Developing a modern shell-model code

Writing a full configuration interaction code for nuclear structure studies

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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 (collaboration with Oak Ridge National Lab)
- 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 shell model codes.
- Codes for one-body transition probabilities such as $M\Lambda$ 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 (open source code) for quantum dots

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The various steps with the addition of Lanczos' and Davidson's algorithms

The first steps will consist of

- Finalize the bit representation of Slater determinants with words of length larger than 64 bits in m-scheme.
- Read a general two-body interaction in m-scheme with pertinent single-particle information
- Write a code for direct methods (Hamiltonians matrices of dimension $n \times n$ with $n \leq 100000$. Here one can use for example Francis' algorithm for direct diagonalization. This implies also setting up the Hamiltonian matrix and properly accounting for the correct phase factor.
- Be able to compute the expectation value of angular momentum (and perhaps isospin).
- Extend the code to include three-body interactions in m-scheme.
- Now extend the code to larger dimensionalities by implementing the Lanczos and Davidson algorithms

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The next steps

With a functioning code for large-scale shell-model problems, the next step is to enable the computation of transition operators and one- and two-body operators. This will allow one to be able to compute various transition probabilities. The code should be able to handle

- $M\Lambda$ and $E\Lambda$
- GT operators
- Double-beta decay operators
- Spectroscopic factors and general two-body operators
- Parallelize the shell-model program

Addition about FCIQMC

A great challenge is to provide benchmark calculations for the two- and three-dimensional electron gas and infinite nuclear matter. Here, a representation of the single-particle energies in a cartesian basis is essential, see for example the PhD thesis of Gustav Baardsen.

The recently developed Full Configuration Interaction Quantum Monte Carlo (FCIQMC) method has gained a lot of attention in quantum chemistry, providing benchmark calculations for the homogeneous electron gas in three dimensions. An exciting extension of the developed shell-model code, could be to start studying infinite nuclear matter with the FCIQMC methods.

A good introduction, with programs as well, is given by Karl Leikanger's thesis