Developing a modern shell-model code

Thesis topics for John Bower

Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University

2016

General motivation

The nuclear shell model plays a central role as a theoretical tool in interpreting nuclear structure experiments. The aim of this thesis is to build on existing shell-model codes like the code developed by us and available, with benchmarks etc at the website of the Computational Environment for Nuclear Structure (CENS) and develop a modern (written in C++ eventually Fortran2008) full configuration interaction environment for nuclear structure studies. These codes should be able to

- Run on the next generation of supercomputers
- Be able to handle both two and three-body interactions
- Be able to handle one- and two-body operators
- Can be extended to FCIQMC studies of finite nuclei and nuclear matter
- Be fully open source and accessible

The CENS project

The CENS site contains

- Shell-model code written in C for identical particles and the proton-neutron case
- Both parallel and serial versions of the above
- Codes for one-body transition probabilities such $M\Lambda$ and $E\Lambda$ transitions but no GT transitions. There is also no code for two-body transition operators and two-body densities
- Codes for three-body forces with identical particles only

These codes can serve as starting point together with the already written FCI code by John.

Efficient algorithms for bit manipulations

In addition to the existing material, there are some useful articles and references for the first steps. The first step is to study efficient representations of the Slater determinants for words with more than 64 bits, allowing thereby for shell-model studies of systems with more than one major shell. Furthermore, the setup of the Hamiltonian matrix elements plays an important role.

In order to study these aspects and write an efficient program, the following articles can be of interest

- Scemana's article on efficient implementation of the Slater-Condon rules
- Simen Kvaal's article on developing an FCI code and open source code for quantum dots

Implementing Lanczos' and Davidson's algorithms

- add references to this
- baby steps

Addition about FCIQMC

- Add notes here