

Tutorial on shell model calculations and the production of nuclear Hamiltonians

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Tutorial of the *Espace de Structure Nucléaire Théorique*

23 April - 27 April 2012

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. If at all possible, participants are requested to bring a Windows or Linux laptop, as the shell model code NUSHELLX may not run on Macs. 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 23-27 April 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://irfu.cea.fr/Sphn/Espace_Theorie/index.php.

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

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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.nsl.mscl.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)
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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 (jholt31@utk.edu)

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. 23 April	Tues. 24 April	Wed. 25 April	Thurs. 26 April	Fri. 27 April
	09h30 Lecture III	09h30 Lecture V	09h30 Lecture VII	09h30 Team Project II
	10h45 Break	10h45 Break	10h45 Break	10h45 Break
11h15 Welcome	11h15 Lecture IV	11h15 Lecture VI	11h15 Lecture VIII	11h15 Team Project III
12h30 Lunch	12h30 Lunch	12h30 Lunch	12h30 Lunch	12h30 Lunch
14h30 Lecture I	14h30 Tutorial I	14h30 Tutorial III	14h30 Tutorial V	14h30 Presentations
15h45 Break	15h45 Break	15h45 Break	15h45 Break	15h45 Break
16h15 Lecture II	16h15 Tutorial II	16h15 Tutorial IV	16h15 Team Project I	16h15 Wrap-up
17h30 End	17h30 End	17h30 End	17h30 End	17h30 End

VIII. ATTENDANCE

The program, consisting of lectures by two organizers as well as tutorials guided by all three organizers, was attended by 24 participants. Of these, five work for CEA/SPhN, eight for CEA/DAM, and nine for other French research institutions. Two attendees were international (Belgium). The majority of the attendees were Ph.D. students as designed, but a few postdocs and researchers also participated.

IX. FINANCIAL BALANCE

The ESNT supported J. Holt for two weeks total, including the week prior to the tutorial for collaboration with the other organizers. The total cost of his stay was xxxx euro. A workshop dinner was held on Wednesday April 25 for a total cost of 497 euros. Lunches for all participants were covered throughout the week for a total of 934,20 euros, with an additional 984 euros spent on transportation from l'Orme des Merisiers to the main CEA site throughout the week. Coffee breaks during the workshop cost 125 euros. The total cost of the workshop therefore summed to 2540,20 + xxxx euros.

X. COMMENTS

Overall, the tutorial was very successful and included positive feedback from many participants. The goals of the program, as listed above, were achieved and the expectations of the organizers were exceeded. The culmination of the tutorial with presentations, focused on shell model calculations of current relevance to nuclear structure theory, displayed the advances made by the participants in the span of one week. While this was the first tutorial of this nature hosted by ESNT, recommendations were made for similar tutorials next year, perhaps a second offering of this program or a new program on energy density functional methods. In general, the organization of the tutorial was satisfactory, with only small complaints concerning the Wifi internet by Linux users.

The additional week spent by J. Holt at ESNT resulted in very fruitful collaborations and progressions of ideas on a variety of topics including pairing and the production of effective interactions from bare two- and three-nucleon forces, in addition to preparation of the lectures and tutorials for the program. The discussions started during these two weeks are expected to continue into this summer and beyond.

The tutorial sessions resulted in the realization that a solutions manual should be developed and disseminated along with the lectures and problem sets on the ESNT website. This task is currently being undertaken and will be completed in the coming months.