Activity #3:
Backflow transformations with CASINO

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In this practical session we will use CASINO to generate a Slater-Jastrow-backflow wave function for an all-electron neon atom, and analyze some of the characteristics of this wave function.

1 Optimizing the backflow parameters

We shall start from a pre-optimized Jastrow factor (actually a rather simple one). Copy the files in `~train07/Neon/` to a working directory, and inspect them.

You will notice that there is an "empty" `BACKFLOW` section at the end of the file. It contains a `mu` (electron-nucleus) term and a `PHI` (electron-electron-nucleus) term.

You must modify the input file in order to carry out the optimization.

- You are going to optimize parameters other than Jastrow parameters, and in particular ones that can change the nodes of the wave function. Therefore you need to set `opt_method` to `madmin` instead of `varmin_linjas`.
- Tell CASINO to use and optimize the backflow parameters by setting `backflow` and `opt_backflow` to `T`.
- Check that you're happy with the number of configurations that are going to be generated in VMC and used in the optimization, as well as with all other parameters (the numbers given should be about fine for our purposes). Feel free to ask about anything you want to know.

Now run CASINO by typing `runqmc nnodes 4`. When finished, type `ve` to choose the best wave function. Save a copy of the initial `correlation.data` elsewhere and replace it with the best parameter file.

1.1 For the brave

Optionally, you can try any of the following:

- Try the optimization methods `emin` and `varmin` (for the latter you'd better set `vm_filter` to `T` in the input file). See which gives better results in this particular case.
- Use a higher expansion order for the backflow `PHI` function to see if you can improve your answer. You can do the same for the Jastrow F term.

2 Checking the DMC energies

Here we want to run three DMC calculations:

- One without a Jastrow or backflow (i.e., with a HF wave function)
- One with a Jastrow
- One with a Jastrow and backflow

The purpose is to compare the three energies and, hopefully, find that the HF and SJ DMC energies are the same, and the BF-DMC energy is lower.

To run a DMC calculation you have to

- Set `opt_method` to `vmc_dmc`
- Choose a target population `nconfig`; use about 100
- Set the VMC parameters so that `nconfig` configurations are written; the VMC run need not be longer than that.

- Choose an equlibration length (`nmove_dmc_equil` and `nblock_dmc_equil`)
- Choose a statistics-accumulation length (`nmove_dmc_stats` and `nblock_dmc_stats`)
- Choose a (small) timestep (`dtdmc`); about 0.002 should do

You will have to work on different directories for each of the three calculations to avoid messing the `correlation.data` files. Use the `use_jastrow` and `backflow` flags to activate or deactivate the Jastrow and backflow as appropriate.

When the calculation is finished, type `graphit`. This will let you visualize the DMC data, so that you can find when the data have become equilibrated. Then type `reblock` and give it the data it requests. When asked about block sizes, hit `CTRL-C` and type `plot_reblock`. Determine the position of the plateau (block size) and re-run `reblock` to obtain the final result.

3 Fancy plots

Add the following block at the end of the `input` file:

```
%block qmc_plot
nodes
2D
100 100
-1 -1 0
-1  1 0
 1 -1 0
0
%endblock qmc_plot
```

This will plot the wave function and nodes as you move one electron in a plane delimited by $(-1,-1,0)$, $(-1,1,0)$, $(1,-1,0)$ and $(1,1,0)$, using a 100×100 grid. Type `runqmc nnodes 1`. Then type `plot_2D -nodes 2Dnodes.dat -surf`, which will feed gnuplot with the data for you to view. Do this for the HF, SJ and BF wave functions and see what the differences are.