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Activities of the ENEA Nuclear Data Project in 2007

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March 2008

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Activities of the ENEA Nuclear Data Project in 2007

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Abstract

Descriptions are given of the nuclear data activities at the Bologna Research Centre of the Italian National Agency for New Technologies, Energy and the Environment (ENEA), in 2007.

March 2008

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General Quantum Mechanics

Scattering in PT-symmetric quantum mechanics

Considerable interest has arisen in non-Hermitian Hamiltonians that exhibit definite transformation properties under parity (P), time reversal (T), and charge conjugation (C), particularly PT-symmetric Hamiltonians which are invariant under the product operator PT, but not under P and T separately.

We have performed a rather general study of the scattering properties of one-dimensional PT-symmetric Hamiltonians [A.1], after defining a 2 x 2 scattering matrix whose entries are the transmission and reflection coefficients for progressive waves T(L→R) and R(L→R), and for regressive waves T(R→L) and R(R→L), respectively. Furthermore, we have shown that Hamiltonians which are PT invariant and whose asymptotic wave functions are eigenstates of PT are necessarily reflectionless:

$$| T(L\rightarrow R)| = | T(R\rightarrow L)| = 1,\ R(L\rightarrow R) = R(R\rightarrow L) = 0$$

Transmission and reflection coefficients have been worked out in detail for some solvable PT-symmetric potentials as examples of application of different methods. Thus, the single and multiple square well have been solved by the matching matrix method, the hyperbolic Scarf potential by direct computation of the asymptotic wave functions, and a family of non-local potentials with separable kernel by the Green function method.

Nuclear Structure Theory

Micro-canonical calculations of nuclear level densities

Our theoretical research programme is focused on micro-canonical formalisms of level densities for open-shell nuclei, where nucleons interact with a mean field generated in a spherical shell model and a residual interaction consisting of proton-proton and neutron-neutron pairing treated exactly in the Richardson formalism, and simplified multipole-multipole interactions responsible for the dynamical deformation of the nuclear system. This system is expected to change with the excitation energy or temperature of the equilibrated system, and is especially important for improved applications of nuclear level densities (for nuclear reactions and astrophysics), where standard phenomenological formula based on experimental systematics cannot be reliably applied.

A major advantage of a micro-canonical approach with respect to a grand-canonical approach is that physical fluctuations of level density versus energy, as observed in recent measurements below the neutron binding energy, are not washed out and should be directly comparable with experimental data. Within the micro-canonical methodology, a rigorous study of nuclear temperature can be performed, and give limitations on the calculations based on grand-canonical approaches.

Preliminary results of level density calculations in the A = 50 mass region were presented at a Workshop on Level Density and Gamma Strength in Continuum, Oslo, 21-24 May 2007 [C.1]. Fig.1 shows the total level density of ^{56}Fe as a function of excitation energy in comparison with experimental data.

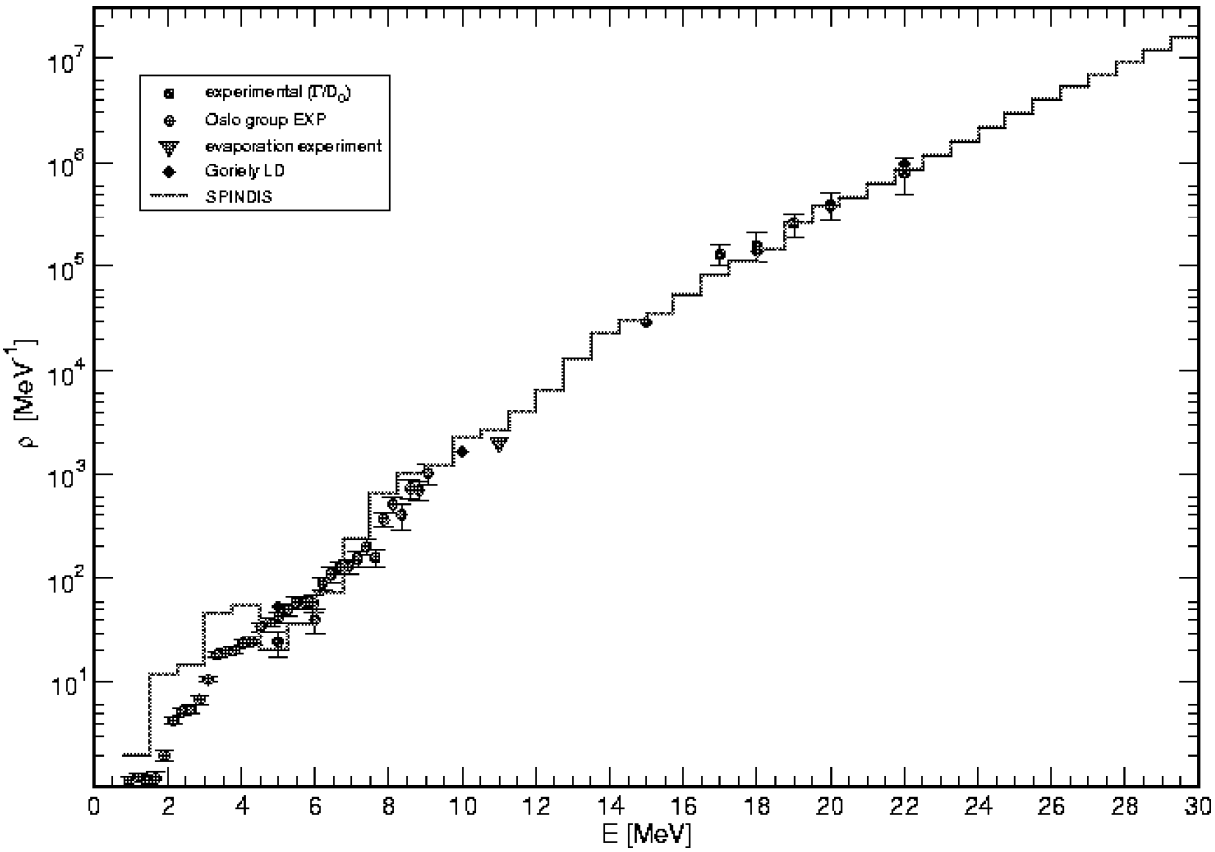

Fig.1. Level density of ^{56}Fe vs excitation energy: histogram depicts micro-canonical SPINDIS calculations; solid dots below E = 10 MeV are experimental data of A. Schiller *et al.*, Phys. Rev. C**68** (2003) 054326.

Nuclear Reaction Theory and Experiments

Measurements of neutron cross sections at the n_TOF facility, CERN

Publication of experimental results obtained in the 2002-04 campaign on the n_TOF facility at CERN [A.6] continued in 2007 with definitive values of neutron capture cross sections of ^{204}Pb [A.2], ^{139}La [A.3] and ^{206}Pb [A.4].

The neutron-magic isotope ^{139}La plays an important role in nuclear astrophysics; this isotope is produced at the second peak of the slow neutron capture process (*s*-process) shaped by the N = 82 nuclei from Ba to Nd, and is particularly well suited for monitoring the *s*-process abundances from Ba up to Pb. Moreover, ^{139}La is relatively easy to observe in stellar spectra, because transition probabilities and hyperfine structure constants of several La levels are known to good accuracy.

Nuclear resonance parameters and capture cross section of ^{139}La have been measured relative to ^{197}Au in the neutron energy range from 0.6 eV to 9 keV, in which 79 resonances have been observed [A.3]. The main nuclear constants obtained in the analysis are the resonance integral, the average gamma widths, spacings and neutron strength functions for *s* and *p* waves. The deduced Maxwellian-averaged capture cross sections are important for the interpretation of the most recent spectroscopic observations in low-metallicity stars.

The *s*-process fraction of the lead isotopes ^{204,206}Pb is mostly produced in thermally pulsing asymptotic giant branch stars, and is defined as the main component of the *s*-process. Moreover, the neutron capture of ^{206}Pb is also important for the design of fast reactors based on Pb/Bi spallation sources. Since 24.1% of natural lead consists of ^{206}Pb, the neutron capture cross section influences the neutron balance of the reactor.

The (n,γ) cross section of ^{204}Pb has been measured in the neutron energy range from 1 eV to 440 keV [A.2]. Within the resolved resonance region between 480 eV and 100 keV, 171 resonances have been observed; an average capture cross section has been determined over the energy range from 100 to 440 keV. The resulting Maxwellian-averaged cross sections are in agreement with previous experiments at kT = 30 keV, but approximately 35% higher than the values reported so far at kT = 5 keV.

The (n,γ) cross section of ^{206}Pb has been measured in the neutron energy range from 1 eV to 620 keV [A.4]. About 130 resonances have been observed and the parameters for 61 of them between 3.36 and 572 keV have been determined. Compared with literature values, the Maxwellian-averaged cross sections derived from the present data are about 20% and 9% lower at kT = 5 and 30 keV, respectively. The new results have a direct impact on the *s*-process abundance of ^{206}Pb, which represents an important test for the interpretation of the cosmic clock based on the decay of ^{238}U.

Preliminary results on neutron capture by other isotopes, such as ^{90,91,92,93,94,96}Zr, ^{186,187,188}Os, ^{197}Au, ^{234}U, ^{237}Np, ^{240}Pu, and neutron-induced fission of ^{233,235}U and ^{245}Cm have been presented at the International Conference on Nuclear Data for Science and Technology, Nice, 22-27 April 2007 [C.2-10] and other conferences [C.11-14]. As an example, Fig. 2 shows neutron capture cross sections of ^{186,187,188}Os in the unresolved resonance region [A.5], compared with previous experimental data and Hauser-Feshbach statistical model calculations.

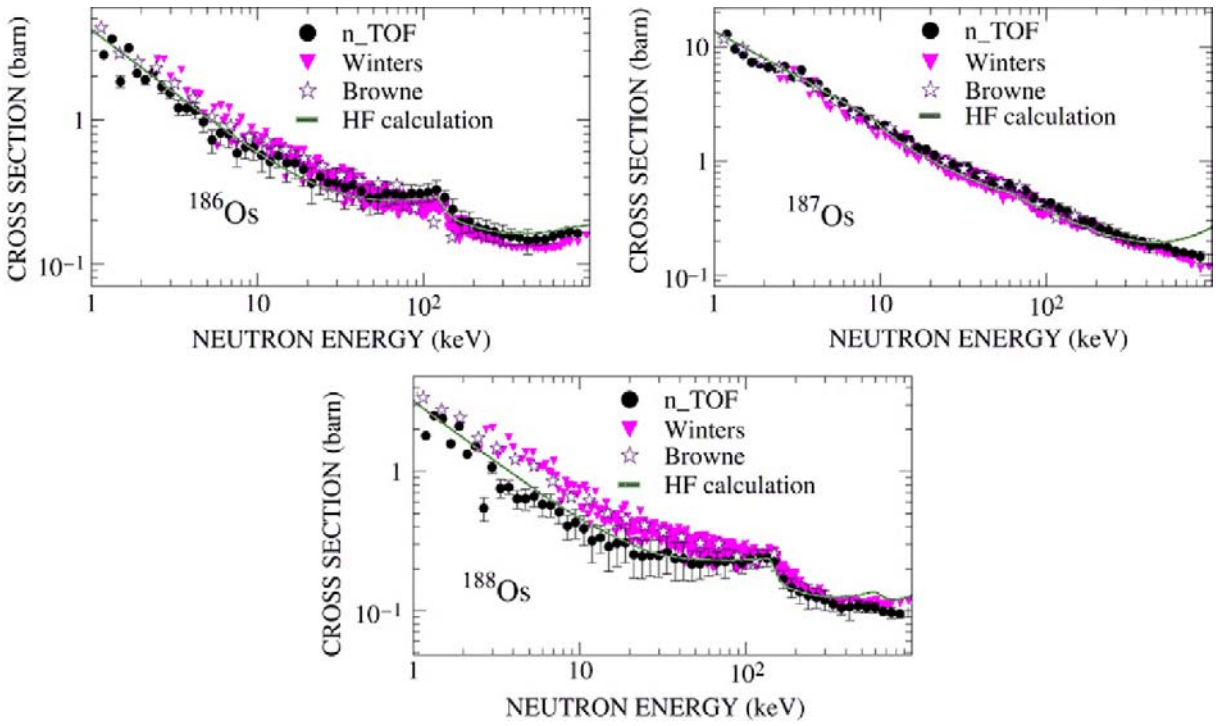

Fig. 2. Capture cross sections of ^{186,187,188}Os in the unresolved resonance region [A.5].

Nuclear Data Processing and Validation

Two multi-group coupled neutron and photon cross section libraries, based on the JEFF-3.1 library of evaluated data produced and distributed by the OECD/NEA Data Bank (Issy-les-Moulineaux, France), were generated for nuclear fission applications. These libraries are named VITJEFF31.BOLIB and MATJEFF31.BOLIB, and were re-processed in AMPX and MATXS format, respectively, through ENEA-Bologna revised versions of the NJOY-99.160 and SCAMPI nuclear data processing systems. A total of 182 files (176 standard files + 6 thermal scattering files for bound nuclides) were processed into the VITAMIN-B6 American library energy group structure (199 neutron groups + 42 photon groups). Eight revised JEFF-3.1 files were also downloaded and processed from the OECD/NEA Data Bank (Bi-209, Ca-46, Cl-35, Cl-37, Cr-52, Fe-58, U-233 and U-234). This set of files was accepted by the JEFF Working Group of the OECD/NEA Data Bank, and contains the revised Ca-46 file prepared at ENEA-Bologna and proposed for the future JEFF-3.2 evaluated data library. A massive data validation of the VITJEFF31.BOLIB library was performed with transport codes on about 90 criticality safety benchmark experiments with thermal, intermediate and fast neutron fission spectrum. Both discrete ordinates (SN) codes XSDRNPM (1D) and DORT (2D) were employed in the calculations. In parallel, the Monte Carlo code MCNP4C2 was used with an ENEA-Bologna generated JEFF-3.1 point-wise (continuous-energy) cross section library in ACE format in order to have reference results consistent with the official JEFF-3.1 data validation results, as obtained by the OECD/NEA Data Bank with the MCNP4C3 Monte Carlo code. Furthermore, two similar multi-group coupled neutron and photon cross section libraries were also produced, based on the recent American evaluated nuclear data library ENDF/B-VII.0. These libraries are named VITENDF70.BOLIB and MATENDF70.BOLIB, and were generated in AMPX and MATXS format, respectively, by means of the ENEA-Bologna versions of the NJOY-99.160 and SCAMPI nuclear data processing systems. Both VITJEFF31.BOLIB and VITENDF70.BOLIB in AMPX format were processed through the ENEA-Bologna 2007 revision of SCAMPI to collapse the two working libraries of self-shielded cross sections into FIDO-ANISN format and an energy group structure (47 neutron groups + 20 photon groups) of the American BUGLE-96 library. These libraries are specifically dedicated to LWR shielding and pressure vessel dosimetry applications, and are called BUGJEFF31.BOLIB and BUGENDF70.BOLIB, respectively.

The NJOY-99.160 version used in the present data processing of the VITJEFF31.BOLIB, MATJEFF31.BOLIB, VITENDF70.BOLIB and MATENDF70.BOLIB fine-group libraries contains an ENEA-Bologna revised patch for the GROUPR module dedicated to extending the group-wise data processing capability to the evaluated data files, *e.g.* 69 JEFF-3.1 nuclear data files, including non-Cartesian interpolation schemes for secondary neutron energy distributions. An original version of this patch was prepared at ENEA-Bologna in 2006 and sent to OECD/NEA Data Bank in order to be used officially for the first time with NJOY-99.112.

A specific correction patch dedicated to the proper calculation of the fluctuation factors for heating in the probability tables generated by the PURR module was developed, tested and sent to the OECD/NEA Data Bank before similar official corrections were publicly announced with the release of NJOY-99.172. The corrections permit proper evaluation of the heat deposition in Monte Carlo MCNP calculations when a specific evaluated file with the unresolved resonance (URR) representation (LSSF=1) is involved. The problem is present in seven JEFF-3.1 files (Fe-58, Re-185, Re-187, U-235, U-238, Pu-240 and Am-241) and in nine ENDF/B-VII.0 files (Zr-90, Re-185, Re-187, Th-232, Pa-231, Pa-233, U-233, U-235 and U-238).

A package of updates and corrections, essential for the processing of both the JEFF-3.1 and the ENDF/B-VII.0 data files, was prepared for the SCAMPI system; this package will be freely released to the OECD/NEA Data Bank in parallel with the VITJEFF31.BOLIB library. The package designated "ENEA-Bologna 2007 Revision of SCAMPI" also allows a potential user of VITJEFF31.BOLIB to process data in AMPX format. The list of modifications prepared last year was further integrated with new corrections. Hence, the RGENDF subroutine in the SMILER module was corrected and modified in order to read GENDF double-precision binary files from NJOY-99. The ENEA-Bologna 2007 revision of SCAMPI includes all the pre-2007 ENEA-Bologna SCAMPI modifications related to the MALOCS and SMILER modules, particularly fission matrix collapsing and the possibility of truncation of the upscatter terms with the full effective use of the IOPT7 options (IOPT7 = 0 , 1, 2 , 3) within MALOCS. As far as SMILER is concerned, we have ensured the possibility of obtaining the total neutron fission spectrum by taking into account both the prompt and delayed components (unlike the official Oak Ridge National Laboratory (ORNL) version of SMILER, which extracts only the prompt component from the GENDF file of NJOY).

All the activities described above were performed in close collaboration with a Russian specialist in nuclear data processing, who had previously worked at the Obninsk Institute of Physics and Power Engineering.

Computer Code Development

ADEFTA Version 4.0 (ADEFTA-4.0) was released in 2007 [R.2]. ADEFTA-4.0 is available from both OECD/NEA Data Bank (Issy-les-Moulineaux, France) and the Oak Ridge National Laboratory Radiation Safety Information Computational Center (ORNL/RSICC, USA):

- **NEA-1708/05 ADEFTA 4.0.** ADEFTA 4.0, Atomic Densities for Transport Analysis;
- **RSICC CODE PACKAGE PSR-543**: ADEFTA 4.0: Atomic Densities for Transport Analysis Script.

ADEFTA is a script file for any UNIX/Linux platform that uses only Bourne shell commands and the "awk" UNIX-Linux utility in order to calculate the atomic densities related to any compositional model for transport analysis. This file can run in Cygwin (http://www.cygwin.com) and so the output is available in Windows as well as in UNIX/Linux.

The output produced by ADEFTA can be useful for applications with many transport codes. However, ADEFTA is of particular value to users of the following:

(a) GIP code included in the ORNL DOORS package, which prepares the macroscopic cross-sections for the DORT and TORT deterministic transport codes (both included in the DOORS package), and
(b) Monte-Carlo MCNP code (Los Alamos National Laboratory (LANL), USA).

Compared with the previous version, ADEFTA 4.0 changes only the format of the output file for MCNP that can be directly used by MCNP with minor editing.

BOT3P version 5.2 (BOT3P-5.2) was released in 2007 [A.7, R.3]. BOT3P-5.2 is available from both the OECD/NEA Data Bank and ORNL-RSICC:

- **NEA-1678 BOT3P-5.2** BOT3P5.2, 3D Mesh Generator and Graphical Display of Geometry for Radiation Transport Codes, Display of Results;

- **RSICC CODE PACKAGE PSR-530:** BOT3P-5.2: Code System for 2D and 3D Mesh Generation and Graphical Display of Geometry and Results for Radiation Transport Codes.

BOT3P is a set of standard FORTRAN 77 language codes developed by the ENEA Nuclear Data Group from August 1997 onwards, and is designed to run on most Linux/UNIX platforms.

BOT3P Version 1.0 was originally conceived as a set of standard FORTRAN 77 language programs in order to give the users of the DORT and TORT deterministic transport codes some useful diagnostic tools to prepare and check their input data files for both Cartesian and cylindrical geometries, including mesh grid generation modules, graphical display and utility programs for post-processing applications. Later versions included options for the production of geometrical material distribution and fixed neutron source data to other deterministic transport codes such as TWODANT/THREEDANT (both included in the LANL DANTSYS package), PARTISN (updated parallel version of DANTSYS) and the sensitivity code SUSD3D (distributed by OECD/NEA Data Bank), and potentially to any transport code through BOT3P binary output files that can be easily interfaced (for example, two-dimensional (2D) and three-dimensional (3D) discrete ordinates neutron, photon and charged-particle transport codes KASKAD-S-2.5 and KATRIN-2.0 developed at the Keldysh Institute of Applied Mathematics (Moscow, Russian Federation)). Thus, users can directly compare for the same geometry the effects stemming from the use of different data libraries and solution approaches on transport analysis results.

BOT3P allows users to model X-Y, X-Z, Y-Z, R-Θ and R-Z geometries in two dimensions and X-Y-Z and R-Θ-Z geometries in three dimensions. A general method to conserve mass of geometrically complex material zones simulated on both Cartesian and cylindrical mesh grids is implemented in BOT3P version 5.0. BOT3P allows users to specify as refined a computation as desired of the possible area/volume error of material zones due to the stair-cased geometry representation, and corrects material densities automatically in order to conserve masses globally. BOT3P can store as binary outputs the detailed material zone distribution map inside each cell of the mesh grid according to a sub-mesh grid refinement defined by the user and the area/volume fraction distribution of the different material zones contained in meshes at zone interfaces. This procedure allows a local density correction (per cell) as an alternative to the approach of a uniform density correction on the whole zone domain, providing the user with the potential to perform material zone homogenization locally and transport analyses with more accuracy. Important additions specifically to address radiation transport analysis for medical applications were introduced in BOT3P-5.1.

BOT3P-5.2 contains new important graphics capabilities that enable users to select space sub-domains of the total mesh grid in order to improve the zoom simulation of the geometry, both in 2D cuts and in 3D. Moreover, the new BOT3P module (PDTM) is a flexible tool that has much improved the interface capability of BOT3P geometrical models to any transport analysis code.

BOT3P was successfully used not only in some complex neutron shielding and criticality benchmarks, but also in power reactor applications (for example in the Westinghouse AP1000 internals heating rate distribution calculations by Ansaldo Nucleare). BOT3P has achieved world-wide recognition, and is currently used by important companies such as Westinghouse Electric Co. NEA/Data Bank received more than 130 dispatch requests for different versions up to the end of 2007.

The following plots provide good representations of the complex modelling capabilities of BOT3P.

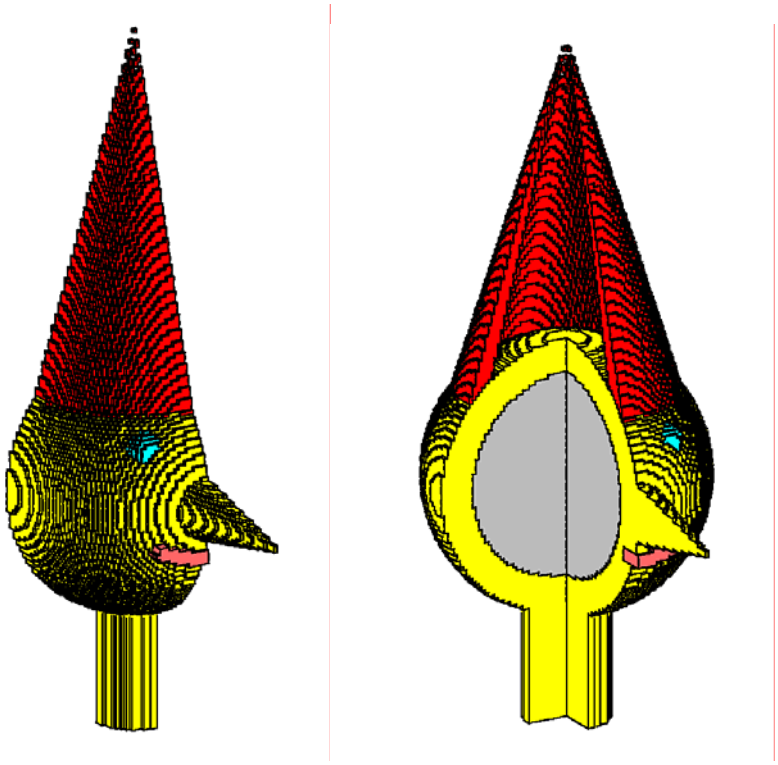

Fig.3: Complex geometry simulation in Cartesian coordinates (120X, 88Y, 200Z).

Publications 2007

Articles

[A.1] F. Cannata, J.-P. Dedonder and A. Ventura, *Scattering in PT-symmetric Quantum Mechanics,* Ann. Phys. **322**, 397-433 (2007).

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[A.3] R. Terlizzi *et al.* (the n_TOF Collaboration), *The ^{139}La(n,γ) Cross Section: Key for the Onset of the s-Process,* Phys. Rev. C **75**, 035807: 1-15 (2007).

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[A.6] F. Gunsing *et al.* (n_TOF Collaboration), *Status and Outlook of the Neutron Time-of-Flight Facility n_TOF at CERN*, Nucl. Instr. Meth. Phys. Res. B **261**, 925-929 (2007).

[A.7] R. Orsi, *Potential Enhanced Performances in Radiation Transport Analysis on Structured Mesh Grids Made Available by BOT3P,* Nucl. Sci. Eng. **157**, 110-116 (2007).

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[C.1] A. Ventura and R. Pezer, *Micro-canonical Level Densities of Non-magic Nuclei,* Workshop on Level Density and Gamma Strength in Continuum, Oslo, 21-24 May 2007; presentation available at http://ocl.uio.no/workshop07/talks.htm.

[C.2] F. Gunsing *et al.* (n_TOF Collaboration), *Neutron Resonance Spectroscopy at n_TOF at CERN,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.3] C. Domingo-Pardo *et al.* (n_TOF Collaboration), *Improved Lead and Bismuth (n,γ) cross sections and their astrophysical impact,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.4] G. Tagliente *et al.* (n_TOF Collaboration), *Measurement of the ^{90,91,92,93,94,96}Zr(n,γ) and ^{139}La(n,γ) cross sections at n_TOF,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.5] K. Fujii *et al.* (n_TOF Collaboration), *Capture Cross Section Measurements of ^{186,187,188}Os at n_TOF: the Resolved Resonance Region,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.6] C. Massimi *et al.* (n_TOF Collaboration), *Measurement of the ^{197}Au(n,γ) Cross Section at n_TOF: Towards a New Standard,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.7] C. Lampoudis *et al.* (n_TOF Collaboration), *The ^{234}U Neutron Capture Cross Section at the n_TOF Facility,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.8] C. Guerrero *et al.* (n_TOF Collaboration), *The Neutron Capture Cross Sections of ^{237}Np and ^{240}Pu and Their Relevance in the Transmutation of Nuclear Waste,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.9] E. Berthoumieux *et al.* (n_TOF Collaboration), *Simultaneous Measurement of the Neutron Capture and Fission Yields of ^{233}U,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.10] M. Calviani *et al.* (n_TOF Collaboration), *Measurement of Neutron Induced Fission of ^{235}U, ^{233}U and ^{245}Cm with the FIC Detector at the CERN n_TOF Facility,* International Conference on Nuclear Data for Science and Technology, Nice, 22-25 April 2007 (to be published).
[C.11] P. F. Mastinu *et al.* (n_TOF Collaboration), *Measurement of the Neutron Induced Fission Cross Section on Transuranic Elements at the n_TOF Facility at CERN,* 11th Latin-American Symposium on Nuclear Physics and Applications, Cuzco, 11-16 June 2007 (to be published).
[C.12] C. Guerrero *et al.* (n_TOF Collaboration), *Application of Photon Strength Functions to (n,γ) Measurements with the n_TOF TAC,* Workshop on Photon Strength Functions and Related Applications, Prague, 17-21 June 2007 (to be published).
[C.13] D. Cano-Ott *et al.* (n_TOF Collaboration), *The n_TOF Facility at CERN,* 8th International Topical Meeting on Nuclear Applications and Utilization of Accelerators, Pocatello, Idaho, 30 July – 2 August 2007 (to be published).
[C.14] M. Calviani *et al.* (n_TOF Collaboration), *Measurements of Fission Cross Sections of Actinides at n_TOF,* 4th International Workshop on Neutron Measurements, Evaluations and Applications, Prague, 16-18 October 2007 (to be published).
[C.15] M. Pescarini, V. Sinitsa, R. Orsi, *ENEA-Bologna Production and Testing of JEFF-3.1 Multi-Group Cross Section Libraries for Nuclear Fission Applications*, International Conference on Nuclear Data for Science and Technology, Nice, 22-27 April 2007 (to be published).
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[R.2] R. Orsi, *ADEFTA Version 4.0: a Program to Calculate the Atomic Densities of a Compositional Model for Transport Analysis,* ENEA/FPN-P9H6-004 Rev.0 (2007).

[R.3] R. Orsi, *BOT3P Version 5.2: a Pre-Post-Processor System for Transport Analysis,* ENEA/FPN-P9H6-002 Rev.0 (2007).

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