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Spin-Polarized NEGF Convergence Guide

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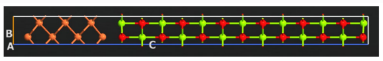
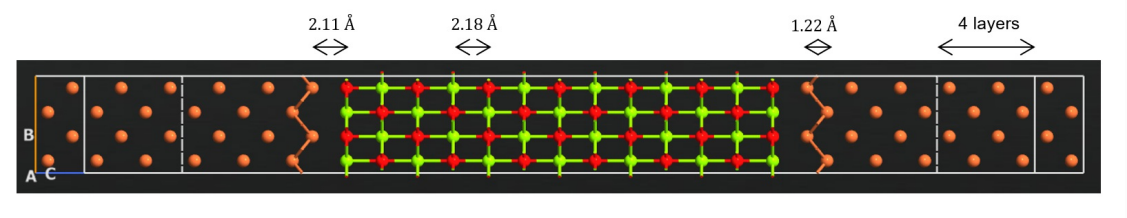
QuantumATK delivers a market-leading and highly optimized implementation of the non-equilibrium Green's function (NEGF) method for spin-polarized electron transport calculations. Achieving fast and reliable convergence of the NEGF calculation to obtain the electronic ground state can sometimes be challenging as discussed in NEGF Convergence Guide for spin-unpolarized devices. This guide provides additional guidance when dealing with spin-polarized devices, e.g., magnetic tunnel junctions (MTJ), see also Spin transport in magnetic tunnel junctions.

Systems investigated

- Fe(001)|MgO reference structure



- Fe(001)|MgO|Fe(001) magnetic tunnel junction (MTJ)



Computational parameters for the reference Fe|MgO structure

- 1×1 lateral unit cell Fe(001)|MgO.
- Dielectric layer: 13 MgO monolayers.
- Ferromagnetic metal: 7 Fe monolayers.
- Norm-conserving pseudopotential: SG15.
- LCAO basis set: `Medium`.
- K-points mesh:
  $21 \times 21 \times 1$.
- Mesh cutoff:
  150 Hartree.
- SCF threshold:
  10^{-5} Hartree
- Forces threshold:
  0.05 eV/Å.
- Geometry optimization: full relaxation of Fe and MgO structure and lattice parameters.

Computational parameters for the Fe|MgO|Fe device

- **Basic parameters**
  - 2×2 lateral unit cell Fe(001)|MgO|Fe(001) junction.
  - Dielectric spacer: 13 MgO monolayers.
  - Norm-conserving pseudopotential: SG15.
  - LCAO basis set: `Medium`.
  - Mesh cutoff:
    150 Hartree.
  - SCF threshold:
    10^{-5} Hartree.

- **Structural parameters taken from a reference Fe(001)|MgO structure**
  - Bulk Fe lattice parameter:
    $a_{\mathrm{Fe}} = 3.00$ Å.
  - Fe-O separation distance:
    $d_{\mathrm{Fe-O}} = 2.11$ Å.
  - Mg-O separation distance:
    $d_{\mathrm{Mg-O}} = 2.18$ Å.

- **Parameters that have been varied**
  - **Electrodes**
    - Length: 4 or 6 Fe monolayers
  - **Bias voltage**
    - Voltage range: 0.0, 0.05 and 0.1 V, as set in the `IVCharacteristics` study object.
  - **K-point sampling**
    - Device calculations:
      11×11 and
      15×15.
    - Electrode calculations:
      $11 \times 11 \times 151$ and
      $15 \times 15 \times 151$.

- Mixing parameters
  - Damping factor: 0.1 and 0.05.
  - Number of history steps: 20 and 12.

Calculating the self-energy matrix

- Green's-function matrix

$$G(\varepsilon) = [(\varepsilon + i\delta_+)S - H - \Sigma^L(\varepsilon) - \Sigma^R(\varepsilon)]^{-1}.$$

Σ^{L} (Σ^{R}) is the self-energy matrix of the left (right) electrode.

1. Method overview

- Equilibrium part
  - `RecursionSelfEnergy`: iterative scheme.
  - `SparseRecursionSelfEnergy`: sparse-matrix version of `RecursionSelfEnergy`.

- Non-equilibrium part
  - `RecursionSelfEnergy`.
  - `SparseRecursionSelfEnergy`.
  - `KrylovSelfEnergy`: iterative Krylov subspace method. The parameter $\lambda_{\min}$ determines the size of the subspace - only modes with a decay slower than $\lambda_{\min}$ are included.
  - `DirectSelfEnergy`: direct diagonalization scheme - all modes included.

2. Practical methods

- In practice, `RecursionSelfEnergy` and `SparseRecursionSelfEnergy` are the methods of choice for both equilibrium and non-equilibrium calculations.
- The best method for equilibrium and non-equilibrium calculations in terms of speed and memory footprint can be chosen by using `DevicePerformanceProfile` to analyze the performance of the device calculation.

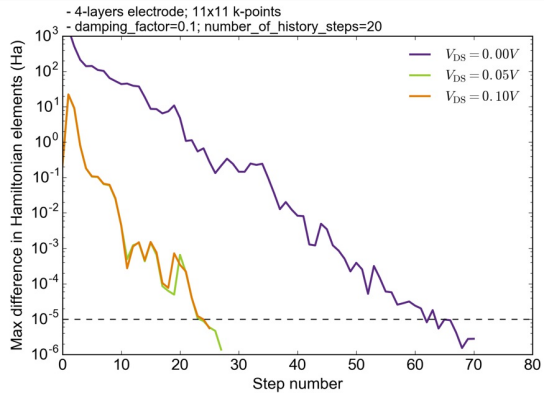
```
# Create the performance profile and print a report.
device_performance_profile = DevicePerformanceProfile(device_configuration)
nlprint(device_performance_profile)
```

```
+-----------------------------------------------------------------------+
| Device Performance Profile (1 process)                                |
+-----------------------------------------------------------------------+
| Contour point timing (s):                                             |
|                                EQ          NEQ                        |
| GreensFunction               5.10         7.49                       |
| SparseGreensFunction        23.59        11.57                       |
|                                                                       |
| Fastest EQ method (by 4.6 times): GreensFunction                      |
| Fastest NEQ method (by 1.5 times): GreensFunction                     |
+-----------------------------------------------------------------------+
| Peak memory usage/process (MB):                                       |
|                                EQ          NEQ                        |
| GreensFunction            1446.13      1913.02                       |
| SparseGreensFunction      1628.67      1589.79                       |
|                                                                       |
| Most memory-efficient EQ method (by 1.1 times): GreensFunction        |
| Most memory-efficient NEQ method (by 1.2 times): SparseGreensFunction |
+-----------------------------------------------------------------------+
```

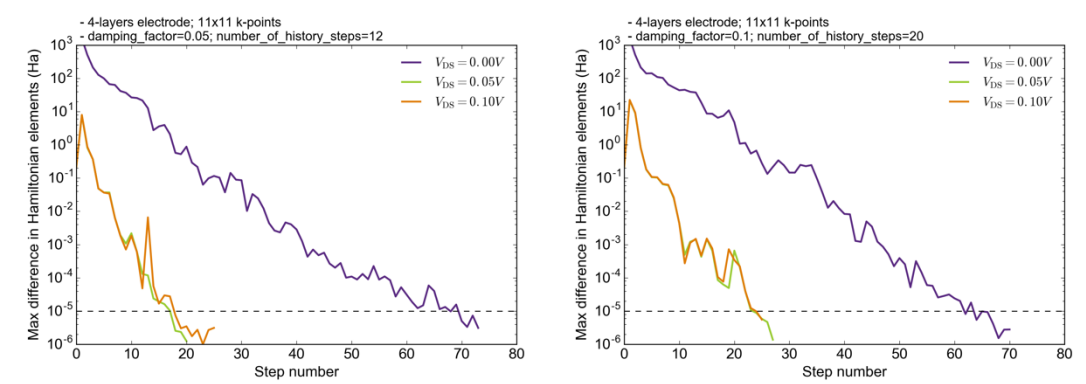
Zero and finite-bias convergence: mixing parameters

- General considerations

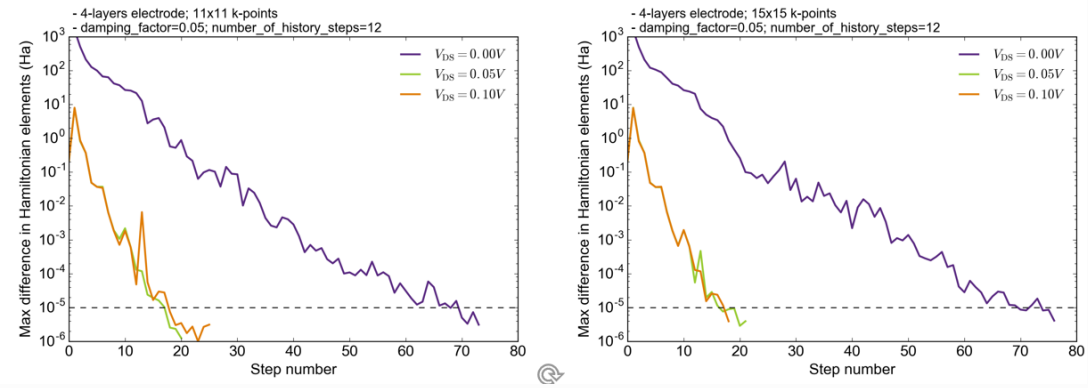
- All calculations converge, independently on the parameters used.
- The convergence is almost unaffected by the variation of the computational parameters.
- Convergence at finite bias voltages is much faster than at zero bias, because the density matrix from the most close bias voltage is used as the initial state.



- If slightly less aggressive mixing parameters are used compared to the default ones (lower `damping_factor` and `number_of_history_steps`), the convergence at zero (finite) bias voltage is slightly slower (faster).



- Increasing the `k_point_sampling` along A and B from 11×11 to 15×15 results in a slightly slower convergence at zero bias voltage, but in a faster convergence at finite bias voltages.

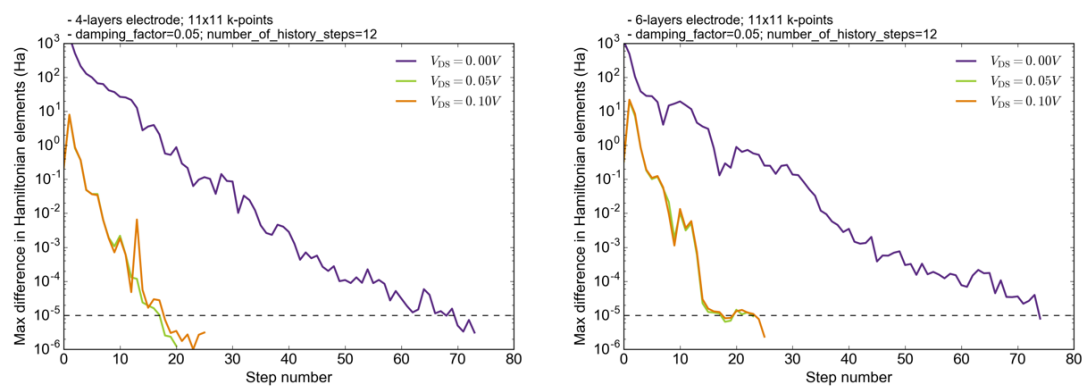


Zero and finite-bias convergence: electrode-length and k-point sampling

- Increasing the electrode length from 4-layers to 6-layers results in a slightly slower convergence at

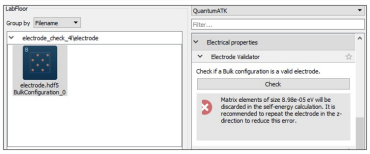
zero-bias voltage. Convergence at finite-bias voltages is very similar.

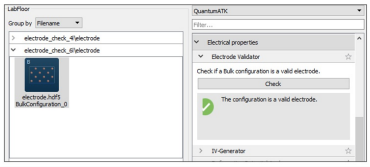
- The 6-layers electrode calculations are more memory intensive than the 4-layers electrode calculations. In case of insufficient memory, it is possible to reduce the memory footprint by re-evaluating the self-energies at each SCF step `storage_strategy=NoStorage()`.



Electrode validator

- The **electrode validator** allows one to check if the electrode repetition is sufficiently long in the C direction. The length of the electrode ultimately depends on the basis set used in the calculations.
- In the present calculations, the four-layers electrode is slightly too short and some matrix elements are discarded. *For production calculations with Fe electrodes and the SG15-Medium pseudopotential/basis set, a 6-layers electrode should be used.*





Contact support

If you failed to converge your device calculation even after following our guidelines, write a post on the online QuantumATK Forum (https://forum.quantumatk.com) or contact QuantumATK support (quantumatk-support@synopsys.com). In both cases, please attach your QuantumATK script and log file.

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