# 4 Exercise 5. Adding a New Potential

There a number of ways to add a new potential function into the Quantics library. The easiest is to set up a dynamic library including the code for the surface - there is no need to recompile the Quantics package.

Take the potential arar.f90 and put it in a directory. Copy the file $QUANTICS_DIR/source/opfuncs/usersrf.f90 to the directory containing the new potential routines and edit it to provide the interface to the new routines. Three routines must be changed

- `udefsrf` : Define the labels to specify the potentials. Change the example label "mysrf" to something new and unique, e.g. ararpot.
- `uvpoint` : Add the call to the potential function. For case(1) edit the "call mysrf(v,gpoint)" to the name of the subroutine in the potential.
- `usersrfinfo` : Add text to be written to the log file. Again edit the text under case(1).

If more than one potential is to added, repeat for each with a new value of `hopilab` associated with the label in `udefsrf`, and new cases in `uvpoint` and `usersrfinfo` to match the new value of `hopilab`.

After this has been done compile the `usersrf.F90` and new routines together to make a shared library `libusrf.so` . Either replace the library with this name in $QUANTICS_DIR/bin/dyn_libs or set the variable LD_LIBRARY_PATH to search the new directory first. A sample Makefile is provided. This needs to be edited to change mysrf.o to the name of your potential file.

Go to a new directory to run the calculation. Set up the operator file. As this is a 1D potential, it is straightforward and is in the files directory as `arar.op`. Edit this file to add the name of the potential as given in the `udefsrf` routine, e.g. ararpot. When Quantics reads the .op file, it finds the label V as part of the Hamiltonian. This is translated as the operator ararpot. Quantics then searches the library routines and finds the operator ararpot defined in the libusrf.so library. This is translated as the number 1 (the value of hopilab), and so when the potential must be calculated the routine uvpoint is called and the first function in that routine used.

There is an input file arar.inp that will diagonalise the Hamiltonian set up in arar.op. Run this calculation. You should now be able to go into the output directory and plot the potential using showsys. You can also see the eigenvalues in the eigval file, and plot them using rdeigval.