARPACK Users Guide* (Philadelphia, SIAM, ISBN 978-0-89871-407-4, 1998)
- [9] M. Rizea, N. Carjan, *Proc. Rom. Acad. A* **16**, 176–183 (2015)
- [10] N. Kornilov, F.-J. Hamsch et al., *Nucl. Sci. Eng.* **165**, 117–127 (2010).