University of Oslo

Master Thesis

Program Documentation

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Chapter 1

Layout

My master thesis was built upon the work of Audun Skau Hansen, who, in 2015, received a Msc due to his work on the homogeneous electron gas. His paper, titled *"Coupled Cluster Studies of infinite systems"*, reviewed two different computational schemes he developed to study the infinite electron gas, using the coupled-cluster method. The layout of his program will be presented here, in the form it was when I first received it. This paper is purely meant to explain the program used for my studies. We start with the program layout.

1.1 Main.cpp

The input parameters for the program are:

- `i0` : The number of first shell
- `i1` : The number of last shell
- `iNp` : The number of particles present
- `rs` : The Wigner-Seiz radius
- `iterations` : Maximum number of iterations
- `dConvergenceThreshold` : The number of decimals in the answer
- `dRelaxation` : Relaxation of amplitude updates
- `uiStatAlloc` : Maximum size of statically allocated vectors. (use 100000 on smaller calculations

All this is presented on program startup.

1.2 Python

1.2.1 "makeIntMatrix"

Currently (as by 01/11/16) the function essentially wants to make a list V_{pppp}, where each element is a numpy matrix where the columns and rows are combinations of SP states. This means, for example, that $V_{pppp}[a,b,c,d] = \langle ab||cd\rangle$. The blocks are identified by a unique number, defined by:

$$k_{unique}(k = k_a + k_b = k_c + k_d) = k_x + k_y\Delta k + k_z\Delta k^2 \tag{1.1}$$

All combinations where $k_{unique}(k_a+k_b) \neq k_{unique}(k_c+k_d)$ give zero, thus is not stored. This is the explicit implementation of the "block"-approach.