Theo4Exp: A THEORY SERVICE FOR EURO-LABS COMMUNITY*

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Received 4 December 2024, accepted 15 January 2025, published online 10 April 2025

A new virtual access facility Theo4Exp provides a variety of computer codes for nuclear structure and reactions, accessible to researchers worldwide. The use of these codes is made simple by the adoption of clear interfaces and the implementation of graphical tools. Results can be easily transmitted, exchanged and compared. The EURO-LABS project, funded within the EC Horizon Europe program, has provided the appropriate framework and dedicated personnel to create this service.

DOI:10.5506/APhysPolBSupp.18.2-A10

1. Introduction

During last years, the nuclear scientific community has been moving towards open science: open access publications, accessibility to experimental data and codes, *etc.* In this context, the creation of user-friendly platforms, in which non-expert users can perform calculations using well-established theory codes, represents a significant and long-awaited advancement. The new virtual access facility Theo4Exp addresses this need by providing a variety of computer codes for nuclear structure and reactions, made easily accessible to researchers worldwide. The use of clear interfaces and the implementation of graphical tools makes it convenient and simple for the user, also providing result as files which can be easily transmitted, exchanged, and compared. It is expected that the new service will create a virtuous circle of

* Presented at the 57$^{\text{th}}$ Zakopane Conference on Nuclear Physics, *Extremes of the Nuclear Landscape*, Zakopane, Poland, 25 August–1 September, 2024.

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increased collaboration between theorists and experimentalists, leading to innovative experiments and facilitating their interpretation.

The EURO-LABS project, accessible via

https://web.infn.it/EURO-LABS

and funded within the EC Horizon Europe program, has provided an appropriate framework and dedicated personnel to create this service. Open to users since February 1st, 2024, Theo4Exp is composed of three installations: one for reaction calculations, Reaction4Exp, and two dedicated to structure calculations, MeanField4Exp and Structure4Exp. The Theo4Exp portal can be found at the main website https://institucional.us.es/theo4exp. Users are granted access to each installation via the application https://iam-eurolabs.ijclab.in2p3.fr developed within the EURO-LABS project, either by providing their institution credentials (if they belong to eduGAIN network) or the ORCID identification.

2. MeanField4Exp

The installation of MeanField4Exp is based on the numerical applications [1–4] of the realistic phenomenological mean-field approach, developed by Jerzy Dudek and collaborators at the University of Strasbourg. The codes have been implemented by Irene Dedes and Abdelghafar Gaamouci at the Institute of Nuclear Physics of the Polish Academy of Sciences (IFJ PAN) in Kraków. The functioning of the MeanField4Exp service benefits from the integration of nuclear structure theory and quantum mechanics methods based on the most recent nuclear mean-field parametrization [4], with advanced mathematical tools. These include inverse problem theory and Monte Carlo simulations for parameter optimization [1, 2], group and group representation theories for nuclear symmetries, and graph theory for studying shape transitions, such as the ones induced by nuclear fission [4]. The service provides access to advanced codes as well as to a comprehensive database containing pre-calculated results.

Users can produce diagrams of nucleonic energy levels or total nuclear energies as functions of various deformation parameters. Potential energy maps allow for studying shape coexistence and evolution as functions of proton and neutron numbers, as well as of angular momentum, addressing Jacobi and Poincaré shape transitions. Two examples of results provided by MeanField4Exp are shown in figures 1 and 2. Figure 1 illustrates the energy of selected isotopes of thorium as a function of quadrupole deformation, whereas figure 2 displays a contour map of the energy of ^{222}Th as a function of the quadrupole and octupole deformation parameters. Important extensions to the capabilities of the current system are underway.

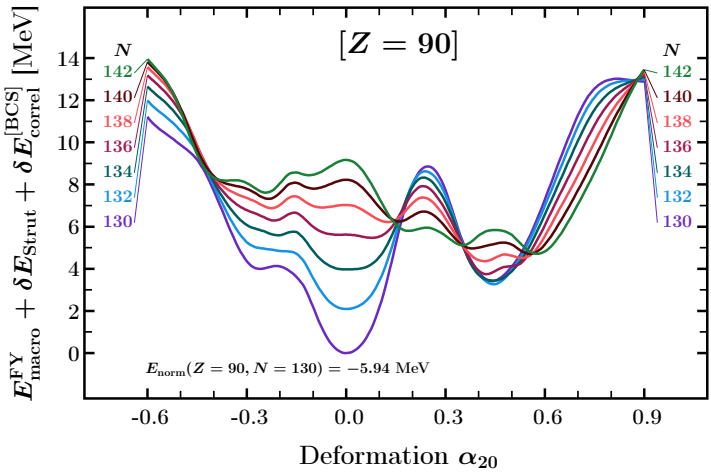

Fig. 1. Comparison of the total energies of selected isotopes of thorium as functions of the quadrupole deformation.

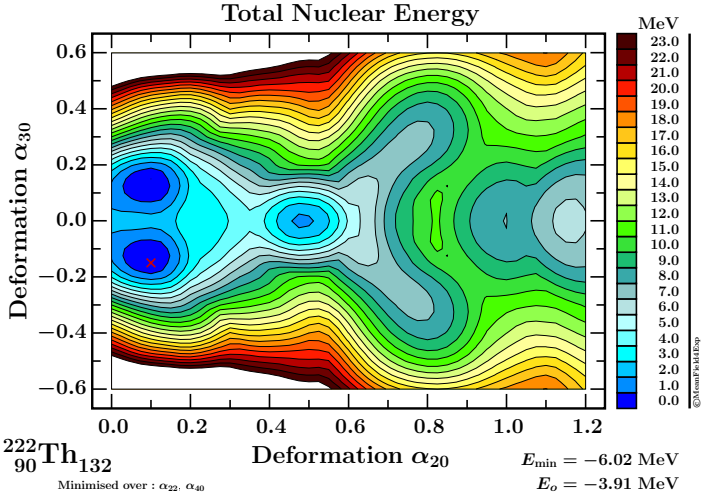

Fig. 2. Potential energy surface of ^{222}Th as a function of quadrupole α_{20} and octupole α_{30} shape degrees of freedom.

3. Reaction4Exp

The Reaction4Exp installation, hosted at Universidad de Sevilla (Spain) and implemented by Carla Muñoz-Chimbo, provides codes for the calculation of observables measured in different kinds of direct reactions, including presently Coulomb breakup, elastic, and inelastic scattering. All the results

are presented in the text format as well as graphically displayed and can be downloaded. We plan to shortly include the study of transfer reactions and the production of double-folding potentials from nuclear density distributions.

Coulomb breakup is calculated in a semi-classical formalism, the Equivalent Photon Model [5], and makes use of the code [6] developed by José A. Lay-Valera at Universidad de Sevilla. This program provides differential Coulomb breakup cross sections from external transition probabilities, as functions of both angle and energy. In Fig. 3, the angular distribution of the breakup differential cross section for $^{11}\mathrm{Li} + {}^{64}\mathrm{Zn}$ at 72 MeV is shown.

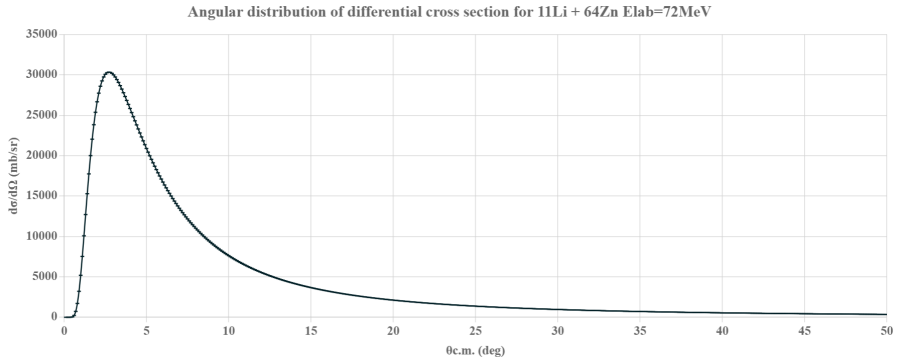

Fig. 3. Example of the results obtained using the Equivalent Photon Model: Angular distribution of the breakup differential cross section for $^{11}\mathrm{Li} + {}^{64}\mathrm{Zn}$ at 72 MeV.

Elastic-scattering calculations are performed according to the Optical Model formalism by introducing an optical potential to describe the interaction between the projectile and target. The code provides angular distributions for the reaction considered at a given energy in the laboratory frame. Figure 4 shows the angular distribution of the elastic differential cross section for $^{3}\mathrm{He} + {}^{14}\mathrm{C}$ at 72 MeV. The decomposition in the near- and far-side components is also shown. It is also possible to obtain the classical trajectories and deflection function as a function of the impact parameter, using a code developed by Mario Gómez-Ramos at Universidad de Sevilla.

The inelastic-scattering code provides cross sections for the population of the excited states of the projectile or target, making use of transition probabilities obtained from a collective model. It is based on the Coupled-Channels formalism, and the cross sections can also be computed in the first-order approximation, known as Distorted Wave Born Approximation (DWBA). Figure 5 shows the differential cross sections for the inelastic-scattering reaction: $n + {}^{238}\mathrm{U}$ at 3.5 MeV, leading to the first excited states of the target.

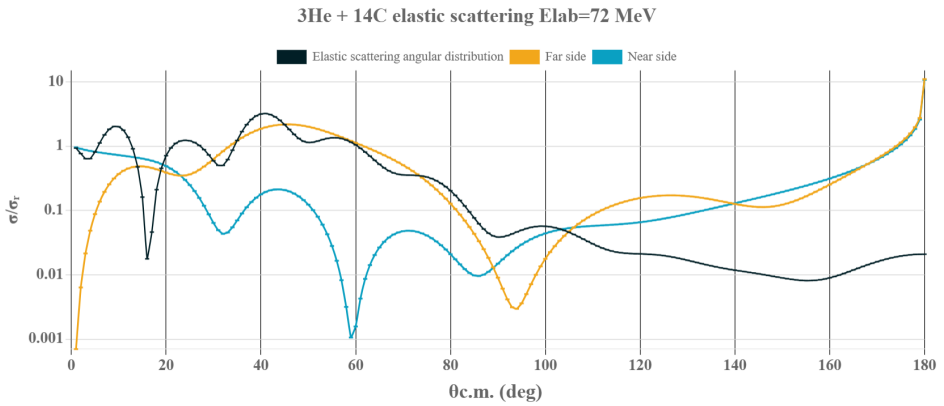

Fig. 4. Example of the Optical Model application: the angular distribution of the elastic differential cross section for $^{3}\mathrm{He} + {}^{14}\mathrm{C}$ at 72 MeV.

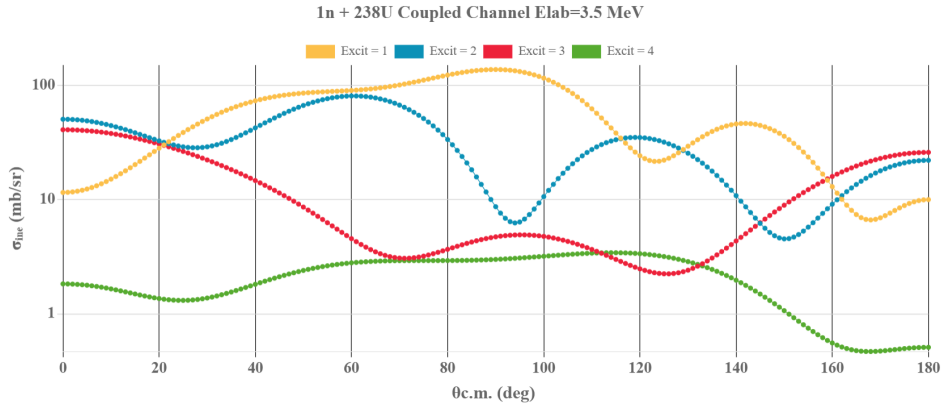

Fig. 5. Example of the Coupled Channels approach: Differential cross sections for the inelastic excitation to the first excited states of the target in the $n + {}^{238}\mathrm{U}$ reaction at 3.5 MeV.

The Optical Model, Coupled Channels, and Distorted Wave Born Approximation calculations are performed with the Fresco code [7], (see `https://www.fresco.org.uk`), which was developed by Ian J. Thompson (Lawrence Livermore National Laboratory, USA and University of Surrey, UK).

4. Structure4Exp

The Structure4Exp installation, hosted at the University of Milan (Italy), and set up by Imane Moumene, offers two types of codes. The first category includes two codes that are designed for the calculation of basic spectroscopic properties of spherical nuclei throughout the mass table. Ground-

state properties such as masses and radii, as well as vibrational excited states, are provided. For each excited state, the codes give the transition strengths associated with the usual isoscalar, isovector, and electromagnetic operators. One can visualize how this strength is distributed among giant resonances and low-lying vibrational states. One of these two codes is based on self-consistent Hartree–Fock (HF) plus Random Phase Approximation (RPA), developed by Colò and co-workers [8]. This is suitable for double-magic nuclei, or for nuclei with closed sub-shells both for neutrons and protons. Figure 6 shows an example of the results given by the code, in the case of the isovector dipole strength of ^{132}Sn. The other code is based on Hartree–Fock+Bardeen–Cooper–Schrieffer (HF+BCS) plus Quasiparticle RPA (QRPA), and has been developed by Colò and Roca-Maza [9]. Both codes employ a Skyrme-type effective force.

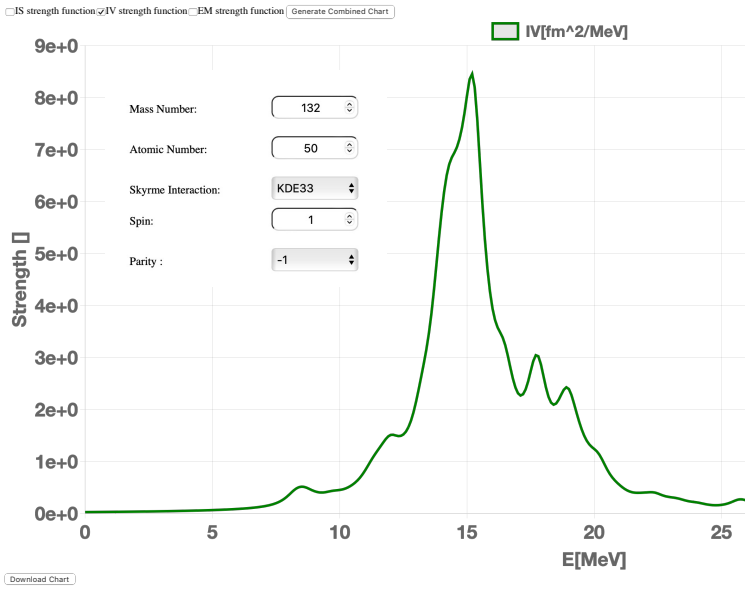

Fig. 6. Example of a result in the case of the isovector dipole strength calculated in RPA using the Skyrme force KDE033 in ^{132}Sn. The inset shows the input mask that the user has to fill.

The installation also offers the possibility to run the shell-model code KSHELL [10]. This has been developed by N. Shimizu and collaborators at the Centre for Computational Sciences of the University of Tsukuba. The code has been implemented with the help of Giovanni Di Gregorio (Caserta University and INFN Napoli) and Angela Gargano (INFN Napoli). Calculations can be performed in different valence spaces, with a selection of appro-

priate interactions. Users can specify the energy levels to be determined, and the program provides energy, occupation numbers, main contributing configurations, and, if requested, E2 and M1 electromagnetic transition rates. One can compare in several cases the QRPA and shell-model results.

5. Conclusions and outlook

Although the Theo4Exp Virtual Access facility has been running for few months only and is still in incomplete form, there is already a lot of interest from external users. New services are planned to be offered and we also envision ways to interact with the users' community.

This work has made use of the Virtual Access facility Theo4Exp funded by the European Union's Horizon Europe Research and Innovation programme under Grant Agreement No. 101057511. This work is also part of the I+D+i project PID2020-114687GB-I00 funded by MCIN/AEI/10.13039/501100011033.

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