Computational Study of Scission Neutrons in Low-Energy Fission: Stationary and Time-Dependent Approaches

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Abstract. The emission of scission neutrons from fissioning nuclei is of high practical interest. To study this process we have used the sudden approximation and also a more realistic approach that takes into account the scission dynamics. Numerically, this implies the solution of the bi-dimensional Schrödinger equation, both stationary and time-dependent. To describe axially symmetric extremely deformed nuclear shapes, we have used the Cassini parametrization. The Hamiltonian is discretized by using finite difference approximations of the derivatives. The main computational challenges are the solution of algebraic eigenvalue problems and of linear systems with large sparse matrices. We have employed appropriate procedures (Arnoldi and bi-conjugate gradients). The numerical solutions have been used to evaluate physical quantities, like the number of emitted neutrons per scission event, the primary fragments' excitation energy and the distribution of the emission points.

1 Introduction

During the last years, there has been an increasing interest in the simulation of fundamental processes in quantum systems by numerical methods. In this context, the solution of the Schrödinger equation plays a major role in the investigation of phenomena

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like nuclear fission and fusion, atomic and nuclear collisions, laser-atom interaction. In the present paper we focus on the scission neutrons, subject of present interest, important for nuclear applications. Among the neutrons emitted during fission, one can distinguish chronologically three categories: the scission neutrons (10^{-21}-10^{-20} s), the prompt neutrons (10^{-18}-10^{-16} s) and the delayed neutrons ($> 10^{-16}$ s). The last two components form the large majority of fission neutrons and have been extensively studied. The scission neutrons were less investigated, but are recently receiving an increasing attention. Estimated to represent 10-30% of the total number of neutrons, this kind of neutrons are considered responsible for important effects observed in the fission process (see [1–7]) and are essential ingredients in numerical reactor simulations. One possible approach to study the emission of scission neutrons is the sudden approximation [8]. This implies the numerical solution of an eigenvalue problem associated to the bi-dimensional stationary Schrödinger equation for independent neutrons in axially symmetric extremely deformed nuclear shapes. We have used a grid-based procedure, in which the equation is discretized by finite difference approximations of the derivatives. We are led to an algebraic eigenvalue problem with large (sparse) matrix, which is solved by the Implicitly Restarted Method of Arnoldi. In the sudden approximation the scission is seen as a sudden transition between two different nuclear configurations. By calculating the bound state wavefunctions just-before-scission (ϵ_i) and immediately-after-scission (ϵ_f), one can evaluate physical quantities like: the number of scission neutrons per fission event and the excitation energy of primary fission fragments. An alternative approach is to consider the last stage of the fission process as a time dependent fast (diabatic) process. By solving the bi-dimensional time-dependent Schrödinger equation (TDSE) with a potential variable in time between ϵ_i and ϵ_f, one can study the scission process in a more realistic model. The numerical solution of TDSE is obtained by a Crank-Nicolson scheme, which requires the solution of large sparse linear systems that was obtained by a variant of the bi-conjugate gradient method. Transparent Boundary Conditions have been implemented, to avoid reflexions on the numerical boundaries.

A similar time-dependent approach was applied in [9] to a different sequence of nuclear shapes during fission, namely to the descent of the fissioning nucleus from the saddle point to the scission point. The numerical calculation capabilities being quite limited at that time, the authors had to neglect the spin-orbit coupling, use a non-diffuse nuclear potential (square well) and a much smaller spatio-temporal grid.

In the following we present some details on the physical problem, on the mathematical model and on the numerical procedures. Also, some results in a definite case will be shown.

2   The bi-dimensional Schrödinger equation

To obtain the bound states, one has to solve the eigenvalue problem:

$$\mathcal{H}\Psi = E\Psi, \tag{2.1}$$