EPJ Web of Conferences **322**, 07002 (2025) https://doi.org/10.1051/epjconf/202532207002
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Non-Equilibrium Aspects of Fission Dynamics within the Time Dependent Density Functional Theory

Aurel Bulgac[1,*], *Matthew* Kafker[1], *Ibrahim* Abdurrahman[2], and *Ionel* Stetcu[2]

[1]Department of Physics, University of Washington, Seattle, WA 98195, USA
[2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Abstract. We will cover briefly the time-dependent density functional theory approach, extended to include pairing correlations, to induced fission of ^{238}U(n,f), ^{241,243}Pu, and ^{238}Np, and also results on scission neutrons and a number of very nontrivial aspects of induced fission.

1 Introduction

For all results reported here we performed extensive fully microscopic studies of fission dynamics within the time-dependent density functional theory (TDDFT) extended to include pairing correlations, with controlled numerical approximations and without introducing any unchecked assumptions or simplifications. The theoretical framework is described and was reviewed in great detail in Refs. [1–3] and the corresponding codes are accessible on GitHub.

2 Induced fission of odd-mass and odd-odd nuclei

We performed studies of the induced fission dynamics of nuclei with either odd number of neutrons for the compound fission systems ^{238}U(n,f) [23 trajectories], ^{240}Pu(n,f) [42 trajectories], ^{242}Pu(n,f) [7 trajectories], and with both odd proton and neutron numbers for ^{237}Np(n,f) [48 trajectories], where in each case the number of trajectories describe various initial nuclear shape deformations characterized by quadrupole and octupole momenta (Q_{20}, Q_{30}) near the outer fission barrier and various odd quasiparticle states of the respective fissioning compound nucleus, constructed using the standard prescription outlined in Refs. [4–7]. In addition, for comparison, we have performed additional calculations also for the induced fission of ^{235}U(n,f) [24 trajectories], ^{239}Pu(n,f) [7 trajectories] and for the odd nucleon systems ^{237}Np(n,f) [11 trajectories], ^{238}U(n,f) [6 trajectories], ^{240}Pu(n,f) [13 trajectories], and ^{242}Pu(n,f) [2 trajectories], treating them as even-even nuclei for a total of 63 trajectories. The total 121+63 = 184 TDDFT trajectories for these nuclei is comparable (or maybe even bigger) with perhaps of all of the rest of the world TDDFT fission trajectories obtained for even-even nuclei by other authors since 2015, see review talk of D. Vretenar for some references. The simulations have been performed in a simulation box $30^2 \times 60$ fm^3 with a lattice constant of 1 fm and following the dynamics for up to about 30,000 to 60,000 times steps or longer in some cases. These simulations were performed with the energy density functional SeaLL1 [3] by evolving $2\times 2\times 4\times 30^2\times 60 = 864,000$ complex, coupled, nonlinear PDEs in 3D+time, see Refs [1–3, 8–11] for details. This proves that inspite of the complexity of these simulations, using a total number of quasiparticle states $2\times 2\times 30^2\times 60 = 216,000$, such simulations can be performed on a large variety of supercomputers available worldwide nowadays. Detailed extensive results of these simulations will be submitted for publication soon.

Ever since the development of a microscopic description of pairing correlations by Bardeen *et al.* [12] and the recognition that they are also most likely crucial in explaining nuclear properties [13], the treatments of fermion systems with odd numbers of particles have relied on the so called Pauli blocking approximation. The extra odd nucleon carries a non-vanishing angular momentum and as a result the nuclear mean field breaks time-reversal invariance. The compound nucleus breaks the gauge symmetry as well and has a negative particle parity. The rotational symmetry and sometimes spatial parity are also broken. From the theoretical point of view these are rather inconvenient features, resulting in a significant number of technical difficulties, and which forced most theoretical treatments to adopt approximations and assumptions. In nuclear large amplitude collective motion the Pauli blocking approximation has been used almost always, see the most recent and detailed studies of the fission of odd-mass nuclei, where Pauli blocking in conjunction along with the equal filling approximation [14] have been implemented [6, 7].

Overall the FF properties in the induced fission of even-even, odd-mass, and odd-odd nuclei are very similar, but the widths of total kinetic energy, FF neutron and charge distributions are typically twice as large as in the case of induced fission of even-even nuclei. Often there is a difference in the times the two FFs reach scission, when

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[*] e-mail: bulgac@uw.edu

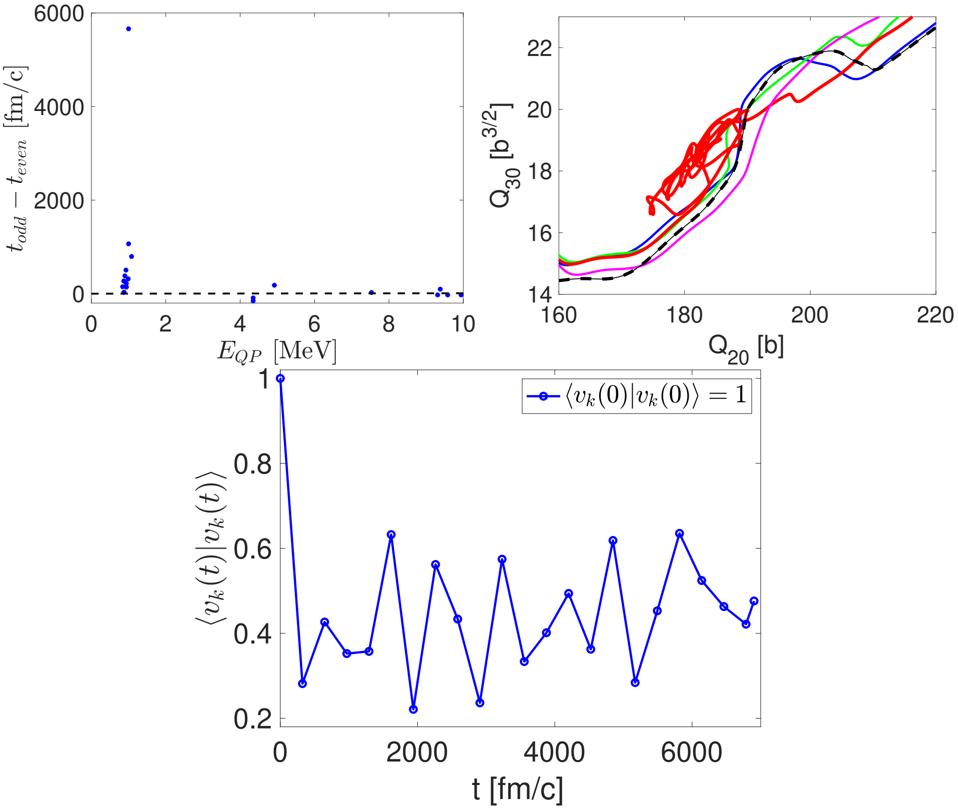

Figure 1. In the upper row left panel we display the time difference to full spatial separation of the two fission fragments (FFs) between the case of an even-even and odd-mass nuclei. The odd-mass system is treated with an exact odd-neutron and even-proton numbers respectively. The odd-mass nucleus is treated as having an even-neutron and an even-proton numbers, with the average $N = 147$ and $Z = 92$ respectively for ^{239}U and then a quasiparticle state is excited as described in Refs. [4, 5]. In the upper row right panel we show several TDDFT trajectories for the fission of an odd-nucleon nucleus with solid lines and for reference a TDDFT trajectory for an even-even nucleus with average $N = 147$ and $Z = 92$, with a dashed-thin solid line. Unlike the TDDFT trajectories, in which typically the quadrupole moment Q_{20} typically increases in time in the case of fission of odd-nucleon systems the nucleus encounters a "bumpier" potential energy surface in the (Q_{20}, Q_{30}) plane towards scission and the system it gets "confused" following a much more "challenging obstacle course," see upper row right panel. In the second row we show the occupation probability of the initial odd-nucleon state as a function of time. For time $t = 0$ the occupation probability was obtained by constructing the corresponding canonical occupation probabilities [10]. For $t > 0$ apart from one canonical quasiparticle state with occupation probability 1, the rest of the quasiparticle states are all double occupied with probabilities less than 1.

the corresponding initial quasiparticle state has a relatively low excitation energy, typically smaller than the pairing gap, see Fig. 1. In that case the TDDFT trajectory is significantly more complicated as the system spends quite a lot of time "deciding"' which path to follow on the potential energy surface. Such a situation has been encountered for some almost symmetric TDDFT trajectories [8, 9] in the case of fission even-even compound nuclei.

An unexpected feature is the violation of the Pauli blocking approximation, see Fig. 1, used for more than 6 decades in nuclear physics. During the time evolution, as was demonstrated in Ref. [11], even if the system is started in a fully canonical basis, in the subsequent time evolution the quasiparticle states are not anymore canonical states, and at each time step one has to identify the new canonical set of wave functions. One can clearly see that the single odd quasiparticle state initially occupied with probability 1 in canonical basis, ceases to maintain the same occupation probability. However, at each time $t > 00$ there is only one canonical state occupied with exactly probability 1. We expect that this is a feature to be observed in any nuclear Large Amplitude Collective Motion (LACM) of an odd fermion system, in either excited states of a nucleus or in heavy-ion collisions. A clear example when such a situation is encountered is when the angular momentum of the initial odd fermion is $\approx A^{1/3}$, since such a state cannot exist with a significant occupation probability in either FF [8, 9, 15, 16].

3 Scission neutrons and nontrivial aspects of fission dynamics revealed in TDDFT framework

The scission neutrons have been conjectured to exist by Bohr and Wheeler [17] and more than 50 years after discovery of nuclear fission Wagemans [18] stated (see his introductory remarks) that they most likely do not exist. Wagemans's remarks are notable in another respect also, he never refers to Meitner and Frisch breakthrough paper [19] and instead gives all the credit to Bohr and Wheeler [17] for explaining the nature of nuclear fission, even though Bohr and Wheeler refer to Meitner and Frisch in their paper and even the name nuclear fission was coined by Meitner and Frisch. The experimental search and various theoretical models predicted the existence of scission neutrons with contradicting conclusions and properties in the following years, as either dominating the number of emitted neutrons by fission fragments (FFs) or being almost absent. In a very recent paper [20] we have reported the results of our most comprehensive theoretical analysis of scission neutrons within the Time-Dependent Density Functional Theory (TDDFT) extended to superfluid fermionic systems and predicted an extensive range of their properties. We invite the reader to consult this publication [20], including the quite extensive supplement.

In recent publications [10, 11] we have presented several new aspects of the fission process, which were never discussed in literature. We have demonstrated that the fission dynamics from saddle-to-scission has an intrinsically non-Markovian character and consequently various previous attempts to describe this process using various stochastic or kinetic approaches are inadequate. Moreover, since in nuclear LACM the occupation probabilities of single-particle states with large momenta have very long tails $\propto C/p^4$, where p is the local single-particle momentum, a significant repopulation of the quasiparticle states occurs during the fission dynamics and theoretical modeling with a reduced basis set of single-particle states, such as (TD)BCS+TDHF or even TDDFT with a limited number of quasiparticle states lead to inaccurate predictions of the FFs properties, or even fail to lead to fission.

4 Conclusions

TDDFT, extended to include a correct description of the dynamics of the pairing correlations, is arguably the most advanced microscopic quantum tool available today, and it is based on solid independent knowledge of basic nuclear properties of nuclei with $A \geq 16$. In this approach only 7 parameters well known for a long time are needed: energy and equilibrium density of symmetric nuclear matter, surface tension, symmetry energy and its density dependence, spin-orbit and pairing strengths), and this leads to a one of the most accurate descriptions of the binding energies, charge radii, one- and two-neutron separation energies, single-particle spectra of magic nuclei, etc., see Ref. [3], and it is used in TDDFT to describe fission dynamics. We described briefly several recent developments in a fully microscopic description of fission dynamics. i) The TDDFT approach to the emission of scission neutrons, a topic still not settled either theoretically or experimentally, was conjectured in 1939 [17] soon after nuclear fission explanation of fission [19]. ii) The non-Markovian aspects of the fission descent, which is distinct from the earlier demonstrated clear dissipative character of fission dynamics. iii) A first peak to some of our preliminary results from the first TDDFT treatment of the induced fission of a large class of odd nucleon compound nuclei. A overall arching conclusion emerges from these studies: fission dynamics is an intrinsically non-equilibrium process, which requires a detailed time-dependent microscopic description, without the inclusion of unchecked assumptions, phenomenology and parameter fitting, and uncontrolled approximations and simplifications.

Acknowledgement

The funding for A.B. and M.K. from the Office of Science, Grant No. DE-FG02-97ER41014 and also the partial support provided by NNSA cooperative Agreement DE-NA0003841 is greatly appreciated. The work of I.A. and I.S. was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. The Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy Contract No. 89233218CNA000001. This research used resources of the Oak Ridge Leadership Computing Facility, which is a U.S. DOE Office of Science User Facility supported under Contract No. DE-AC05-00OR22725.

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