Superfluidity is a generic feature of various quantum systems at low temperatures and it is in particular important for the description of dynamics of low energy nuclear reactions. The Time-Dependent Density Functional Theory (TDDFT) is, to date, the only microscopic method which takes into account in a consistent way far-from-equilibrium dynamics of pairing field and single-particle degrees of freedom. The local version of TDDFT, so-called TDSLDA, is particularly useful for the description of nuclear reactions and is well-suited for leadership class computers of hybrid (CPU+GPU) architecture. The preliminary results obtained for collisions involving both medium-mass and heavy nuclei at the energies around the Coulomb barrier are presented.

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1. Introduction

The Time-Dependent Superfluid Local Density Approximation (TDSLDA) is a versatile tool to investigate a variety of phenomena involving superfluidity in Fermi systems including atomic nuclei. TDSLDA originates from time-dependent density functional theory, which become nowadays a standard theoretical tool for studies of interacting many-body Fermi systems and offers a universal approach to the quantum many-body dynamics (see Refs. [1–3] and references therein). The superfluid extension of TDDFT has been triggered by the discovery of high-temperature superconductivity and resulted in the creation of nonlocal TDDFT for superconductors [4, 5]. It has been possible, however, to formulate the problem using local pairing

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field [6]. The justification for the so-called SLDA (Superfluid Local Density Approximation) has been developed in a series of papers (see, e.g., a review [7] and references therein) and it has been shown to be very accurate for nuclei and cold atomic gases [8, 9]. The recent studies of various low-energy nuclear reactions and in particular induced fission [10–15] has proved that the TDSLDA is capable of describing nuclear processes, where pairing correlations play a crucial role.

In the following, we will present selected aspects of superfluid dynamics in low-energy nuclear reactions. We consider two particular cases associated with two different types of collisions. In the first one, we will consider a mass-symmetric collision of superfluid nuclei which have different phases of the pairing field, giving rise to solitonic excitation between two colliding nuclei. The second example concerns collisions of a light and a heavy superfluid nuclei, and is oriented towards investigation of an effect of superfluidity on the quasi-fission process in reactions leading to the formation of superheavy elements (SHEs).

2. Computation background

There are a variety of computational methods to approximate the static solution of TDSLDA. They usually involve a number of diagonalizations of the Hamiltonian matrix, which is a quite computationally demanding task as the size of the matrix is of the order of the lattice size. The one employed in this work is known as the Conjugate-Orthogonal Conjugate-Gradient (COCG) method (see Ref. [16] for a detailed description). Its main advantage is that it does not require diagonalizations during the iteration process, namely, both normal and anomalous densities are constructed through evaluation of Green’s function of the problem.

The typical procedure applied in the context of the presented studies is the following:

1. Two nuclei are placed inside a box, symmetrically at the relative distance of 40 fm, and an external potential $V_{\text{ext}}(r) \approx V_0|x|$ which generates constant force pointing towards center of the box $x = 0$ is used to counteract the Coulomb repulsion. The grid spacing is 1.25 fm in all directions, and the box size is $80 \times 25 \times 25$ fm$^3$.

2. Self-consistent iterations are executed using COCG code [16], and the density solution found is inputted into a diagonalisation code in order to extract the quasi-particle wave functions.

3. The wave functions are then evolved solving TDSLDA equations, which are formally equivalent to the time-dependent Hartree–Fock–Bogoliubov equations (see Ref. [8] for a review).
For a thorough description of this process, the reader is directed towards the supplementary material of Ref. [13]. In this work, the full Skyrme functional (SLy4) is used, including the spin-orbit term.

3. Nuclear collisions within TDSLDA

Nuclear collisions simulated within the TDSLDA framework take into account dynamics of both single-particle and pairing degrees of freedom during the collision process [17]. The pairing field is a complex field and, therefore, its excitations consist both of variations of the magnitude and the phase, \( i.e. \Delta(r,t) = |\Delta(r,t)|e^{i\phi(r,t)} \). In particular, the combination of both the phase and magnitude variations may lead to a long-lived solitonic excitations observed in superfluid systems [18] and also predicted recently in the case of nuclear collisions [13].

This section will now provide a mainly qualitative summary of the results of our investigations to date. It is split into two subsections. In one subsection, we discuss the results obtained for solitonic excitations, and in the other one, we discuss pairing dynamics in the context of quasi-fission.

3.1. Solitonic excitations

Collisions of two superfluid nuclei may differ not only by the magnitude of the pairing gap but also by the phase. The latter quantity is not controlled in nuclear systems but may lead to observable effects [13, 19]. Namely, a nonzero phase difference creates a long-lived solitonic structure between colliding nuclei, where part of the kinetic energy is stored. This in turn creates an additional barrier for fusion which a projectile needs to overcome. In order to investigate possible consequences of this effect, medium mass-symmetric collisions are considered. In this process, the magnitude of pairing field of both nuclei is the same and the only effect comes from the pairing phase difference. Therefore, the mass-symmetric head-on collisions of \(^{90}\text{Zr} + ^{90}\text{Zr}\) and \(^{96}\text{Zr} + ^{96}\text{Zr}\) were investigated within the TDSLDA framework, with the goal of determining the change of the barrier height for capture as a function of the relative phase difference \(\Delta\phi\) between colliding nuclei. By comparing \(^{90}\text{Zr} + ^{90}\text{Zr}\) (zero pairing gap) to \(^{96}\text{Zr} + ^{96}\text{Zr}\) (\(\approx 1\) MeV pairing gap), one may deduce the magnitude of this increase relative to the magnitude of the pairing gap. The previously reported results in Ref. [13] were performed with the Fayans functional without the spin-orbit term. In the present work, the full SLy4 functional has been applied. The timescale under which it was checked whether nuclei split was approximately \(10^4\) fm/c. It is observed that \(^{90}\text{Zr} + ^{96}\text{Zr}\) collisions indeed produce the gauge-angle-dependent barrier for capture, confirming the earlier results. Consequently, the effective barrier for capture in \(^{96}\text{Zr} + ^{96}\text{Zr}\) is enhanced as
compared to $^{90}\text{Zr} + ^{90}\text{Zr}$, where no effect is observed. The SLy4 functional produces weaker enhancement of the barrier compared to the value reported in Ref. [13], in agreement with empirical analysis of Ref. [20]. The reduction is suspected to be due to that when the spin-orbit interaction is not included, there is no spin-orbit splitting, and pairing is likely stronger, due to higher degeneracies of single-particle levels. The details of this study will be reported elsewhere.

3.2. Mass-asymmetric collisions

The mass-asymmetric collisions of $^{48}\text{Ca} + ^{252}\text{Cf}$ and $^{50}\text{Ti} + ^{252}\text{Cf}$ offer the possibility to investigate the influence of pairing on the mechanism of the formation of SHEs. Here, we report preliminary results concerning tip collisions within the CM energy range of 200–300 MeV for $^{48}\text{Ca} + ^{252}\text{Cf}$, and 220–300 MeV for $^{50}\text{Ti} + ^{252}\text{Cf}$. Notice that the projectile $^{48}\text{Ca}$ is essentially in a normal state, while $^{252}\text{Cf}$ possess nonzero pairing gap for both protons and neutrons. The projectile $^{50}\text{Ti}$ possess a nonzero proton pairing. Therefore, these two reactions represent interesting cases to investigate the collision of normal and superfluid systems and to compare it to the case of superfluid on superfluid collisions.

From the results, we found the heavy fragment to be close to a doubly-magic nucleus, regardless of the nuclei involved in the collision and energy. Although the split was similar in terms of proton and neutron numbers, it was generally found that the contact time of the two nuclei was several $1000\, \text{fm}/\text{c}$ longer for $^{48}\text{Ca} + ^{252}\text{Cf}$. This occurs when the amount of kinetic energy that the heavy fragment carries away is noticeably smaller (5–10 MeV). Visually comparing the collisions of $^{48}\text{Ca} + ^{252}\text{Cf}$ (Fig. 1) and $^{50}\text{Ti} + ^{252}\text{Cf}$ (not shown), it appears that the resultant nucleus is more elongated for $^{48}\text{Ca} + ^{252}\text{Cf}$ before fissioning. The larger elongation should reduce the magnitude of the Coulomb repulsion between the fragments, thereby reducing their kinetic energies after fission.

Comparing the contact times for the two cases to similar collisions in TDHF calculations, it is found that the contact time is approximately 2–3 times longer for TDSLDA. The important effect of the $^{48}\text{Ca} + ^{252}\text{Cf}$ collision consists of the pairing transfer from the superfluid heavy nucleus to the initially-normal light projectile. Such an effect is surprising at first sight as it corresponds to inducing pairing correlations in the system which is heated up due to collision and is otherwise in the normal state. However, one needs to take into account that a nucleus is in a nonequilibrium state. Moreover, the pairing properties in the nuclear system depends on the level density at the Fermi surface, which may be changed at finite excitation energy and thus allow for pairing correlations to set in. A similar effect known as “pairing reentrance” has been predicted in hot rotating atomic nuclei [21, 22].
Fig. 1. Snapshots before ($t = 0$ fm/c, left) and after ($t \approx 10200$ fm/c, right) a tip collision of $^{48}\text{Ca} + ^{252}\text{Cf}$. The centre-of-mass energy in this example is 230 MeV.

4. Conclusion

$^{48}\text{Ca} + ^{252}\text{Cf}$ and $^{50}\text{Ti} + ^{252}\text{Cf}$ collisions were performed within the TD-SLDA framework, and reaction dynamics were compared to investigate the quasi-fission process. It was found that contact times for $^{48}\text{Ca} + ^{252}\text{Cf}$ were generally significantly longer than that obtained for $^{50}\text{Ti} + ^{252}\text{Cf}$. This coincided with a reduction in the kinetic energy after collision for $^{48}\text{Ca} + ^{252}\text{Cf}$. It was also observed that the superfluidity is transferred to the initially-normal projectile $^{48}\text{Ca}$ as a result of nonequilibrium single-particle and pairing field dynamics. In the future, we plan to reperform the same calculations but with a different orientations of the $^{252}\text{Cf}$ nucleus.

$^{90}\text{Zr} + ^{90}\text{Zr}$ and $^{96}\text{Zr} + ^{96}\text{Zr}$ collisions were also compared to see how a solitonic excitation created between the two fragments would affect the fusion threshold energy. By creating a $\pi$ phase difference between the two superfluid nuclei, it was found that this threshold increased by 5 MeV for $^{96}\text{Zr} + ^{96}\text{Zr}$ compared to no phase difference, but no increase was found for $^{90}\text{Zr} + ^{90}\text{Zr}$. In the future, we plan to reperform the calculations with a larger pairing gap. Finally, we plan to determine whether the analysis presented in this paper is independent of the functional being used.

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