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LIST OF ACRONYMS AND ABBREVIATIONS

HF	Hartree-Fock
BCS	Bardeen Cooper Schieffer
HF-BCS	Hartree-Fock- Bardeen Cooper Schrieffer
HFB	Hartree-Fock-Bogolyubov
TDHF	Time-Dependent Hartree-Fock
EDF	Energy-density functional
RPA	Random-Phase Approximation
QRPA	Quasi-particle Random-Phase Approximation
EOS	Equation Of State

Executive Summary

This deliverable report describes the status of the development and validation of two codes dedicated to the description of small and large amplitude collective motion in atomic nuclei. A first code, called Quasi-Particle Random-Phase Approximation (QRPA), has been developed to describe collective excitations in open-shell nuclei opening new perspectives. A time-dependent version of this theory, called Time-Dependent Hartree-Fock + BCS (TDHF+BCS), allowing to describe consistently small and large amplitude nuclear dynamics was also further developed and finalised. The two computer packages have been finalised during the ENSAR2 period. Results of the two approaches, which are *a priori* equivalent in the case of small amplitude collective vibrations, have been compared successfully with each other.

Introduction

During the four years of the project, the members of the TheoS JRA have continuously worked on the QRPA and TDHF+BCS package with the aim of improving the codes and preparing a version that could be released to the worldwide scientific low-energy nuclear physics community. A summary of the progresses made as well as the status of the deliverable D11.4 is given below.

Section 1: QRPA theory and code for the description of small amplitude collective vibration in atomic nuclei

The Milano node of the TheoS JRA has a strong expertise in mean-field and DFT models, as testified by review articles as well as lectures in addition to articles in peer-reviewed journals. In particular, the group has had a strong focus on the calculation of excitations within small-amplitude, fully self-consistent formalisms. Among these excitations, we should point out collective modes like giant resonances as the most relevant ones. We should also point out that this focus on giant resonances is motivated by their importance also for the study of the nuclear equation of state (EOS). As is well known, only self-consistent RPA allows connecting, so far, the isoscalar monopole resonances with the nuclear incompressibility or the dipole resonances with the density-dependence of the symmetry energy.

One of the outcomes of this long-standing activity has been the publication, back in 2013, of the Random-Phase Approximation (RPA) code [1]. This code is the evolution of codes that were already developed in the 1980s and 1990s. However, the efforts carried out in the first decade of this century have allowed to remove all approximations that were still existing and were affecting the accuracy of the results. This code has been downloaded and quoted by many groups, including nuclear theorists, experimentalists, and recently also atomic physicists (in the arXiv paper 2002:02227v2 [physics.atom-ph]. The code has been used to calculate finite nuclear size effects on atomic energy levels and the bound-electron g-factor). How this code has been used as a benchmark to compare with TDHF is described in Section 3 of this report.

This RPA code employs Skyrme-type effective interactions or energy functionals. These have been quite successful during the last decades in describing bulk nuclear properties.

The main limitation of the RPA code is that it is limited to spherical systems and to closed shells. One of the objectives of the ENSAR2 project was the delivering of a new code that can overcome at least one of these shortcomings. QRPA can be applied to open-shell nuclei and we had planned to deliver the spherical QRPA code. This is an extension of the RPA code, which includes the pairing interaction between neutrons or protons. The code treats this interaction self-consistently, in the very same manner as the RPA code is fully self-consistent in the so-called mean-field channel. It can start from either a HF-BCS or HFB description of the nuclear ground state. It has to be noted that many ground-state codes of this type (mainly HFB) are available to the general users, but this is not the case for QRPA with Skyrme interactions.

At present, the code is fully tested. It has been used for calculations of the low-lying dipole and quadrupole strengths (see, e.g., Ref. [2]) or as a basis for calculations beyond the mean field [3]. The present activity is focused on improving the readability and user-interface of the code. Within the ENSAR2 timeline, we expect to distribute the code by making it available on the web page of the project. We envisage the publication in a specialised journal at a slightly later time.

SECTION 2: TDHF-BCS THEORY AND CODE TO DESCRIBE NUCLEAR DYNAMICS FROM SMALL TO LARGE AMPLITUDE COLLECTIVE MOTION.

The IPN Orsay/CNRS node of the TheoS JRA has a long-standing experience in the development of time-dependent approaches dedicated to the study of phenomena occurring in collisions of atomic nuclei. The Time-Dependent Hartree-Fock (TDHF) model offers a unique framework to describe small and large amplitude collective motion in a fully microscopic framework where the quantum nature of nucleons is explicitly treated. After the first applications of this theory to heavy-ion reactions in 1976, enormous efforts have been made to continuously improve this approach. Because of the numerical complexity, a new generation of TDHF codes without symmetries and using state-of-the-art effective interactions consistent with nuclear structure models was only achieved around 2000. Despite this major progress, superfluidity, which is an important ingredient in nuclei, was still missing in dynamical models until very recently. In the years 2013-2014, a first version of dynamical models including superfluidity in the BCS approximation was developed by the Orsay node. This code will be called hereafter TDHF+BCS. This new numerical programme has allowed, for instance, to describe the effect of pairing correlations on collective motion, fusion reactions or one- and two-particle transfer in heavy-ion reactions.

The version of the TDHF+BCS code available at the beginning of the ENSAR2 project was still an intermediate working version with many aspects to be improved. One of the goals of the deliverable D11.4 was to provide a clean standard version in order (i) to render it more versatile for applications by our group, and (ii) to provide a package that could be eventually given to the interested community worldwide. During the period of the ENSAR2 project, the code has been continuously improved along the line of the deliverable D11.4. A first releasable version of the code has been achieved in 2017. This version was used, for instance, in [4] to obtain the internal excitation of fragments after nuclear collisions. It has also allowed to complete with success the study of Ref. [5] dedicated to the description of fission including quantum collective fluctuations (milestone MS40 of the ENSAR2 project). For this, more than 1000 TDHF+BCS trajectories were needed and the availability of the novel standard version of the code was decisive. A final validation of the TDHF+BCS code was finally made by performing calculations of the isoscalar and isovector dipole response of atomic nuclei and comparing it with the result of the QRPA code discussed in Section 1. This important step, which is described further in Section 3, was useful to further clean up the TDHF+BCS code and figure out possible future improvements. During the period in which the code was improved, a detailed documentation was also written in order for the new users to be able to handle the code rapidly. The code is now available to the scientific community upon request. Regular advertisements were and will be made during workshops and conferences. The TDHF+BCS package has already been distributed to several groups worldwide including groups in Belgium, Algeria, Turkey, Italy and Japan.

Section 3: comparison/validation of the QRPA and TDHF+BCS approaches

The INFN-LNS node of the TheoS JRA has a long-standing expertise in the study of nuclear collective motion, within the framework of dynamical approaches (in the small amplitude limit) and RPA calculations, mainly in the semi-classical approximation.
Collective excitations are at the crossroad between nuclear structure and nuclear reactions. In fact, they are the optimal laboratories where clear connections between various methods can be made. In particular, dynamical approaches, such as TDHF, and RPA calculations should provide convergent results for the small-amplitude nuclear response. Thus, this kind of investigations can also be considered as a validation of the (Q)RPA and TDHF(+BCS) codes elaborated by the TheoS nodes. We have performed TDHF calculations, employing Skyrme functionals, to investigate the small-amplitude dipole response of selected neutron-rich nuclei and Sn isotopes. A detailed comparison with RPA calculations was presented in [6]. A quite good agreement between the two approaches was observed for the Isoscalar (IS) and Isovector (IV) dipole strengths, and the transition densities of the main excitation modes. Pairing effects were neglected in this case because they do not play a role in the magic nuclei considered in the analysis. Moreover, in the open-shell spherical systems, that we also considered, pairing is known to affect more the low-lying quadrupole and octupole states than the dipole response.

TDHF results were also confronted with Vlasov calculations [6,7] to explore up to which extent a semi-classical picture can explain the properties of the nuclear response. This comparison has evidenced the importance of shell effects and quantal intrinsic gradient terms in shaping isoscalar and isovector density profiles of the ground-state configuration. In particular, HF calculations are generally associated with smoother isoscalar density profiles, with respect to the ones deduced within the semi-classical approximation. Whereas the quantal IV dipole strength is quite well reproduced by Vlasov calculations, significant differences were observed in the low-energy domain of the IS response, concerning the energy and the relative weight of the different peaks [6]. Considering that this region is populated by surface excitation modes, this observation can be ascribed to the different density profiles and the different treatment of surface effects and gradient terms in quantal and semi-classical approaches. Moreover, shell effects can affect significantly the details of the low-lying states, especially as far as the Pygmy Dipole Strength (PDS) is concerned.

The TDHF/RPA comparison performed in [6] can be considered as a further proof of reliability of both codes. The TDHF (+BCS) code was also exploited to tackle various aspects of dissipative nuclear dynamics. In particular, in Ref. [8] we investigated fusion vs quasi-fission dynamics in heavy-ion collisions close to the Coulomb barrier, with the aim of probing the impact of several ingredients of the nuclear effective interaction, such as incompressibility, symmetry energy and surface terms, on the final reaction outcome.

Conclusion

The deliverable D11.4 has been completed successfully without encountering unexpected problems. Two computer programmes were improved and finalised during the ENSAR2 period. The QRPA package extends previous versions by including superfluid effects and offers the possibility to describe open shell nuclei. The second programme, TDHF-BCS, can treat both small- and large-amplitude collective motion and tackle dissipative reaction dynamics. In the small-amplitude sector, the two new codes were validated by comparing their results for specific giant resonances in atomic nuclei. This important step has shown that results obtained with these two computer programmes are consistent with each other. This comparison was an important validation of the two models. For both QRPA and TDHF+BCS, a package is now ready for being released to the international community.