Program for Nuclear Talent course on *Many-body methods for nuclear physics, from Structure to Reactions* at Henan Normal University, P.R. China, July 16-August 5 2018

Kevin Fossez[1]

Morten Hjorth-Jensen[2]

Baishan Hu[3]

Weiguang Jiang[4]

Thomas Papenbrock[4]

Ragnar Stroberg[5]

Zhonghao Sun[4]

Yu-Min Zhao[6]

[1]National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA
[2]National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA
[3]School of Physics, Peking University, Beijing 100871, P.R. China
[4]Oak Ridge National Laboratory and Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA
[5]Departmentof Physics, Reed College, Portland, OR, 97202 and Department of Physics, University of Washington, Seattle, WA 98195-1560, USA
[6]School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, P.R. China

March 2018

Motivation and introduction

To understand why matter is stable, and thereby shed light on the limits of nuclear stability, is one of the overarching aims and intellectual challenges of basic research in nuclear physics. To relate the stability of matter to the

underlying fundamental forces and particles of nature as manifested in nuclear matter, is central to present and planned rare isotope facilities.

Important properties of nuclear systems which can reveal information about these topics are for example masses, and thereby binding energies, and density distributions of nuclei. These are quantities which convey important information on the shell structure of nuclei, with their pertinent magic numbers and shell closures or the eventual disappearence of the latter away from the valley of stability.

During the last decade, the study of nuclear structure and the models used to describe atomic nuclei are experiencing a renaissance. This is driven by three technological revolutions: accelerators capable of producing and accelerating exotic nuclei far from stability; instrumentation capable of detecting the resulting reaction products and gamma radiation, often on an event-by-event basis, in situations where data rates may be many orders of magnitude less than has been traditional; and computing power adequate to analyze the resulting data, often on-line, and to carry out sophisticated theoretical calculations to understand these nuclei at the limits of stability and to unravel what they tell us about nuclei and their structural evolution.

The nuclear shell model plays a central role in guiding our analysis of this wealth of experimental data. The shell model provides an excellent link to the underlying nuclear forces and the pertinent laws of motion, allowing nuclear physicists to interpret complicated experiments in terms of various components of the nuclear Hamiltonian and to understand a swath of nuclei by following chains of isotopes and isotoones over wide ranges of nucleon numbers. The nuclear shell model allows us to see how the structure of nuclei changes and how the occupation of specific nucleonic orbits affects the interplay of residual interactions and configuration mixing. The computed expectation values and transition probabilities can be directly linked to experiment, with the potential to single out new phenomena and guide future experiments. Large-scale shell-model calculations represent also challenging computational and theoretical topics, spanning from efficient usage of high-performance computing facilities to consistent theories for deriving effective Hamiltonians and operators. Alltogether, these various facets of nuclear theory represent important elements in our endeavors to understand nuclei and their limits of stability.

However, the dimensionalities of interest for shell-model studies exceed quickly present computational capabilities of eigensystem solvers. In order to be able to describe nuclear systems with many more degrees of freedom as well as providing better effective operators, approximative many-body methods like **Coupled Cluster** (CC) theory or the **In-Medium Similarity Renormalization Group** (IMSRG) approach have lately gained wide interest and applicabilities in the nuclear many-body community.

It is the goal and motivation of this course to introduce and develop the nuclear structure tools needed to carry out forefront research using the shell model and many-body methods like CC theory and the IMSRG method as central tools, with applications to both structure and reaction theory studies, including continuum contributions and resonances. After completion, it is our

hope that the participants have understood the overarching ideas behind central theoretical tools used to analyse nuclear structure experiments.

This three-week TALENT course on nuclear theory will focus on the Many-body methods for nuclear structure and reactions, focusing on nuclear shell model and/or coupled cluster theory and in-medium SRG with applications to structure and reactions. Via hands-on projects and series of exercise, the participants will have been exposed to the necessary tools and theoretical models used in modern nuclear theory.

Format: We propose approximately forty-five hours of lectures over three weeks and a comparable amount of practical computer and exercise sessions, including the setting of individual problems and the organization of various individual projects. The course starts July 16 (with arrival on July 15) and ends (the course) on August 3. A three days workshop will be organized from August 4 to August 6. The mornings will consist of lectures and the afternoons will be devoted to exercises meant to shed light on the exposed theory, and the computational projects. These components will be coordinated to foster student engagement, maximize learning and create lasting value for the students. For the benefit of the TALENT series and of the community, material (courses, slides, problems and solutions, reports on students' projects) will be made publicly available using version control software like *git* and posted electronically on github.

As with previous TALENT courses, we envision the following features for the afternoon sessions:

- We will use both individual and group work to carry out tasks that are very specific in technical instructions, but leave freedom for creativity.

- Groups will be carefully put together to maximize diversity of backgrounds.

- Results will be presented in a conference-like setting to create accountability.

- We will organize events where individuals and groups exchange their experiences, difficulties and successes to foster interaction.

- During the school, on-line and lecture-based training tailored to technical issues will be provided. Students will learn to use and interpret the results of computer-based and hand calculations of nuclear models. The lectures will be aligned with the practical computational projects and exercises and the lecturers will be available to help students and work with them during the exercise sessions.

- These interactions will raise topics not originally envisioned for the course but which are recognized to be valuable for the students. There will be flexibility to organize mini-lectures and discussion sessions on an ad-hoc basis in such cases.

- Each group of students will maintain an online logbook of their activities and results.

- Training modules, codes, lectures, practical exercise instructions, online logbooks, instructions and information created by participants will be merged into a comprehensive website that will be available to the community and the public for self-guided training or for use in various educational settings (for example, a graduate course at a university could assign some of the projects as homework or an extra credit project, etc).

Objectives and learning outcomes: At the end of the course the students should have a basic understanding of

- Configuration interaction methods (nuclear shell-model here) as a central tool to interpret nuclear structure experiment

- Central many-body methods like Coupled Cluster theory and the In-Medium Similarity Renormalization Group approach

- How to compute nuclear structure properties with these methods

- Have an understanding of single-particle basis functions and the construction of many-body basis states built thereupon. Examples are basis states from a Woods-Saxon potential, harmonic oscillator states and mean-field based states from a Hartree-Fock calculation. The single-particle basis states are orthonormal and are used to construct a corresponding orthonormal basis set of Slater determinants.

- Develop an understanding of what defines an observable.

- Understand how theory can be used to interpret experimental quantities (separation energies and shell gaps for example).

- Understand how second-quantization is used to represent states and compute expectation values and transition probabilities of operators

- Understand how to study resonances and contributions from continuum states

- Understand how the Hamiltonian matrix is constructed from this orthonormal basis set of many-body states (linear expansion of Slater determinants)

- The students will also learn to understand the basic elements of effective shell-model Hamiltonians and how to interpret the calculated properties in terms of various components of the nuclear forces (spin-orbit force, tensor force, central force etc). We will provide the students with the necessary tools to perform such analyses.

- Develop a critical understanding of the limits of many-body studies and how these can be related to interpretations of data such as results from in-beam and decay experiments.

Teachers and organizers

The local organizers are

1. Chun-Wang Ma at Henan Normal University, Xinxiang, Henan 453007, P.R. China

2. Furong Xu at School of Physics, Peking University, Beijing 100871, P.R. China

3. Shan-Gui Zhou at the Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100864, P.R. China

In addition Qiao Chunyuan will help with administrative matters. You can reach her at the email address qiaochunyuan919@126.com.

Thomas Papenbrock and Morten Hjorth-Jensen will also function as student advisors and coordinators.

The teachers are

1. Kevin Fossez at National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA

2. Morten Hjorth-Jensen at National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

3. Baishan Hu at School of Physics, Peking University, Beijing 100871, P.R. China

4. Weiguang Jiang at Oak Ridge National Laboratory and Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA

5. Thomas Papenbrock at Oak Ridge National Laboratory and Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA

6. Ragnar Stroberg at Departmentof Physics, Reed College, Portland, OR, 97202 and Department of Physics, University of Washington, Seattle, WA 98195-1560, USA

7. Zhonghao Sun at Oak Ridge National Laboratory and Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA

8. Yu-Min Zhao at School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, P.R. China

Course Content and detailed plan

Lectures are approximately 45 min each with a small break between each lecture. The morning sessions are scheduled to end around 1230pm. Every Friday we will have presentations from each group, where a summary of what has been achieved is presented.

Lectures and preparatory material on second quantization are all available at the Github address of the course, or go to URL:https://nucleartalent.github.io/ManyBody2018/doc/web/course.ht for an easier read.

Furthermore, we strongly recommend that you read chapter 8 and 10 of Lecture Notes in Physics 936. This text contains also links to all codes we will discuss, in addition to the codes we have placed in the "program folder of the course":"https://nucleartalent.github.io/ManyBody2018/doc/web/course.html

The acronyms here stand for the different teachers:

1. KF: Kevin Fossez

2. MHJ: Morten Hjorth-Jensen

3. WJ: Weiguang Jiang

4. TP: Thomas Papenbrock

5. RS: Ragnar Stroberg

6. ZS: Zhonghao Sun

7. YMZ: Yu-Min Zhao

Week 1.

Day		Lecture Topics and lecturer
Monday	9am-1230pm	Welcome and introduction (Organizers)
		Second quantization and Hamiltonians (MHJ)
	1230pm-230pm	Lunch +own activities
	230pm-6pm	Getting started with Pairing Hamiltonian
Tuesday	9am-11am	Full configuration interaction theory (MHJ)
	1130am-1230pm	Pairing in Nuclear Physics (YMZ)
	1230pm-230pm	Lunch +own activities
	230pm-6pm	
Wednesday	9am-1030am	Full configuration interaction theory and the pairing model problem(M
	11am-1230pm	Pairing in Nuclear Physics (YMZ)
	1230pm-230pm	Lunch +own activities
	230pm-6pm	
Thursday	9am-1230pm	Full configuration interaction theory (MHJ)
		Hartree-Fock theory and links to Coupled Cluster theory
	1230pm-230pm	Lunch +own activities
	230pm-6pm	
Friday	9am-1230pm	
	1230pm-230pm	Lunch +own activities
	230pm-6pm	Group presentations of weekly work

Week 2.

Day		Lecture Topics and lecturer	
Monday	9am-1230pm	Introduction to Coupled Cluster (CC) theory (TP)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		Pairing m
Tuesday	9am-1230pm	Developing a CC code for the pairing model (TP)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		Start writi
Wednesday	9am-11am	Infinite matter and CC theory (TP)	
	1130am-1230pm	Quantum Computing and CC theory (ZS)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		Finaliz
Thursday	9am-1030am	Summary of CC theory and infinite matter (TP)	
	11am-1230pm	Machine learning applied to CC theory (WJ)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		Start wr
Friday	9am-11am	From structure to reaction theory (TP)	
	1130am-1230pm	Summary of second week and links to IMSRG (TP+RS)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm	Group presentations of weekly work	

Week 3.

Day		Lecture Topics and lecturer	
Monday	9am-1230pm	SRG theory (KF and RS)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		C
Tuesday	9am-1230pm	IMSRG and infinite matter (RS)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		Start cod
Wednesday	9am-1030am	Summary IMSRG theory (RS)	
	11am-1230am	Bergreen basis, the continuum and IMSRG (KF)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		
Thursday	9am-1230pm	Bergreen basis, the continuum and IMSRG (KF)	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm		
Friday	9am-1030am	Summary Bergreen basis, the continuum and IMSRG (KF)	
	11am-1230pm	Summary of school	
	1230pm-230pm	Lunch +own activities	
	230pm-6pm	Final group presentations	

Teaching and projects

The course will be taught as an intensive course of duration of three weeks, with a total time of 45 h of lectures, 45 h of exercises, with the possibility to complete a final assignment if credits are needed.

The organization of a typical course day is as follows:

Time	Activity
9am-1230pm	Lectures, project relevant information and directed exercises
1230pm-230pm	Lunch
230pm-6pm	Computational projects, exercises and hands-on sessions
6pm-7pm	Wrap-up of the day and eventual student presentations

Audience and Prerequisites

You are expected to have operating programming skills in in compiled programming languages like Fortran or C++ or alternatively an interpreted language like Python and knowledge of quantum mechanics at an intermediate level. Preparatory modules on second quantization, Wick's theorem, representation of Hamiltonians and calculations of Hamiltonian matrix elements, independent particle models and Hartree-Fock theory are provided at the website of the course. Students who have not studied the above topics are expected to gain this knowledge prior to attendance. Additional modules for self-teaching on Fortran and/or C++ or Python are also provided.