Table of Contents

Transmission spectrum of a spin-polarized atomic chain

Version: 2016.3

Downloads & Links

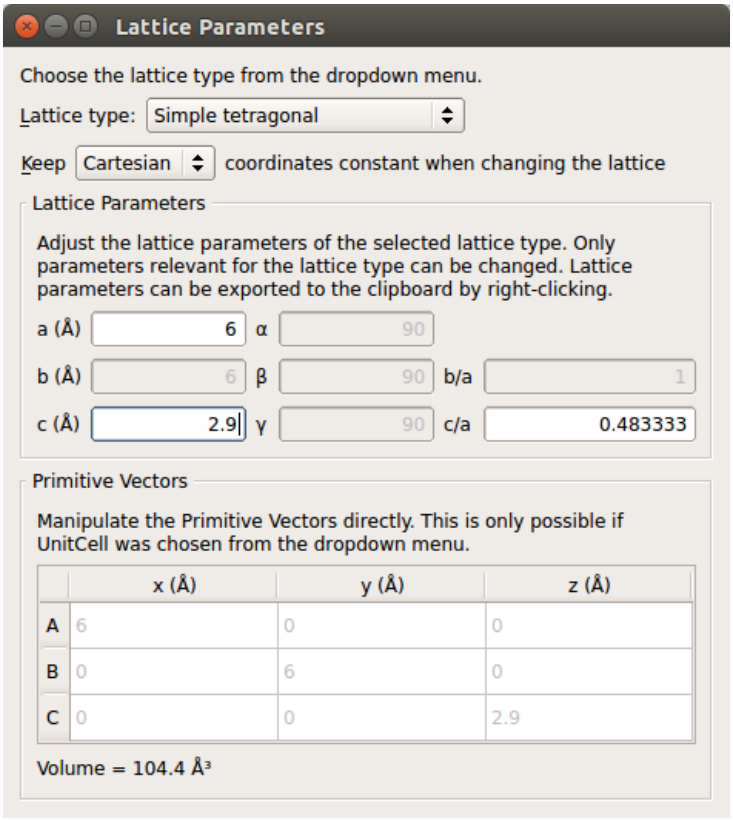
PDF version
carbon_para.py
carbon_anti.py
Basic QuantumATK Tutorial
ATK Reference Manual

In this tutorial, you will learn how to build an atomic-chain device, and calculate the spin-polarized transmission spectrum for two cases where the electrodes have parallel and anti-parallel spin-polarizations.

You will use a chain of carbon atoms to make the calculations run fast. Carbon is not naturally magnetic, but when the atom spacing in the chain is large enough – but not too large – the electronic ground state is actually spin-polarized. This system is of course highly artificial, and only chosen for the purpose of illustrating the methodology.

Building the 1D carbon chain

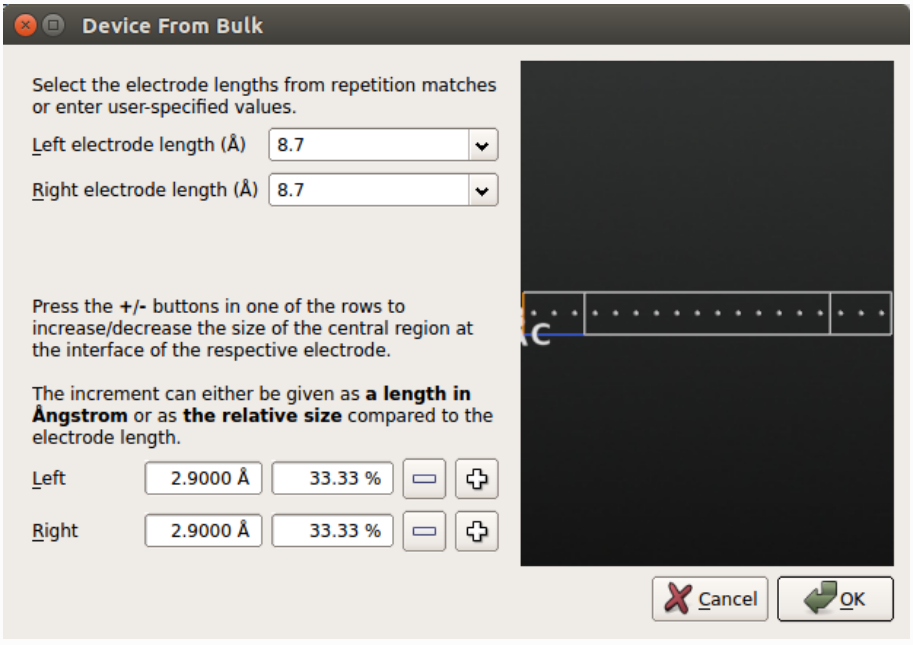
1. Open the QuantumATK **Builder**.
2. In the **Stash**, click Add ▸ New Configuration. This creates a hydrogen atom.
3. Select the hydrogen atom in the 3D view and use the **Periodic Table** tool to convert the atom to carbon.
4. Open the Bulk Tools ▸ Lattice Parameters tool and change the lattice type to **Simple tetragonal**. Then set the lattice constants to a = 6 Å and c = 2.9 Å.



Tip

Periodic boundary conditions will be employed along the A and B directions, so we use the large a = 6 Å unit cell vector to minimize electrostatic interactions between repeated images of the chain along A and B.

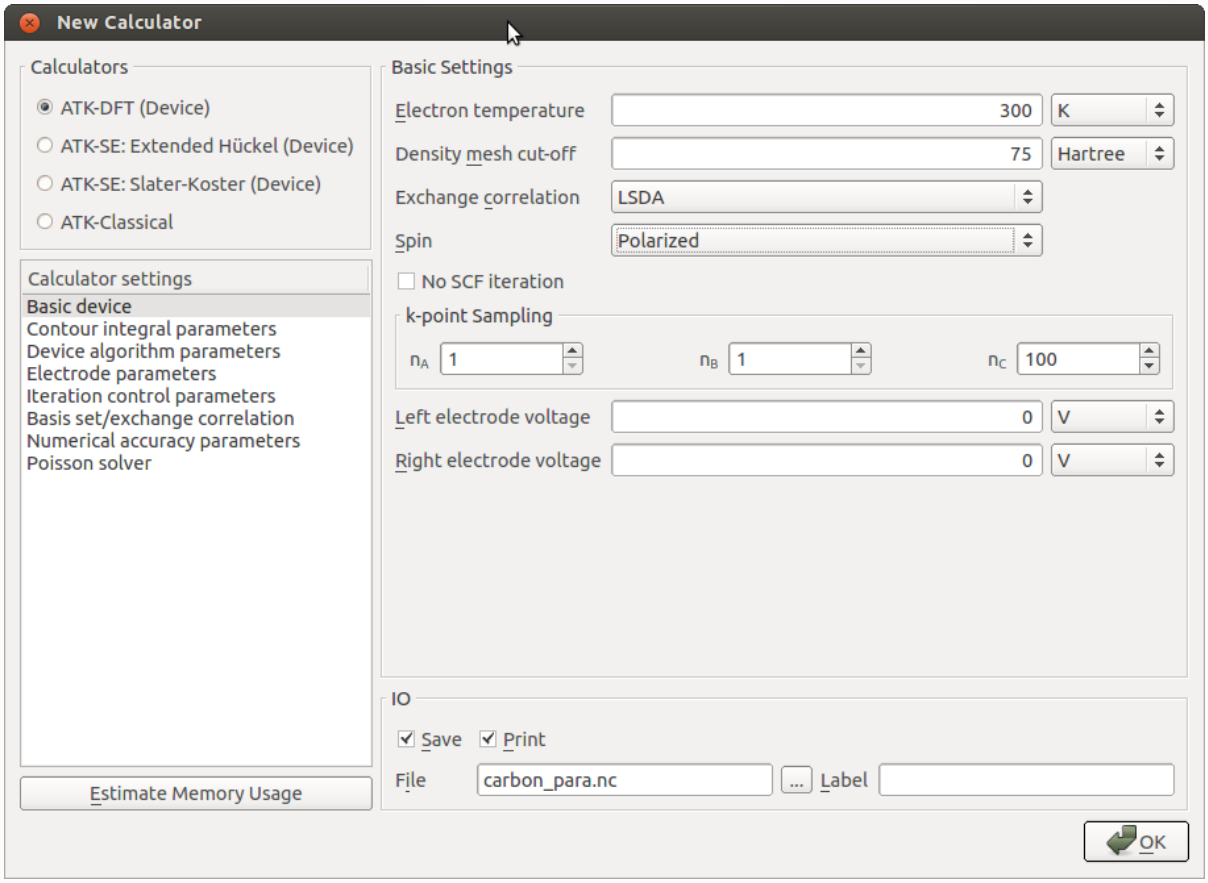
5. Click Coordinate Tools ▸ Center to center the atom in the unit cell.
6. Use the Bulk Tools ▸ Repeat plugin to repeat the system 12 times in the C direction.
7. Use the Device Tools ▸ Device from Bulk plugin to create the carbon-chain device. The automatically suggested electrode length of 8.7 Å is adequate, so just click *OK*.



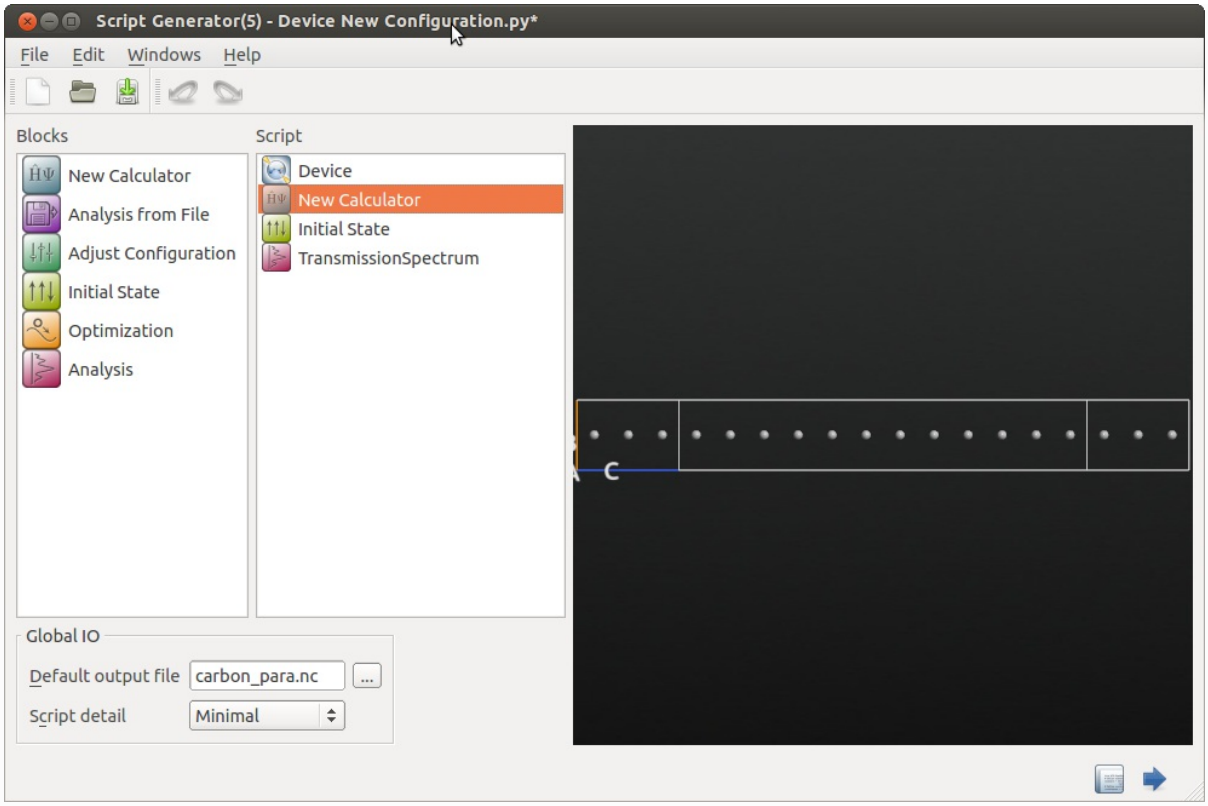
Spin-parallel transmission spectrum

You will now set up a NEGF-DFT calculation with parallel spins throughout the device, and compute the electronic transmission spectrum for this spin configuration.

1. Send the device configuration to the **Script Generator** by using the **Send to** icon in the lower-right corner of the Builder.
2. Set the **Default output file** to `carbon_para.nc`.
3. Add a New Calculator block to the script, and double-click it to open it.
4. Set the *Spin* to **Polarized**. The exchange–correlation functional will automatically switch to **LSDA**.



5. Add an Initial State block, which defines the initial spin populations. Open it and select **User spin** (all atoms now start out at maximum spin-up polarization).
6. Add a Analysis ▸ TransmissionSpectrum block. Default parameters are fine for this 1D carbon chain.



7. The QuantumATK Python script is now ready. Send it to the **Job Manager**, save the script as `carbon_para.py`, and run the calculation – it should only take a few minutes to run.

Note

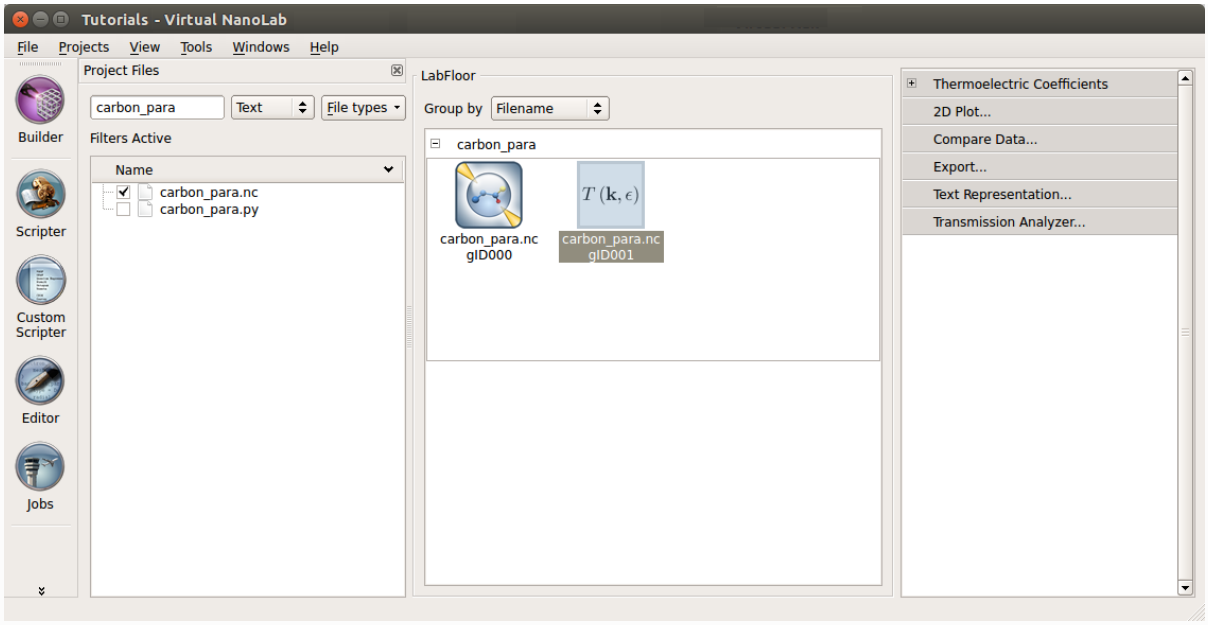
Do not close the Script Generator window – you will need it later on.

Tip

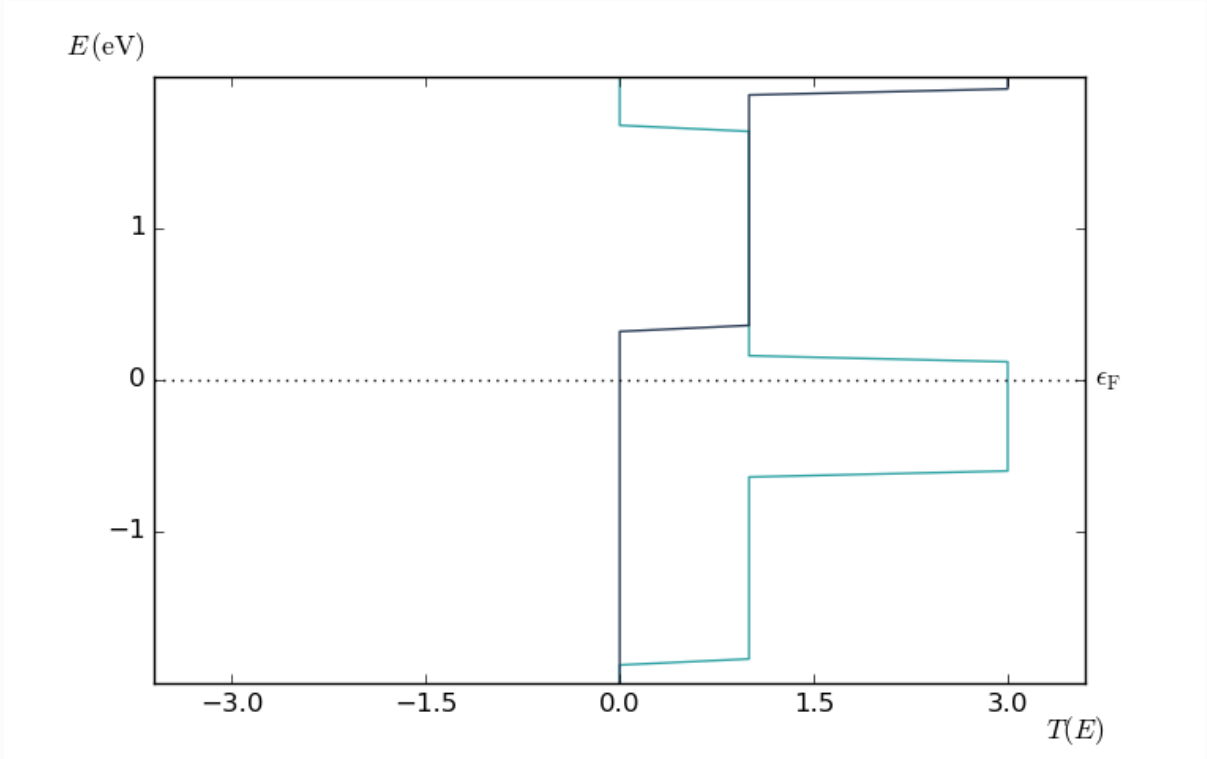
By inspecting the QuantumATK log file, note that the populations for the up/down (*DM[U]*/ *DM[D]*) electronic states are nearly the same on all atoms, as expected in an ideal system. The small differences are primarily due to the fairly low default density mesh cut-off.

Analysis

The calculated **TransmissionSpectrum** analysis object should now be available on the QuantumATK LabFloor.



Select the TransmissionSpectrum and use the **Transmission Analyzer** to plot the spin-parallel transmission spectrum.



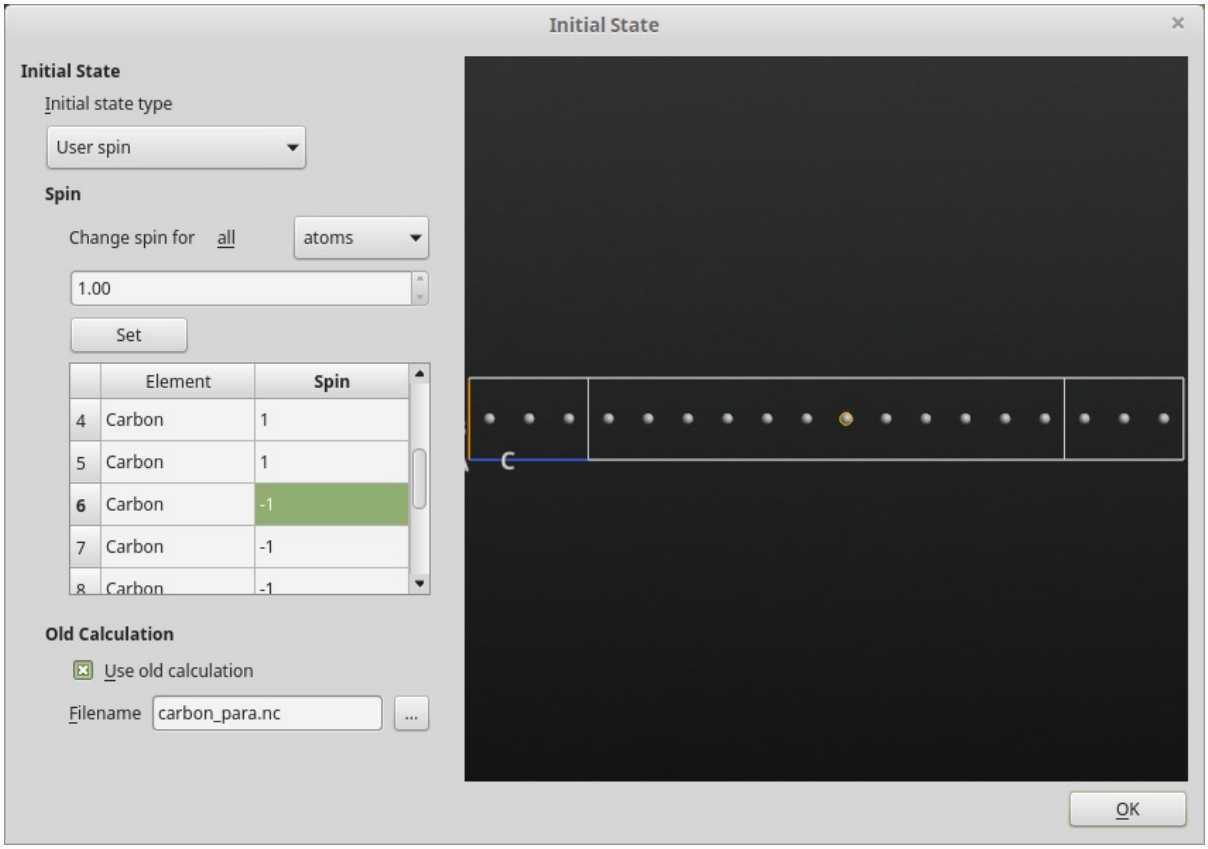
Both the up (light blue) and down (dark blue) spin components of the transmission spectrum are plotted, and they are significantly different: The spin-down transmission is zero at the Fermi level, where the (unitless) spin-up transmission is 3.

Spin anti-parallel transmission spectrum

You will now do the spin anti-parallel calculation and compare the transmission spectrum to that of the spin-parallel case. The already computed spin-parallel ground state will be used as an initial guess for the anti-parallel calculation.

Return to the **Script Generator** window and modify the settings:

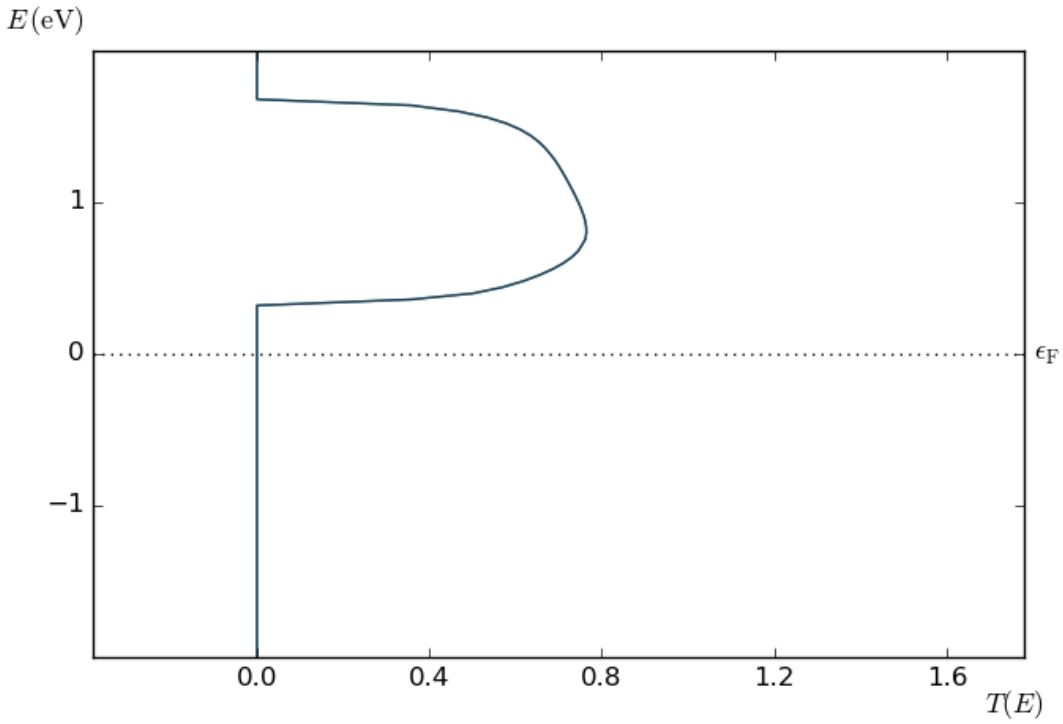
1. Change the **Default output file** to `carbon_anti.nc`.
2. Double-click the InitialState block and modify the following parameters:
   - Set the *initial state type* to **User spin**
   - Set the spin on atoms with index 6 to 11 to -1.
   - Tick **Use old calculation** and set the *Filename*, from where to read the spin-parallel ground state, to `carbon_para.nc`.



3. That's it! Save the script as `carbon_anti.py` and run it using the **Job Manager**.

Analysis

When the calculation finishes, use again the **Transmission Analyzer** to plot the transmission spectrum contained in `carbon_anti.nc`. The two spin components have, in this case, identical transmission spectra, as expected from the symmetry of the device.



Tip

If you inspect the QuantumATK log file from the anti-parallel calculation, you will see that the spin is indeed flipped in the right part of the device, where the spin-down density matrices, *DM[D]*, have higher occupations than the spin-up ones, *DM[U]*.

```
+-------------------------------------------------------------------------------+
| Density Matrix Report                          DM[U]     DM[D]      DD        |
+-------------------------------------------------------------------------------+
|   0   C   [   3.000 ,   3.000 ,   1.450 ]    2.99639   1.00028  -0.00333     |
|   1   C   [   3.000 ,   3.000 ,   4.350 ]    3.00324   0.99997   0.00321     |
|   2   C   [   3.000 ,   3.000 ,   7.250 ]    2.99536   1.00105  -0.00359     |
|   3   C   [   3.000 ,   3.000 ,  10.150 ]    3.00271   1.00275   0.00546     |
|   4   C   [   3.000 ,   3.000 ,  13.050 ]    2.96897   1.01659  -0.01444     |
|   5   C   [   3.000 ,   3.000 ,  15.950 ]    2.92841   1.08262   0.01103     |
|   6   C   [   3.000 ,   3.000 ,  18.850 ]    1.08262   2.92840   0.01101     |
|   7   C   [   3.000 ,   3.000 ,  21.750 ]    1.01660   2.96897  -0.01444     |
|   8   C   [   3.000 ,   3.000 ,  24.650 ]    1.00275   3.00271   0.00546     |
|   9   C   [   3.000 ,   3.000 ,  27.550 ]    1.00105   2.99535  -0.00359     |
|  10   C   [   3.000 ,   3.000 ,  30.450 ]    0.99997   3.00325   0.00322     |
|  11   C   [   3.000 ,   3.000 ,  33.350 ]    1.00027   2.99629  -0.00344     |
+-------------------------------------------------------------------------------+
```

Regarding the use of the spin-parallel calculation as initial state, QuantumATK will actually flip the density matrix if the initial spin (which is set in the InitialState block) is less than zero. Also, the spins in both electrodes are automatically set to match the spin configuration in the corresponding electrode extensions.

Finally, mark both the parallel and anti-parallel transmission spectra on the LabFloor, and use the **Compare Data** plugin to directly compare the total transmission in both cases. The transmission in the spin-parallel state (blue) is significantly larger than that of the anti-parallel state (green) over most of the sampled energy window around the Fermi level.