

Nuclear coupled-cluster theory
David J. Dean
ORNL

Abstract

The quantum-many body problem appears in many fields of science and dictates the behavior of many systems ranging from nanoscale materials, to quantum dots, to chemical structure and bonding, to atomic nuclei. Scientists across these fields have found that predictive theory in these complex systems often requires the application of high-performance computing and advanced computational techniques to the problem of interest. The beauty of the quantum many-body problem in nuclei is especially pronounced as we experimentally and theoretically probe regimes of very short-lived and rare isotopes. Many of these isotopes are hard to make in the laboratory and yet some of them play important roles in the production of ordinary elements during stellar burn and explosions and other applications.

In this talk, I will assess where we stand today in computationally solving the nuclear problem and how future rare isotope facilities will impact our understanding of nuclei. I will discuss the science that goes into and comes out of the nuclear problem, and then turn to implementations of coupled-cluster theory for the problem. Specific to the nuclear problem is the presence of a real three-body force. I will describe its inclusion into the coupled-cluster algorithm. Another interesting feature of the nuclear problem is weak binding that occurs in very unstable nuclei. I also will describe our work to solve the complex coupled-cluster problem utilizing a Berggren ensemble of single-particle basis states, thus enabling us to predict life times of particle unstable nuclei. I will also demonstrate recent successes of coupled-cluster theory in describing medium mass nuclei in the Ca and Ni regions.

Oak Ridge National Laboratory is operated by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.