

Generating QMC trial wave functions using CASTEP (15 minutes)

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1 Generating trial wave functions

Every QMC calculation needs a trial wave function. The first approximation to the trial wave function is usually a single Slater determinant of Kohn–Sham orbitals from a density functional theory (DFT) code. These orbitals may be expanded in plane waves, Slater functions or Gaussians. In this exercise, we will use the CASTEP plane-wave basis code to generate a trial wave function.

2 CASTEP

The CASTEP code was developed by Mike Payne and co-workers at Cambridge and is freely available to UK academics. It is also commercially available as part of the Materials Studio suite of software. For information about CASTEP, please see

<http://www.castep.org/>

3 CASTEP→CASINO example: an isolated neon atom

3.1 Periodicity

Although a plane-wave basis can in principle only be used to describe 3D-periodic systems, it is quite possible to study 0D-, 1D- and 2D-periodic systems by creating a unit cell with an appropriately large region of vacuum in the non-periodic directions. Furthermore, we normally re-represent the orbitals in a localised “blip” basis before performing QMC calculations, allowing us to discard unwanted periodicity.

In this worksheet we will study an isolated neon atom. The files can be found in the Ne_atom directory.

3.2 Pseudopotentials

With the possible exceptions of hydrogen, helium and lithium, plane-wave DFT calculations require the use of pseudopotentials. Suitable Hartree–Fock pseudopotentials for the QMC calculations can be found at

<http://vallico.net/casinoqmc/pplib/>

These pseudopotentials can be used in CASTEP for generating QMC trial wave functions.¹

Neon pseudopotentials are provided in the Ne_atom directory in case there are network problems at TTI, but you might like to check that you can download them. Open the above link to the pseudopotential library in your browser, then click on neon. To download the pseudopotential, right-click on “Tabulated” in the first row of the table and save the file as ne_pp.data. To download the corresponding atomic wave functions (needed by CASTEP), right-click on the bullet point next to “2s²2p⁶ 1S (GS)” in the first row of the table and save the file

¹You are better off using DFT pseudopotentials for geometry optimisation, etc.

as `ne_pp.awfn`. You now have the pseudopotential files needed by CASTEP. The `ne_pp.data` and `ne_pp.awfn` files you have just downloaded should be the same as the ones in the `Ne_atom` directory.

3.3 Running CASTEP

CASTEP requires (i) an `xxx.cell` file, specifying the geometry of the system, (ii) an `xxx.param` file, holding the other calculation parameters and (iii) pseudopotential files. The seed-name “xxx” can be chosen by the user for convenience.

The format of the `xxx.cell` and `xxx.param` files is very similar to that of CASINO’s input file. Furthermore, an analogue of CASINOHELP exists. E.g., to find information about the **cut_off.energy** parameter, type `castep.serial -help cut_off.energy`. To list all the keywords, type `castep.serial -help all`.

Open up the `neon.cell` file in your favourite text editor.

- The first block specifies that we are using a cubic box of volume $10 \times 10 \times 10$ bohr³.
- The second block specifies that there is a single neon atom at the origin.
- The third block tells us that we are using the `ne_pp.data` pseudopotential.
- The fourth block tells us that we are using a single **k** point at Γ .
- The last line tells CASTEP to exploit symmetry.

Open up the `neon.param` file in your favourite text editor.

- Hopefully most of the parameters are self-explanatory. If there are any parameters you are unsure about, use `castep.serial -help (parameter)`.
- One particularly important parameter is **cut_off.energy**, which defines the number of plane waves in the basis. In general, you should make sure your DFT energy is converged with respect to the cut-off energy before starting QMC.

Now you are ready to run CASTEP. Type `castep.serial neon` and wait a minute or so for it to run. Type `ls`. Several new files should have appeared, including `neon.castep`, which contains a summary of the DFT calculation. Have a look through this file.

We have generated our DFT orbitals, but we now need to convert them into a format that CASINO can read.

3.4 Running CASTEP2CASINO

The next step is easy. Type `castep2casino neon`. A new file called `neon.casino` should appear. Please type `mv neon.casino pwfn.data`, to give this file the name (`pwfn.data`) that CASINO expects.

3.5 Running BLIP

The `pwfn.data` file contains the DFT orbitals in a plane-wave basis. As discussed in the worksheet on finite-size errors, it is more efficient to represent the orbitals in a “blip” basis in real space. This also allows us to dispense with the unwanted 3D-periodicity.

Type `blip`. Choose a multiplicity of “2”, choose, e.g., “1000” points for the overlap calculation, answer “n” to the question about a kinetic-energy calculation, say “y” to the reduced-periodicity question, and enter the intended periodicity of “0”. (A periodicity of 0 means we are looking at an isolated system.) A `bwfn.data` file should appear; this holds the same orbitals as `pwfn.data`, but represented in a blip basis.

3.6 Running CASINO

By now you are hopefully an expert at running CASINO calculations. Have a brief look at the `input` file and then type `runqmc -B` to run CASINO. The calculation is set up to perform VMC without a Jastrow factor for a non-periodic system.

Use reblocking analysis to obtain the final energies and error bars. How does the kinetic energy “*K*” compare with the DFT kinetic energy reported in the `out` file (it can also be found in the header of the `pwfn.data` file)?

You have now generated an initial QMC trial wave function using CASTEP. If you wished, you could now proceed to optimise a Jastrow factor and perhaps a backflow function, and then perform DMC calculations.