

Practical session #3: visualising backflow

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In this practical session we will use CASINO to generate a Slater–Jastrow–backflow wave function for a two-dimensional electron gas, and analyse some of the characteristics of this wave function.

1 Optimising the backflow parameters

We shall start from a pre-optimised Jastrow factor.

- Copy the files for the 2D HEG example to a working directory by typing

```
mkdir -p ~/your-name/thursday/act1
cd ~/your-name/thursday/act1
cp ~/CASINO/examples/electron_phases/2D_fluid/* .
```

- Edit the `correlation.data` file and add the following at the bottom:

```
START BACKFLOW
Title
  2D HEG
Truncation order
  3
START ETA TERM
Expansion order
  8
Spin dep
  1
Cut-off
  0.d0 1
Parameters
END ETA TERM
END BACKFLOW
```

This is an “empty” BACKFLOW section containing an ETA (electron–electron) term only, since there are no nuclei in this system.

- Inspect the `input` file. Notice the `free_particles` block. Make sure you understand what the information contained therein means (else ask). Modify the `input` file so that it corresponds to a single-cycle optimisation run for the Jastrow and backflow parameters by setting the following keywords:

```
runtype          : vmc_opt
vmc_nstep         : 50000
vmc_nblock        : 10
vmc_nconfig.write : 5000
opt_method        : madmin
opt_cycles        : 1
opt_jastrow       : T
opt_backflow      : T
backflow          : T
```

All of these keywords are already present in the `input` file.

- Run CASINO.
- Use `envmc` to view the VMC energies before and after optimisation, as we did on Tuesday in the optimisation activity. For book-keeping purposes, type `cp correlation.data cdata.0`,

then `cp out out.1`. Then replace `correlation.data` with the optimised parameters, `cp correlation.out.1 correlation.data`, and type `cleanup`.

2 Fancy plots

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

```
%block qmc_plot
nodes
2D
100 100
-4.5 -4.5 0.0
-4.5 4.5 0.0
4.5 -4.5 0.0
0
%endblock qmc_plot
```

This block instructs CASINO to plot the wave function and nodes as you move one electron in a square corresponding to almost the entire simulation cell, sampled with a 100×100 grid.

Set `runtype : plot` and run CASINO.

- Type `plot_2D -nodes 2Dnodes.dat -jpeg`, which produce a JPEG, which you can open with `xv 2Dnodes.dat.jpg`.
- Produce plots for both the Hartree–Fock and the Slater–Jastrow wave functions (we recommend using different directories for each case, to avoid mixing the files). In order to switch wave functions you simply need to modify the values of `use_jastrow` and `backflow` in the `input` file.
- What differences do you see in the plots? Is this what you expected?