Tutorial on shell model calculations and the production of nuclear Hamiltonians

A. Signoracci*

Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France

T. Duguet†

Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France and National Superconducting Cylcotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

J. Holt‡

Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany and ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

Tutorial of the *Espace de Structure Nucléaire Théorique*

13-17 May 2013

CEA/SPhN, Orme des Merisiers, build. 703, room 135, F-91191 Gif-sur-Yvette Cedex

I. EXECUTIVE SUMMARY

A weeklong program will be held at the Espace de Structure Nucléaire Théorique (CEA/Saclay, France) to educate young researchers on the application of Configuration Interaction techniques in nuclear physics. Each day will be split into a lecture component and a tutorial component, where the participants will gain hands-on experience running shell model codes to produce nuclear level schemes and transition properties for comparison to existing experimental data. As a result, laptops are mandatory. Instructions on downloading and installing NUSHELLX will be given in advance of the program.

To register, please send an email expressing your interest to Angelo Signoracci (angelo.signoracci@cea.fr). While there is no program fee, only lunches on 13-17 May will be supported by the ESNT. All other costs (travel, hotel, dinner, etc.) must be covered by the participants or their institutions. Practical details are available at the ESNT website at http ://esnt.cea.fr, including a link to the program, lectures, and tutorials from the 2012 tutorial (accessed directly at http ://esnt.cea.fr/Phocea/Page/index.php ?id=18).

II. SCIENTIFIC CONTENT

Configuration Interaction theory, including nuclear shell model theory, simplifies the nuclear many-body problem by selecting an inert core of occupied single particle levels as a vacuum with zero point energy. The description of a nucleus with more neutrons and protons than the core is given by valence particles constrained to occupy a model space of single particle orbits outside the core, reducing the allowed configuration space of the nucleons.

After selecting an appropriate core and model space, two problems remain : determining an effective interaction and solving the Schrödinger Equation in the reduced model space. Empirical interactions have been determined for many standard model spaces, and shell model codes such as ANTOINE and NUSHELLX have been developed to solve the eigenvalue problem.

The reduction in allowed configurations (i.e. in the number of degrees of freedom) leads to the definition of an *effective* Hamiltonian, as the interactions between nucleons in the model space must account for effects due to contributions from outside the model space, both from the core and from excluded higher-energy orbits. In principle, the effective

---

*Electronic address: angelo.signoracci@cea.fr

†Electronic address: thomas.duguet@cea.fr

‡Electronic address: holt@theorie.ikp.physik.tu-darmstadt.de

interaction should be determined using a procedure that starts from a microscopic Hamiltonian combining two and three nucleon interactions, that overcomes the repulsive short-range part of standard microscopic interactions via renormalization group methods, and that employs many-body perturbation theory techniques to renormalize the interaction into the model space of interest.

Shell model calculations, often based on empirical interactions, have provided reasonable theoretical predictions of properties such as energies, transitions, and decays in medium-mass nuclei for comparison to experiment. Unfortunately, even though shell model codes are publicly available, only a limited number of experimentalists have learned the procedure to calculate nuclear properties of interest to their research. Those who have often find the lack of standard effective interactions in many regions of the nuclear chart, especially exotic regions accessible with current rare isotope beam facilities, problematic for their calculations. Furthermore, empirical interactions are often unreliable or employed in truncation schemes that lack consistency with their derivation and therefore do not exhibit predictive power.

This program proposes to educate interested researchers in nuclear physics, experimentalists or theorists, on the modern implementation of Configuration Interaction theory. Topics will include background in nuclear structure theory, basics of the shell model, descriptions of the implementations of shell model codes, focusing on NUSHELLX, and the development of a procedure to produce effective interactions through the renormalization of microscopic interactions using renormalization group methods and many-body perturbation theory techniques.

The program is designed to operate as a tutorial : morning sessions will focus on formalism and instruction on the theoretical techniques, while afternoon sessions will involve hands-on training in calculations (laptop mandatory). The program will culminate in the production of an effective interaction and a realistic calculation of an exotic nucleus, with a comparison to experiment.

III. GOALS OF THE PROGRAM

In summary, the goals of the program are

1. To outline the underlying formalism and theoretical background to nuclear shell model codes
2. To provide shell model codes and instruction on their utilization
3. To perform standard shell model calculations
4. To produce effective interactions in the nuclear medium from underlying microscopic interactions
5. To culminate in a practical application to a realistic case of interest for nuclear structure

IV. USEFUL REFERENCES

– NuShellX@MSU, B. A. Brown and W. D. M. Rae, http ://www.nscl.msu.edu/~brown/resources/resources.html
– E. Caurier and F. Nowacki, Acta Phys. Pol. B **30**, 705 (1999) ;
http ://sbgat194.in2p3.fr/ theory/antoine/menu.html
– J. Holt et al., arXiv :1009.5984
– A. Signoracci, B. A. Brown, and M. Hjorth-Jensen, Phys. Rev. C **83**, 024315 (2011)
– T. Otsuka et al., Phys. Rev. Lett. **105**, 032501 (2010)
– F. Nowacki and A. Poves, Phys. Rev. C **79**, 014310 (2009)
– E. Caurier et al., Rev. Mod. Phys. **77**, 427 (2005)
– B. A. Brown, Prog. Part. Nucl. Phys. **47**, 517 (2001)
– M. Hjorth-Jensen, T. T. S. Kuo, and E. Osnes, Phys. Rept. **261**, 125 (1995)

V. LECTURES

– Angelo Signoracci (angelo.signoracci@cea.fr)

1. Lecture I *"Shell Model formalism I"*
2. Lecture II *"Shell Model formalism II"*
3. Lecture III *"Introduction to NUSHELLX I"*
4. Lecture IV *"Introduction to NUSHELLX II"*
5. Lecture VII *"Derivation of effective interactions"*

– Jason Holt (holt@theorie.ikp.physik.tu-darmstadt.de)
  1. Lecture V *"Non-empirical shell model from realistic interactions I"*
  2. Lecture VI *"Non-empirical shell model from realistic interactions II"*
  3. Lecture VIII *"Inclusion of three-body forces"*

VI. TUTORIALS AND TEAM PROJECTS

The program devotes significant time to hands-on experience setting up and running standard shell model codes, in order to prepare the participants for future calculations relevant to their research. The program will culminate with a set of realistic calculations of recent experimental interest, which will be performed in groups and guided by the lecturers. Each group (≈ 5 people per group), starting essentially from scratch, will produce calculations, tabulate the results, and present their findings on the final day of the program. To prepare the groups for this assignment, tutorials will cover the following topics :

1. Tutorial I *"Implementation and running of NUSHELLX I"*
2. Tutorial II *"Implementation and running of NUSHELLX II"*
3. Tutorial III *"Selection of model space and (empirical) interactions"*
4. Tutorial IV *"Producing effective interactions for any model space from microscopic interactions"*
5. Tutorial V *"Inclusion of three-body forces"*

VII. PROGRAM

Mon. 13 May	Tues. 14 May	Wed. 15 May	Thurs. 16 May	Fri. 17 May
	09h30 Lecture III	09h30 Lecture V	09h30 Lecture VIII	09h30 Team Project II
	10h45 **Break**	10h45 **Break**	10h45 **Break**	10h45 **Break**
11h15 Welcome	11h15 Lecture IV	11h15 Lecture VI	11h15 Tutorial IV	11h15 Team Project III
12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**
14h30 Lecture I	14h30 Tutorial I	14h30 Lecture VII	14h30 Tutorial V	14h30 Presentations
15h45 **Break**	15h45 **Break**	15h45 **Break**	15h45 **Break**	15h45 **Break**
16h15 Lecture II	16h15 Tutorial II	16h15 Tutorial III	16h15 Team Project I	16h15 Wrap-up
17h30 **End**	17h30 **End**	17h30 **End**	17h30 **End**	17h30 **End**