Twente Quantum Transport (TQT) code User's Guide

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1 Introduction

This document provides an introduction to the "Twente Quantum Transport (TQT)" code, what it does, how it does it, and what is required of the user to produce reliable and accurate results. The code was written to calculate spin and charge transport properties of metals like the resistivity, spin Hall angle, spin-flip diffusion length, Gilbert damping, spin-transfer torque (STT) and spin-orbit torque (SOT), spin accumulation, chemical potential, etc. This document is meant to teach you how to run the code. To perform calculations accurately, you must nevertheless be aware of what is going on inside the code. Though the details of *how* the TQT code does these things is more or less documented in the published papers [1, 2, 3], a quasi-complete mathematical summary of this is given in later chapters.

Central to the method is the scattering formalism [4] for a two-terminal device [5]. The system under investigation (e.g. a thermally disordered crystalline material) is attached to "reservoirs" by semi-infinite leads that support well-defined scattering states (Fig. 1). For crystalline leads, these states are right- and left-propagating Bloch states that are incident upon the scattering region and either reflected from it or transmitted through it. The probability amplitude that the νth right-propagating state incident from the left lead with spin σ' is scattered into the μth right-propagating state with spin σ in the right lead defines the transmission matrix element $t_{\mu\nu}^{\sigma\sigma'}$ where μ or ν are crystal momenta and band indices of the scattering states. Similarly, the reflection matrix $r_{\mu\nu}^{\sigma\sigma'}$ can be defined for right-propagating states that are reflected back into left-propagating states in the left lead. Denoting leads as left ($\mathcal{L}$) and right ($\mathcal{R}$) for a two-terminal system, we have two transmission matrices $\mathbf{t}_{\mathcal{L}\mathcal{R}}$ and $\mathbf{t}_{\mathcal{R}\mathcal{L}}$, for electrons coming from left- and right-leads, and, similarly, two reflection matrices $\mathbf{r}_{\mathcal{L}\mathcal{L}}$ and $\mathbf{r}_{\mathcal{R}\mathcal{R}}$. Together, they form the scattering matrix $\mathbf{S}$

$$\mathbf{S} = \begin{pmatrix} \mathbf{r}_{\mathcal{L}\mathcal{L}} & \mathbf{t}_{\mathcal{R}\mathcal{L}} \\ \mathbf{t}_{\mathcal{L}\mathcal{R}} & \mathbf{r}_{\mathcal{R}\mathcal{R}} \end{pmatrix} \tag{1}$$

that contains all the information needed to study a number of important physical properties of the system. The best known such property is the conductance G that can be expressed according to the Landauer-Büttiker formalism as [5, 6]

$$G = \frac{e^2}{h} \text{Tr}\{\mathbf{t}\mathbf{t}^\dagger\} \ . \tag{2}$$

The scattering formalism is not restricted to calculations of the conductance. For example the Gilbert damping can be directly determined from the scattering matrix when spin-orbit coupling (SOC) is included [7, 8, 9]. Once the scattering problem has been solved, we have a full description of the scattering wave functions throughout the scattering region allowing us to calculate spin and charge currents [3, 10] from which other transport properties can be determined.
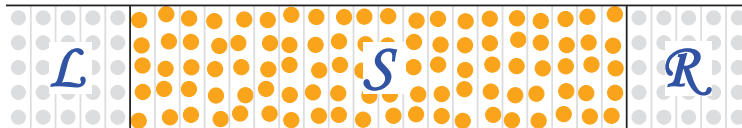

Figure 1: A sketch of a two-terminal configuration for the scattering problem. The scattering region ($\mathcal{S}$) comprising a thermally disordered lattice is sandwiched between left ($\mathcal{L}$) and right ($\mathcal{R}$) semi-infinite leads that have translational symmetry. A current flows from left to right in the direction of the z-axis.

2 Running the code

The TQT package contains two main programs: *bandfull.x* to calculate a band structure $k(\varepsilon)$ and *htrans.x* to calculate the scattering matrix **S** from which transport properties can be determined. *bandfull.x* will be discussed first since it forms essentially a subset of *htrans.x* and is simpler.

2.1 *bandfull.x*

The program *bandfull* calculates the band structure along a certain vector in **k**-space, as defined by the input. The files that are needed to run a calculation are the following:

- band.conf
- geom_b
- atomlist
- atoms/

The "band.conf" file contains the instructions to the program about how the calculation should be run. These are settings like energy range and sampling density, i.e. parameters that affect the numerical accuracy of the results, and inputs like whether spin orbit coupling should be included, i.e. parameters which affect the results qualitatively. A complete list of possible inputs is given in the *output* file, which is always generated when running the code.

The "geom_b" file contains a description of the geometry of the system whose bandstructure is being calculated. It also contains some more subtle information like the hopping range which should be taken into account. The **k**-vector along which the band structure is calculated is determined by the perpendicular translational vector.

The "atomlist" contains, as implied, a list of the atoms in the system.

As implied by the "/" symbol, "atoms/" is a folder, which must contain a file for each of the atoms mentioned in the "atomlist" file.

If all of these are present, one can call the "TQT/bin/bandfull.x" executable and produce a band structure along the given vector within the given energy range. The output will be written out into a few files. The "output" file contains information generated during the run. The bandstructure itself is output in the "plotdown.b" and "plotup.b" files. As of writing, these outputs are identical, both up and down states are written out in both files.

That is all one needs to know to calculate a band structure.

2.2 *htrans.x*

The program *htrans* calculates transport properties of the system in question. The output slightly different to the band structure calculation, but has the same general structure. The input files are

- trans.conf
- geom_l
- geom_m
- geom_r
- atomlist
- atoms/

The similarities with the band structure inputs are clear. For completeness, here is a short description of each of the files.

The "trans.conf" file contains the instructions to the program about how the calculation should be run. These are settings like **k**-point density, i.e. parameters that affect the numerical accuracy of the results, and inputs like whether spin orbit coupling should be included, i.e. parameters which affect the results qualitatively. A complete list of possible inputs is given in the *output* file, which is always generated when running the code.

The "geom_l" file is similar to the "geom_b" file for the band structure calculation. It describes the geometry of the left lead in much the same way as the "geom_b" file describes the geometry of the band structure system. It contains the exact same inputs.

The "geom_m" file specifies the scattering region, i.e. the system which is actually being studied. It has the same structure as the lead geometries, but here the perpendicular translational vector actually has no meaning.

The "geom_r" file is the geometry of the right lead.

The "atomlist" contains, as implied, a list of the atoms in the system.

As implied by the "/" symbol, "atoms/" is a folder which must contain a file for each of the atoms mentioned in the "atomlist" file.

Calling the "/TQT/bin/htrans.x" executable will calculate transport properties of the system. Some properties are only calculated when explicitly "turned on" in the trans.conf file, most importantly the interatomic currents. The output of the transport calculation is given in the "transout.h5" file. This is a special packaged file which cannot easily be opened; a program like "HD5Viewer" is needed to open it. It contains a folder structure so that all the generated values are grouped together for clarity. The postprocessing programs, which will be discussed further on in this document, take their data from this "transout.h5" file.

3 Details of the input files

Here we discuss the details of what the input files have to look like.

3.1 Geometry files

The geometry files "geom_*" (with *= l, m or r) all have the same format. An example of a geometry file is given in Fig. 2. Let us go through the variables one by one. The variable names are given on the right, after the # symbols.

- NP is the number of atoms in the geometry. To be specific, it is the number of atoms for which coordinates are given in the list below.

- NMTR is the number of translation vectors (explained below) that should be taken into account when computing the Hamiltonian for a specific cluster of atoms. This will usually be 3, in some cases 4.

- TR_PERP is the number of *perpendicular* translation vectors that should be taken into account when computing the cluster. Usually it is safe to keep this at 1.

- CUTRAT is the cutoff radius for the size of the sphere for which interactions between atoms are included in the calculation of the Hamiltonian. The second parameter in this line does not concern us at this point, in LMTO calculations it should be omitted (it is only used in EMTO calculations).

Figure 2: The geometry file for the left lead, or the geometry file for a bandstructure calculation. The geometry describes the FCC lattice for platinum, with the perpendicular translational vector pointing in the [111] direction.


```
------========== GEOMETRY  FILE ==========-------
    1       3       1                        # NP,  NMTR,TR_PERP
    2.700000    7.415106                     # CUTRAT
    3       3                                # SC_SIZE
      0.7071068      0.4082483      0.5773503  # SCALING FACTORS
      1.000000      0.000000                 # 1ST TRANSL. VECTOR
     -0.500000      1.500000                 # 2ND TRANSL. VECTOR
      0.000000      1.000000      1.000000   # PERP.TR. VECTOR
      0.000000      0.000000      0.000000   Pt_B
------========== END OF GEOMETRY ==========-------
```

- SC_SIZE describes the "SuperCell Size" and is not relevant for the band structure calculation, where it will always be "1 1", but for transport calculations, the size of the lateral supercell in the leads needs to be large enough (i) to match with the size of the scattering region and (ii) to adequately describe disorder. The numbers are the number of translational vectors which define the lateral supercell.

- SCALING FACTORS are scaling parameters (lattice parameters in nm?) for all of the coordinates given below this point. This is so that the values written for the coordinates can be nice, round numbers, as they are in the example.

- 1ST TRANSL. VECTOR is the first vector which describes the lateral supercell in 2D.

- 2ND TRANSL. VECTOR is the second vector which describes the lateral supercell in 2D. In this case, the two translational vectors describe a close packed plane. Note that these vectors cannot have components in the z-direction.

- PERP. TR. VECTOR describes how the layers defined by the 1ST and 2ND translational vector are stacked to form the full crystal. In the example, the vector describes the ABC stacking of the close-packed planes of the FCC lattice.

- Pt_B are the coordinates of the atom. In this case, there is only one. The total number of atoms should equal NP. Every atom needs three coordinates as well as a label. This label should be identical to the one mentioned in "atomlist" as well as the file in the "atoms/" folder.

3.2   Config files

The *.conf files (*= band or trans) also have a similar structure, though some inputs are only relevant for the band structure calculation and others only for the transport case. Fig. 3 contains an example of the band.conf file for a particular calculation. Note that this is not necessarily a complete list of all possible flags, but it does contain the minimum.

- NUM_POINTS is the number of points the energy range should be divided into

- ENERGY_FROM is the lower energy bound

Figure 3: Example of a band.conf file, which contains flags for a band structure calculation.

- ENERGY_TO is the upper energy bound

- KPAR is the parallel **k** vector for which the band structure should be calculated.

- EIGVAL_SOLVER is not a necessary tag. It determines which solver should be used, but 15 is almost always the best one.

- SO_ON is the tag turns on spin orbit coupling. It is not necessary, if ommitted it will be assumed =0.

- EQUATION_TYPE determines what equation is actually solved. There are multiple options; one can choose to only solve the [P-S] equation, or just the two-centre Hamiltonian [H], or the three-center one [H-HOH]. Switching to the EMTO code also goes via this tag. Then the Kink matrix [K] is the Hamiltonian.

A detailed list of each flag can be generated by running the code with an empty .conf file.

Fig. 4 is an example of a trans.conf file. Some tags are identical to the band.conf file, others are different.

Figure 4: Example of a trans.conf file, which contains flags for a transport calculation.

- LOGLEVEL determines the verbosity level of the output

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- EQUATION_TYPE determines the equation type to be solved (see band.conf case)

- ENERGY_OFFSET sets the energy level away from the Fermi level defined by the atoms. Via this tag one can calculate Fermi level dependent properties, if one wishes.

- EIGVAL_SOLVER is identical to band.conf, usually set at 15.

- BZ_NUM_KPOINTS is important; it determines the density of the **k**-point grid in the parallel **k** vector defined by the lateral supercell. The total number of **k**-points equals $(2*N-1)^2$, where $N =$BZ_NUM_KPOINTS. This way, the **k**-grid is guaranteed to include the Γ point, and is symmetric about it.

- DO_IATCU sets whether or not the interatomic currents should be calculated.

- SO_ON is the spin orbit coupling.

- DO_LEFT_TO_RIGHT determines if the left-to-right calculation should happen.

- DO_RIGHT_TO_LEFT determines if the right-to-left calculation should happen. To obtain reliable results for interatomic currents and chemical potentials, both left-to-righ and right-to-left should be done.

There are many other tags which can be set, which affect the calculation in one way or another. A complete list can be generated by running the code with an empty .conf file. Even with a non-empty .conf file, the "output" file will contain a complete list of the possible flags.

4 Potential files

If you were given potential files in a "atoms/" folder with an "atomlist" file, you need not be too concerned with what is in them. If you trust the capabilities of the person that made them, that is. The outcome of the calculation depends on the electronic potentials you input for the atoms, especially in the details. Therefore, it is important that any user of this code understands the potentials they are using, where they came from, and why they may or may not be adequate for the calculation. To name an example, when doing a transport calculation for Platinum, it matters whether the input potential has self-consistenly included spin orbit coupling or not, since it changes the density of states at the Fermi level. Since our transport happens at the Fermi level, this has substantial effect on the outcome of (e.g.) the value of the spin Hall angle. Understanding what is written in the potential files is one thing, generating them is another. We do not concern ourselves with this for the moment. Let us instead look at an example and describe the flags.

Figure 5 contains an example of a potential file, in this case for iron (Fe). In order of appearance, the parameters are the following (note that they are comments; in principle only the numbers are needed to be a valid file):

- NL is the number of partial waves (3 is spd, 4 is spdf).

- line with FEB are the screening parameters, there are 3 of them for spd, 4 of them for spdf.

- empty line are the atomic number and Wigner Seitz radius

- EF is the Fermi level

- potential shift can be used to raise or lower the potential by a constant, if necessary

- Swap spin not sure what this does, actually

- NS is the number of spins (1 or 2)

- FEB this line is the number of radial points.

Figure 5: Example of a potential file, which contains parameters for the electronic potential inside a sphere, as well as the radial potential $V(r)$.

Figure 6: Example of an atomlist file for a system containing only one type of Pt atom.

- everything after is the potential.

Generally, these values are determined by the way the potential was generated. The values should not really be tinkered with, since they are determined by a self-consistent DFT calculation (hopefully). If you would like to change one of the parameters, chances are you are going to have to do a self-consistent calculation and extract potentials from there. A notable exception is the Potential shift parameter, which can be adjusted freely, should one be so inclined. I myself have never touched this value, for what it's worth.

The atomlist file is very straightforward, any example of it will be selfexplanatory. See figure 6. Note that the mass is a comment and does not actually play a role in the transport calculation. The only relevant parts are the number of atoms, their labels and their filenames in the "atoms/" folder. Note that they can be different, although it is usually convenient to keep them the same.

5 Examples

In the /TQT/ directory, one can find a subdirectory called /samples/ which contains examples of some calculations, with all the necessary files included. We will discuss three calculations here. They will be

1. a band structure calculation (for Pt)

2. a Fermi surface projection calculation (for a Cu|Co [111] interface)

3. a spin Hall calculation (for Pt)

5.1 Band structure of Pt [111]

In the /samples/band/Pt111-SOC/ folder, you can find all the files you need to calculate the band structure of Pt in the $\Gamma \to L$ direction. This **k**-vector orientation is fully determined by the perpendicular translational vector. A different high symmetry line can be accessed by rotating the geometry. All of the files are provided, all you need to do is run the calculation, either on the machine you are using or the cluster. Band structure calculations can be quite quick, so they can be done locally, but in general it is good practice to use the cluster for such things. How to submit jobs is a question for another document. It is a good idea to look at the input files (geometry and config) and think about what changing some of these parameters would do to the band structure. For instance, turning off spin orbit coupling has a substantial effect.

After running the calculation, a few new files will appear in the folder. There is the "output" file, which contains a list of all possible flags, and the values that were used in the calculation as well as two plot*.b files, which contain the band structure points. You can use your favourite plot-software to visualise the bands and confirm that they are correct. In Fig. 7, the expected output is plotted.

5.2 Fermi surface projection of CuCo [111]

Now we are going to use the transport code to calculate the Fermi surfaces of Cu and Co, as well as the projection of the one on the other, for the [111] interface. The files are in /samples/transport/CuCo111/. We will make an edit to the trans.conf file, right now the number of BZ points is very low; let us edit it from 2 to 50. Also, we will comment out the BZ_SYM and BZ_INVE tags. They are ways of saving computing time by making use of the symmetry of the Brillouin zone, but they make the postprocessing a little more complex, so we omit them for the moment. If you have done this, you can run the /TQT/bin/htrans.x executable and obtain the transout.h5 file. This will contain all the output data we are interested in.

The HDF5 file which contains the output is not straightforwardly opened. One needs a viewer (I use HD5Viewer), or one needs to extract the relevant tables with Python or Matlab. My advice is to download the viewer first and look through the HDF5 folder, so that one gets an idea of what is where. There are two relevant folders at this point; the /bz/ folder and the /trans/ folder. In the /bz/ folder, there is a table called 'k' which contains the (k_x, k_y) information. The /trans/ folder contains information for each of the **k**-points.

The nmodesl table is the number of modes in the left lead. The nmodesr table is the number of modes in the right lead. The ll, lr, rl, and rr tables contain reflection and transmission values for each **k**-point.

/HD/:q

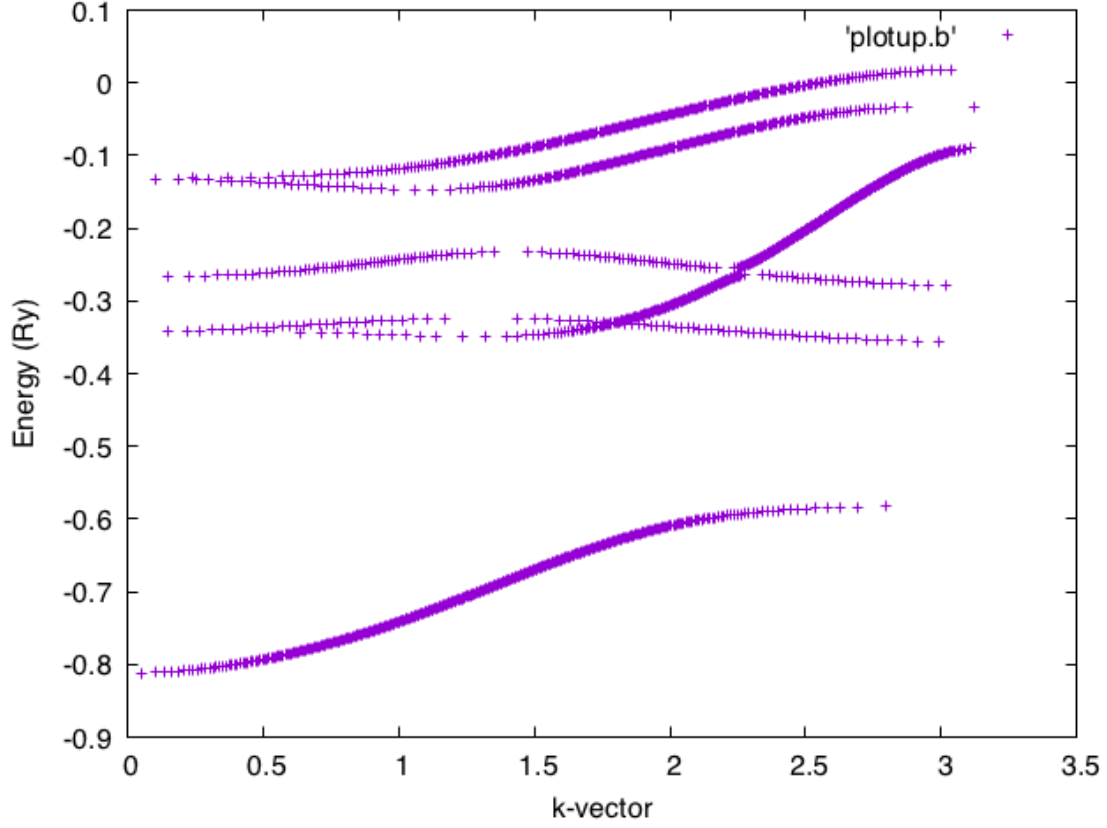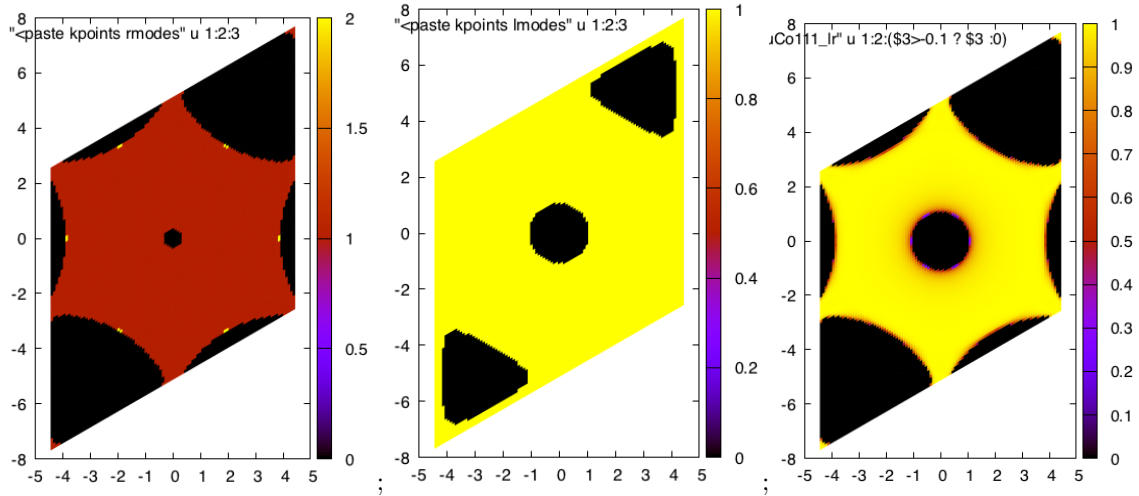Figure 7: Band structure of Pt $[\Gamma \to L]$ in LMTO basis.

Figure 8: Left: Co majority spin Fermi surface projection. Middle: Cu Fermi surface projection. Right: CuCo [111] transmission probabilities.

5.3 Spin Hall angle of Pt

In this example we will calculate the spin Hall angle of Pt using the files in the folder /samples/transport/Pt111SHA/. It is a little bit more involved since as you can see, there are no geometry files yet. We will be generating these and introducing temperature in the form of Gaussian disorder as part of the example. After the calculation is done, we will use another program to extract the interatomic currents from the HDF5 output file and convert them into a usable format. From these currents we can determine the spin Hall angle.

We will use the *db2geom.x* program to generate the geometry. The file "multilay_input" contains the information about the geometry we are going to generate. In order of appearance,

- "number of slabs" is the number of different layers making up the system. For example, one might be interested in a Pt|Au interface in which case there would be 4 layers. The reason we have to include two outer layers without any displacement has to do with the implementation of the code.

- "supercell" is the lateral supercell size. The memory usage scales rapidly with this quantity, since the lead-scattering region coupling scales poorly with it. One should be careful to use supercells which are large enough.

- "number of configurations" refers to the number of disorder configurations over which we will average. Whether we are interested in thermal disorder or alloy disorder, an ensemble average needs to be carried out.

- "D" is the rms displacement that characterizes a Gaussian distribution. Units? Individual atom displacements are random (well, as random as a computer can be) and will have a root mean square value equal to this number. Because it's Gaussian, the average displacement will be zero. One can generate geometries for multiple rms displacements in one go, by defining e.g. D = 0.127, 0.130.

- "K" is an integer describing the length of the scattering region as a number of atomic layers. Because we calculate the resistivity of a material from the slope of a resistance versus length curve, we need to specify the length. Multiple lengths are separated by commas, e.g. K = 60,80,100

- "Slabs" section. The first string "Pt_SOC_sc" is the label of the atom type. This must be the same as one of the files in /TQT/potdb/. The atom-data will be pulled from there.

- "scvec" these vectors describe the FCC lattice. This code is only meant to generate geometries for that specific system (don't ask me why). There are other programs included in the package which can generate geometries more freely, as well as implement thermal disorder, but we don't discuss them here.

- "nlay" is the number of layers of this atom type, with the given stiffness and rms values.

- "stiff" describes how stiff the lattice should be with regards to lattice matching.

- "rms" is the root mean square displacement of the Gaussian disorder. It represents temperature. Units? Relationship to "D"?

To run the db2geom.x code in this folder with the "multilay_input" file explained above, simply type ~/TQT/bin/db2geom.x. This generates the (output files "dirlist" and "dirloop" as well as the) directory "D0.127/K100/" which contains a "number of configurations" folders, cf-i (i=1-"number of configurations") each with its own geometry files (i: interface; l: left lead; m: middle, scattering region; r: right lead)

- geom_i

- geom_l
- geom_m
- geom_r
- "atomlist", a link to a list of atomic species (e.g. bulk Pt, interface Pt, surface Pt) and
- "atoms", a link to the corresponding directory of potential files,
- vis.pdb, a file which specifies the scattering geometry (a list of atoms detailing the atomic species and its position in the scattering region).

One more thing needs to be done: the trans.conf file needs to be copied into each of the cf-i configuration folders by hand. The db2geom.x program doesn't do this, unfortunately. The "runscript" file is the job script which can be submitted to the compute nodes by running "sbatch runscript".
After the job has finished, there will be output files called

- "andout"
- "output"
- "times"
- "transout.h5"

in each of the cf-i configuration folders. The program (qofz) which extracts the currents and processes them is smart enough to read the "dirlist" files which are present in each of the sub-folders, so that we can run it from the top folder and still process all of them. To do so, execute ~/TQT/bin/qofz.x from D0.127. The processed currents will be output in a folder in /D0.127/K100/plots. One can extract the SHA simply by looking at the average value of the third column of Lxcur_ps.dat and the second column of Lycur_ps.dat (multiplied by minus one). These values are the j_{sy}^{x} and $-j_{sx}^{y}$ currents which are generated by the spin Hall effect.
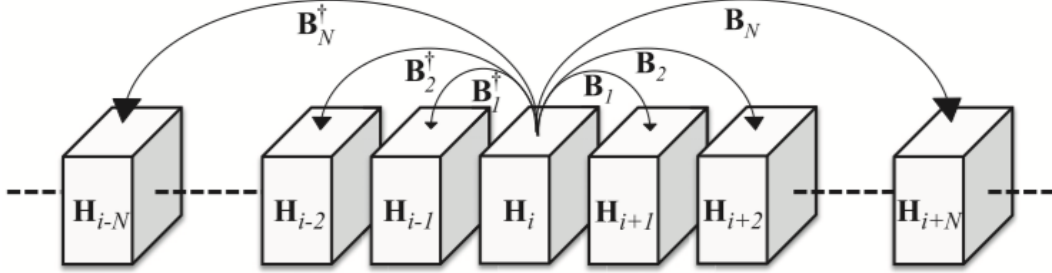
6   What the code actually does

The previous sections were all concerned with how to run the code, but it's useful for any user to know what is actually happening when one presses run. In this section I will try to give an comprehensible overview of what the code does.

6.1   The scattering problem

In essence, we are simply solving the time-independent Schrödinger equation

$$(\mathbf{H} - E\mathbf{I}) \Psi = 0 \,, \tag{3}$$

for some system under study. We are interested at transport properties at the Fermi level, so that the energy $E = E_F$ can be inserted. Transport is modeled by the same procedure as the very first Quantum Mechanics exercise one does as a student: there is an incoming wave from the left and we calculate the probability of transmission through a barrier or over a step. In the analogy, the barrier is the scattering region and the semiinfinite spaces to the left and to the right of the barrier are the leads.

We could very well do this very calculation; vacuum can be simulated by filling the leads with empty spheres so that this precise problem is being studied. In practice, we are interested in the behaviour of electrons in solids, so for the leads we usually choose the same material as the scattering region. This also makes sure that the lattice is properly matched. The electronic properties of the leads manifest mathematically as boundary conditions for the Schrödinger equation.

6.2   Eigenstates of the leads

Though the title of this subsection suggests that it is only relevant for the transport calculation, it is actually important for the band structure calculation as well. In reality, the routine which calculates the eigenstates of the leads is the same as the band structure calculator. We consider an infinitely long wire partitioned into layers which each contain N_O atom centred orbitals and are coupled to N layers on either side. An illustration of this system can be seen in fig. Fig. 9. By defining matrices $\mathbf{B}_l := \mathbf{H}_{i,i+l}$ and $\mathbf{B}_l^\dagger := \mathbf{H}_{i,i-l}$ we can write down the time-independent Schrödinger equation simply as

$$(E\mathbf{I} - \mathbf{H}_i) \Psi_i + \sum_{l=1}^{N} \left(\mathbf{B}_l \Psi_{i+l} + \mathbf{B}_l^\dagger \Psi_{i-l} \right) = 0 \,. \tag{4}$$

On the other hand, we can write the wave function in the l layer in terms of the wave function in the $l-1$ layer by multiplying it with a Bloch factor,

$$\Psi_l = \lambda \Psi_{l-1} \tag{5}$$

where $\lambda \in [0, 1]$. Inserting this equation into the Schrödinger equation leads to a generalized eigenvalue problem

$$\left(E\mathbf{I} - \mathbf{H}_0\right)\Psi_0 + \sum_{l=1}^{N-1}\left(\mathbf{B}_l\Psi_l + \mathbf{B}_l^\dagger\Psi_{l-1}\right) + \mathbf{B}_N^\dagger\Psi_{-N} = -\lambda\mathbf{B}_N\Psi_{N-1}\,, \tag{6}$$

where $i = 0$ has been assumed. The solutions to this equation can be separated into right-moving and left-moving states, which determine the boundary conditions on the scattering problem. The eigenvalues themselves are nothing more than a Bloch factor, i.e. $\lambda = e^{-ikz}$, so that the value of k can be extracted from it. This is what the band structure calculator does. The transport calculation also needs the eigenvectors in a particular way. It constructs matrices

$$\mathbf{U}(\pm) = (\mathbf{u}_1(\pm)...\mathbf{u}_{N_O}(\pm)) \tag{7}$$

which contain the right (left) moving eigenvectors. Any right (left) moving wave can then be expanded as the linear combination of eigenvectors

$$\Psi(\pm) = \mathbf{U}(\pm)\mathbf{C}(\pm)\,, \tag{8}$$

where $\mathbf{C}(\pm)$ is a vector of coefficients. Defining diagonal eigenvalue matrices as $\mathbf{\Lambda}(\pm) = \delta_{nm}\lambda_{mn}(\pm)$, the translation of the wave function at layer i over some number of layers l can be written as

$$\Psi_{i+l} = \mathbf{F}^l(+)\Psi_i(+) + \mathbf{F}^l(-)\Psi_i(-)\,. \tag{9}$$

This will be useful in the next section, when we define the solution for the whole system.

6.3   Solution for the whole system

In this section we will introduce the scattering region in between the two leads and match the wave funciton properly. The scattering region will be treated as one giant block with a Hamiltonian $\mathbf{H}_S$, which describes all of the hopping between atoms inside the region. There will be some range of interaction between the scattering region and the leads, such that in order to competely encapsulate the hopping, we need only include some finite number of lead layers into the scattering mechanism. That is, we assume there are $N+1$ lead layers which have some interaction with the scattering region. These layers are labeled $-N, .., 0$. Figure 10 shows what the geometry looks like.

Within the language used earlier, the scattering region takes the form of a giant meta-layer sandwiched between the leads, which each consists of an infinite number of layers. When considering the Schrödinger equation for the system, we note there must be some finite number of lead-layers $N+1$ which directly interact with the scattering region. That is, in the left lead, for any layer with index $-(N+j)$ where $j > 0$, we can use the solution found in the last subsection to write

$$\mathbf{\Psi}_{\mathcal{L},-N-j} = \mathbf{\Psi}_{\mathcal{L},-N-j}(+) + \mathbf{\Psi}_{\mathcal{L},-N-j}(-) \tag{10}$$
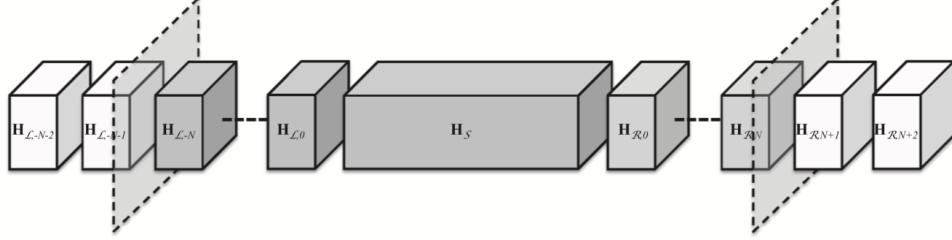
$$= \mathbf{F}_{\mathcal{L}}^{-j}(+)\mathbf{\Psi}_{\mathcal{L},-N}(+) + \mathbf{F}_{\mathcal{L}}^{-j}(-)\mathbf{\Psi}_{\mathcal{L},-N}(-) \tag{11}$$

$$= \left[\mathbf{F}_{\mathcal{L}}^{-j}(+) - \mathbf{F}_{\mathcal{L}}^{-j}(-)\right]\mathbf{\Psi}_{\mathcal{L},-N}(+) + \mathbf{F}_{\mathcal{L}}^{-j}(-)\mathbf{\Psi}_{\mathcal{L},-N}\,. \tag{12}$$

For the layers with index $n \in [-N, 0]$ of the left lead, the Schrödinger equation reads

$$\left(E\mathbf{I} - \mathbf{H}_{\mathcal{L},n}\right)\Psi_{\mathcal{L},n} + \sum_{l=1}^{-n}\mathbf{B}_{\mathcal{L},l}\Psi_{\mathcal{L},n+l} + \mathbf{B}_{\mathcal{L}\mathcal{S},n}\Psi_S + \sum_{l=1}^{N}\mathbf{B}_{\mathcal{L},l}^\dagger\Psi_{\mathcal{L},n-l} = 0\,. \tag{13}$$

Figure 10: Geometry of the finite scattering region with attached leads. The number of lead layers N is chosen such that there is no interaction between the scattering region and the (white) infinite leads.

The first term contains the on-layer contributions, the second term is the hopping from layer n to all layers with a higher (closer to 0) index, the third term is all hopping from layer n to the scattering region, and the last term is any hopping from layer n to any layer with a lower (i.e. more negative) index. It is within this term that we can use (12). The Schrödinger equation becomes

$$\left(E\mathbf{I} - \mathbf{H}_{\mathcal{L},n}\right)\mathbf{\Psi}_{\mathcal{L},n} + \sum_{l=1}^{-n}\mathbf{B}_{\mathcal{L},l}\mathbf{\Psi}_{\mathcal{L},n+l} + \mathbf{B}_{\mathcal{L}\mathcal{S},n}\mathbf{\Psi}_S + (1-\delta_{N,-n})\sum_{l=1}^{N+n}\mathbf{B}_{\mathcal{L},l}^{\dagger}\mathbf{\Psi}_{\mathcal{L},n-l} + \sum_{l=N+n+l}^{N}\mathbf{B}_{\mathcal{L},l}^{\dagger}\mathbf{F}_{\mathcal{L}}^{-l+N+n}(-)\mathbf{\Psi}_{\mathcal{L},-N}$$

$$= -\sum_{l=N+n+1}^{N}\mathbf{B}_{\mathcal{L},l}^{\dagger}\left[\mathbf{F}_{\mathcal{L}}^{-l+N+n}(+) - \mathbf{F}_{\mathcal{L}}^{-l+N+n}(-)\right]\mathbf{\Psi}_{\mathcal{L},-N}(+)\,,$$

$$(14)$$

where $\mathbf{B}_{\mathcal{L}\mathcal{S},n}$ is the hopping matrix from layer n to the scattering region. The Schrödinger equation for the right lead is similar, but simpler, since in the right lead, only right-moving states can exist, so for any layer with index $N+j$ where $j>0$, we have

$$\mathbf{\Psi}_{\mathcal{R},N+j} = \mathbf{F}_{\mathcal{R}}^{j}(+)\mathbf{\Psi}_{\mathcal{R},N}\,. \tag{15}$$

The Schrödinger equation for the layers of the right lead with index $n < N + j$ becomes

$$\left(E\mathbf{I} - \mathbf{H}_{\mathcal{R},n}\right) + \sum_{l=1}^{n}\mathbf{B}_{\mathcal{R},l}^{\dagger}\mathbf{\Psi}_{\mathcal{R},n-l} + \mathbf{B}_{\mathcal{R}\mathcal{S},n}^{\dagger}\mathbf{\Psi}_S + (1-\delta_{N,n})\sum_{l=1}^{N-n}\mathbf{B}_{\mathcal{R},l}\mathbf{\Psi}_{\mathcal{R},n+l} + \sum_{l=N-n+1}^{N}\mathbf{B}_{\mathcal{R},l}\mathbf{F}_{\mathcal{R}}^{l-N+n}(+)\mathbf{\Psi}_{\mathcal{R},N} = 0\,. \tag{16}$$

Finally, the Schrödinger equation for the states within the scattering region is

$$\left(E\mathbf{I} - \mathbf{H}_S\right)\mathbf{\Psi}_S + \sum_{l=0}^{N-1}\left[\mathbf{B}_{\mathcal{L}\mathcal{S},l}^{\dagger}\mathbf{\Psi}_{\mathcal{L},-l} + \mathbf{B}_{\mathcal{R}\mathcal{S},l}\mathbf{\Psi}_{\mathcal{R},l}\right] = 0\,. \tag{17}$$

These are all the equations needed to fully solve the system, with one final boundary condition being

$$\mathbf{\Psi}_{\mathcal{L},-N}(+) = \mathbf{U}_{\mathcal{L}}(+)\,. \tag{18}$$

That is, the incoming states are the right-going eigenstates of the left lead. The final set of equations is an inhomogeneous set of linear equations which is relatively sparse, thanks to the TB-LMTOs. The reflection and transmission matrices can be extracted as

$$\mathbf{\Psi}_{\mathcal{L},-N}(-) = \mathbf{U}_{\mathcal{L}}(-)\mathbf{r} \tag{19}$$

$$\mathbf{\Psi}_{\mathcal{R},N}(+) = \mathbf{U}_{\mathcal{R}}(+)\mathbf{t} \tag{20}$$

or rather, in usable form

$$\mathbf{r} = \mathbf{U}_{\mathcal{L}}^{-1}(-)\left[\mathbf{\Psi}_{\mathcal{L},-N} - \mathbf{U}_{\mathcal{L}}(+)\right] \tag{21}$$

$$\mathbf{t} = \mathbf{U}_{\mathcal{R}}^{-1}(+)\mathbf{\Psi}_{\mathcal{R},N} \tag{22}$$

6.4   Interatomic currents

One vital part of the transport code is the interatomic currents, as well as the layer-averaging algorithms it contains. Through the hopping Hamiltonians (which we have to construct anyway), we can in a remarkably simple fashion extract the interatomic (spin) currents from the scattering region.

Let us consider an atom P within the scattering region. The TB-LMTO method has as its basis a set of localised orbitals, such that we can associate every basis function with one particular atom. We write all basis functions localised on P as $|\Psi_P\rangle$. The current at P is simply equal to the change of the electron density in time

$$\begin{aligned}
\frac{\partial}{\partial t} n_P &= \frac{\partial}{\partial t} \langle \Psi_P | \Psi_P \rangle = \frac{\partial}{\partial t} \int \Psi_P(\mathbf{r})^\dagger \Psi_P(\mathbf{r}) d\mathbf{r} \\
&= \int \frac{\partial \Psi_P(\mathbf{r})^\dagger}{\partial t} \Psi_P(\mathbf{r}) d\mathbf{r} + \int \Psi_P(\mathbf{r})^\dagger \frac{\partial \Psi_P(\mathbf{r})}{\partial t} d\mathbf{r} \\
&= \langle \frac{\partial}{\partial t} \Psi_P | \Psi_P \rangle + \langle \Psi_P | \frac{\partial}{\partial t} \Psi_P \rangle .
\end{aligned}$$

Now remembering the time dependent Schrödinger equation, which is

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi , \tag{23}$$

we find an equation for the charge current, solely in terms of the Hamiltonian $\hat{H}$ and the wave function Ψ_P

$$\frac{\partial}{\partial t} n_P = \frac{1}{i\hbar} \left[\langle \Psi_P | \hat{H} | \Psi \rangle - \langle \Psi | \hat{H} | \Psi_P \rangle \right] . \tag{24}$$

We also know, by conservation of charge, that the current at atom P must necessarily equal the sum of all currents between atoms P and every other atom, or in equation form

$$\frac{\partial}{\partial t} n_P = \sum_Q j_c^{PQ}(\Psi_P, \Psi_Q) , \tag{25}$$

and indeed, the equation for the current (24) fits such a form, when we decompose the Hamiltonian $\hat{H}$ into atom-to-atom blocks $\hat{H}_{PQ}$

$$j_c^{PQ} = \frac{1}{i\hbar} \left[\langle \Psi_P | \hat{H}_{PQ} | \Psi_Q \rangle - \langle \Psi_Q | \hat{H}_{QP} | \Psi_P \rangle \right] . \tag{26}$$

The derivation of the expression for the spin currents is very similar. The spin density on each atom is $s_{\alpha,P} := \langle \Psi_P | \sigma_\alpha | \Psi_P \rangle$, with σ_α the Pauli matrices, so that the spin currents become

$$\frac{\partial}{\partial t} s_{\alpha,P} = \langle \frac{\partial}{\partial t} \Psi_P | \sigma_\alpha | \Psi_P \rangle + \langle \Psi_P | \sigma_\alpha | \frac{\partial}{\partial t} \Psi_P \rangle \tag{27}$$

$$= \frac{1}{i\hbar} \left[\langle \Psi_P | \sigma_\alpha \hat{H} | \Psi \rangle - \langle \Psi | \hat{H} \sigma_\alpha | \Psi_P \rangle \right] . \tag{28}$$

which we decompose into interatomic spin currents in the exact same way

$$j_{s\alpha}^{PQ} = \frac{1}{i\hbar} \left[\langle \Psi_P | \sigma_\alpha \hat{H}_{PQ} | \Psi_Q \rangle - \langle \Psi_Q | \hat{H}_{QP} \sigma_\alpha | \Psi_P \rangle \right] . \tag{29}$$

We note that these currents are actually current *densities*, so to find the actual current, we multiply the current densities, which we gather in a tensor $\tilde{j}^{PQ}$ by a volume $V_{PQ} = A_{PQ}|\mathbf{d}_{PQ}|$, where A_{PQ} is an arbritrary cross section which cancels in the integration, and $\mathbf{d}_{PQ}$ is the vector pointing from P to Q.

$$\tilde{j}^{PQ}V_{PQ} = \begin{pmatrix} j^{PQ}_{sx}d_x & j^{PQ}_{sx}d_y & j^{PQ}_{sx}d_z \\ j^{PQ}_{sy}d_x & j^{PQ}_{sy}d_y & j^{PQ}_{sy}d_z \\ j^{PQ}_{sz}d_x & j^{PQ}_{sz}d_y & j^{PQ}_{sz}d_z \\ j^{PQ}_{c}d_x & j^{PQ}_{c}d_y & j^{PQ}_{c}d_z \end{pmatrix} = \mathbf{j}^{PQ} \otimes \mathbf{d}_{PQ} \tag{30}$$

When we group together a group of atoms and call them a layer, there are plenty of interatomic currents between two layers. To ensure that we divide up the current properly between the layers, we define a parameter

$$\beta_{QP,l} = \begin{cases} 0 & \text{if Q is inside layer l} \\ d_{Q,l}/d_z & \text{if Q is outside layer l} \end{cases}, \tag{31}$$

where $d_{Q,l}$ is the distance in the z direction between atom Q and the outer boundary of layer l, and d_z is the distance in the z direction between Q and P. For the spin currents, we need to linearly interpolate between $j^{PQ}_{s\alpha}$ and $j^{QP}_{s\alpha}$ since the spin current is in general not conserved between two atoms.

$$\mathbf{j}^{PQ}(\lambda) = \lambda\mathbf{j}^{PQ} - (1-\lambda)\mathbf{j}^{QP} \qquad \lambda \in [0,1] \tag{32}$$

The part of $\tilde{j}^{PQ}V_{PQ}$ that belongs to layer l then equals

$$\int_{\beta_{QP,l}}^{1-\beta_{PQ,l}} \mathbf{j}^{PQ}(c)\otimes\mathbf{d}_{PQ}dc = \frac{1}{2}\left[(1-\beta_{PQ,l})^2 - \beta_{QP,l}^2\right]\mathbf{j}^{PQ}\otimes\mathbf{d}_{PQ} + \frac{1}{2}\left[(1-\beta_{QP,l})^2 - \beta_{QP,l}^2\right]\mathbf{j}^{QP}\otimes\mathbf{d}_{QP}. \tag{33}$$

The average current density tensor within layer l is

$$\tilde{j}_l = \frac{1}{V_l}\sum_{P,Q}\frac{1}{2}\left[(1-\beta_{PQ,l})^2 - \beta_{QP,l}^2\right]\mathbf{j}^{PQ}\otimes\mathbf{d}_{PQ}. \tag{34}$$

Dividing the scattering region into layers seems unnecessary, but is actually very important to obtain reasonable currents.

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