Thesis project for PhD student Gustav Jansen: Spherical Coupled-Cluster theory for open-shell systems

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Project summary: In the last few years Coupled-Cluster theory has seen a revival in the nuclear structure community. Up until recently Coupled-Cluster theory was implemented in an uncoupled scheme (m-scheme). Although simple in its form, the m-scheme representation puts constraints on the size of the model space and the number particles considered. Recently, Coupled-Cluster with Singles- and Doubles approximation (CCSD) was derived and implemented in a J-coupled scheme. Taking the spherical symmetry of closed shell nuclei into account, and realizing that the Coupled-Cluster Singles- and Doubles similarity transformed Hamiltonian has at most two-body terms, an efficient spherical CCSD code was implemented. This representation reduces the number of non-linear equations and the computational cost dramatically, allowing us to reach into the medium mass region of the nuclear chart. Within the spherical scheme, it is now possible to reach convergence of medium mass nuclei starting from "bare" interactions. Single-reference Coupled-Cluster theory works well for nuclei with closed shells such as ^{4}He, ^{16}O and ^{40}Ca, see Ref. [1]. Extending Coupled-Cluster theory to open-shell nuclei, with one or more particles outside a closed shell is a challenging problem and has been a topic of research for several years. There exist several, complementary, approaches to open-shell systems. The usual approaches are based on multi-reference Coupled-Cluster theory, where the reference state is built from all possible configurations allowed by symmetry. In addition to the growth of numerical and mathematical complexity, these approaches often suffer from intruder states and in some cases the loss of size-extensivity. In extending Coupled-Cluster theory to open-shell system, one would ideally like to keep the simplicity of the single-reference Coupled-Cluster theory, and consistently build upon the single-reference Coupled-Cluster theory for closed shell systems. Equation-of-Motion Coupled-Cluster (EOM-CC) theory provides such a consistent framework. The basic idea behind EOM-CC is to construct the similarity transformed Hamiltonian from the Coupled-Cluster ground state solution, and then diagonalize it within a given sub-space of particle-hole excited reference states. This method can obtain both ground- and excited states of closed and open-shell nuclei. One-particle attached/removed EOM-CC has been the most common method in order to solve for systems with A $\pm$1 particles outside a closed shell. For a given approximation at the Coupled-Cluster level, e.g. CCSD, there is a natural truncation of n-particle-m-hole excitations. For CCSD, there are only 1p (1h) and 2p1h (2h1p) excited states, since any higher exciation can not connect to the similarity transformed Hamiltonian. There is also a natural extension to two-particles

attached and removed EOM-CC, and in principle any number of particles can be added or removed.

In this PhD project we intend to derive and implement all diagrams for two-particle attached/removed EOM-CC. At leading order this will include excitations of the type 2p (2h) and 3p-1h (3h-1p). It is clear that the number of configurations will be large, and eventually become a memory issue when increasing the system size (number of particles and model-space). At leading order we have $n_o n_u^3$ number of configurations where n_o is the number of occupied and n_u the number of unoccupied orbitals. As a first step the equations will be implemented in m-scheme. This approach, does however slightly violate size-extensivity due to unlinked diagrams, it has been shown that this violation affects mostly the high lying spectrum. A method which restores size-extensivity and works for open-shell systems is the Fock-Space Multireference Coupled-Cluster theory by R. Bartlett and M. Musial [2]. We will study how well the two-particle attached/removed EOM-CC approach performs by comparing ground and excited states of ^{6}He with exact diagonalization. Having assessed the quality of this approach, we intend to derive and implement a spherical particle attached/removed EOM-CC code. In this way we can target specific states of interest, and most importantly the dimensionality of the problem will decrease dramatically. Each diagram will be checked against the m-scheme code ensuring correct implementation and derivation. With this fully operational a lot of interesting physics problems can be addressed. Ab-initio calculation of the whole oxygen chain ($^{20-28}$O) will be possible. It will be very useful for obtaining a microscopic understanding of pairing densities in nuclei. Further, it will allow for microscopic calculation of neutrino-less double-beta decay. As a final application this approach will allow for the construction of an effective two-body interaction which can be input in shell-model approaches where particles move with respect to a closed core.

These topics will form the main part of the PhD thesis, providing thereby an unprecendented level of many-body physics in the derivation of effective interactions for configuration interaction. In addition, the codes will be made flexible enough to be able to include studies of hypernuclei, partly studied in Gustav Jansen's Master thesis. Furthermore, this flexibility will allow for studies of atomic systems and quantum dots as well.

The main issue of the thesis will deal with two-body interactions and equations at the level of two-particle-two-hole correlations built from an N-particle Slater determinant. However, if time allows, the inclusion of triples and three-body interactions, is an important and actual

topic.

1. G. Hagen, T. Papenbrock, D. J. Dean and M. Hjorth-Jensen, Phys. Rev. Lett. **101**, in press (2008).

2. R. J. Bartlett and M. Musial, Rev. Mod. Phys. **79**, 291 (2007) and references therein.