Compiling

In its current state, the project is uncompiled. `.cpp` files prefixed with an underscore indicate that they are to be compiled into executables.

There are four main executable files, one for each section of the report:

- `_QB1.cpp` Calculates results for a hydrogen-like lithium atom
- `_QB2.cpp` Models an atom with greens function electron screening
- `_QB3.cpp` Uses the Hartree iterative method
- `_QB4.cpp` Uses the Hartree-Fock iterative method

As well as three additional files for testing other features:

- `_SingleHydrogen.cpp`
  A test file for solving the bare nucleus orbitals for any Z and l. Useful for validating results against hydrogen by using $Z = 1$ and $l = 0$
- `_QB3-fast.cpp`
  An alternative to _QB3.cpp that uses an alternate implementation of the Hartree method that scales better with $n_{splines}$
- `_QB4-fast.cpp`
  An alternative to _QB3.cpp that uses an alternate implementation of the Hartree-Fock method that scales better with $n_{splines}$

These files must be compiled alongside their dependencies:

- `matrix.cpp` A matrix class used in linear algebra systems
- `LP_solvers.cpp` Functions for using `LAPACK`
- `vector_utils.cpp` Utility functions and overloads for vectors
- `spline_eval.cpp` Wrapper functions for `bsplines.hpp`
- `potentials_and_solvers.cpp` Atomic potentials & solvers (e.g. Hartree)

And must be compiled with the flags `-llapack -lblas` to allow the use of the Fortran LAPACK libraries in LP_solvers.cpp, and the `-O3` flag.

e.g., to compile _QB1.cpp:

```
g++ _QB1 _QB1.cpp matrix.cpp LP_solvers.cpp vector_utils.cpp
spline_eval.cpp Potentials_and_Solvers.cpp -llapack -lblas -O3
```

All of these files can be compiled automatically by using the shell script "_compile.sh", and will compile to executables of the same name (including the underscore prefix).

Running / Inputs

All compiled executables are set to take arguments from command line. Arguments must be given in order, and will defer to default values if not provided. E.g.

```
_QB1 120 20001
```

Will run _QB1 with $n_{splines} = 120$ and $n_{grid} = 20001$, and will use default values for r_{Min}, r_{Max} and the output mode / folder. The "_run.sh" shell script will run the main files (_QB[1-4]) with the parameters used to generate the values in the report. Outputs will only save if the specified directory exists.

_QB1 and _QB2

Input	Type	Default	Desc
n_{spline}	Int	60	Number of modes to solve / splines to model with
n_{grid}	Int	5001	Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration
r_{Min}	Double	0.001	Minimum modelling radius
r_{Max}	Double	100	Maximum modelling radius
Output	Bool	False	Whether or not to save results that are too big to save to the screen
Output Folder	String	./outputs/B[i]/	Folder to output results to if output=true

_QB3, _QB4 and Alternatives

Input	Type	Default	Desc
n_{spline}	Int	60	Number of modes to solve / splines to model with
n_{grid}	Int	5001	Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration
r_{Min}	Double	0.001	Minimum modelling radius
r_{Max}	Double	100	Maximum modelling radius
maxits	Int	40	Maximum number of iterations in Hartree and Hartree-Fock
Tol	double	1E-6	Energy change tolerance for
Ens_to_check	Int	5	Number of energy levels to check for convergence in iterative procedures
Output	Bool	False	Whether or not to save results that are too big to save to the screen
Output Folder	String	./outputs/B[i]/	Folder to output results to if output=true

_SingleHydrogen

Input	Type	Default	Desc
Z	Int	1	Atomic number of hydrogen-like atom
L	int	0	'l' number of orbital to model
n_{spline}	Int	60	Number of modes to solve / splines to model with
n_{grid}	Int	1001	Number of grid evenly spaced radial grid points. Must of odd for Simpsons integration
r_{Min}	Double	0.001	Minimum modelling radius
r_{Max}	Double	200	Maximum modelling radius
Output	Bool	False	Whether or not to save results that are too big to save to the screen
Output Folder	String	./outputs/single/	Folder to output results to if output=true

Plotting

To generate the plots in the report, pythons scripts have been added to the pre-made output folders. Activating these should save the relevant plots to the folder.