

Chapter 1

BoltzTraP

This package contains the program **BoltzmannTransportProperties** (**BoltzTraP**) for calculating the semi-classic transport coefficients. The program has documented in Comp. Phys. Commun.[1] and can be obtained at the web site www.chem.au.dk/~webuorg/gm. If you publish results obtained using the program this paper should be sited.

The program has only been interfaced to the WIEN2k code, but could easily be interfaced to other bandstructure codes. Please contribute if you make such an interface.

1.1 Getting started

1.1.1 Unpacking

Run the command `tar xzvf BoltzTrap.tgz`

This will unpack into three directories and two files

<code>SRC_BoltzTrap101</code>	The source code
<code>CoSb3</code>	Example files
<code>Bi2Te3</code>	Example files
<hr/>	
<code>BoltzTraP.pdf</code>	Paper describing the program
<code>README.pdf</code>	This file

1.1.2 Compiling

The distribution includes a makefile for the intel fortran compiler and the mkl libraries. Once you have successfully compiled the program you should have an executable named `BoltzTrap`.

Furthermore the script `x_trans` can be found in the directory.

1.1.3 Running test examples

The distribution includes two examples: `CoSb3` and `Bi2Te3`. Both examples are also described in the BoltzTraP paper[1] To run the examples you must change to one of these two directories

CoSb₃

Once you are in the `CoSb3` directory you can run BoltzTrap by the following command (Remember the capital letters)

```
"path to BoltzTrap"/x_trans BoltzTraP
```

The `x_trans` script will make a file called `BoltzTrap.def` and executes BoltzTrap. The `BoltzTrap.def` file names the input and output files (described below)

Bi₂Te₃

The `Bi2Te3` example includes spin-orbit coupling in the Hamiltonian. Therefore the example should be by the following command:

```
"path to BoltzTrap"/x_trans BoltzTraP -so
```

Notice the `-so` option. This will tell the program to read the eigenvalues from the file `case.energyso` (see `Boltztrap.def`) and the program will then automatically know the each state contains only one electron.

1.2 Using the program

1.2.1 Input files

To run the program you must have a file describing the parameters for BoltzTraP named case.intrans (where case is the name of the directory). Furthermore you need a file with the band-structure and the crystal structure, case.energy(so) and case.struct, where case is the name of the directory. Presently case.energy(so) and case.struct have to be in the format of the WIEN2k code.

WIEN	Format of DOS. Till now only WIEN is supported
0 0 0 0.0	iskip idebug setgap gapchange iskip is not presently used and idebug sets the level of output setgap=1 will force the gap to be gapchange (in Ry)
0.55475 0.0005 0.4 240.	Fermilevel (Ry), deltae, ecut, number of valence electrons deltae determines the stepsize of the DOS grid ecut gives the range around efermi in which the bands are included
CALC	CALC (calculate expansion coeff, Eq.(p1), NOCALC (read from file)
5	lpfac, number of latt-points per k-point lpfac=5: five times as many \mathbf{R} points are used as \mathbf{k} points were input
BOLTZ	run mode (only BOLTZ is supported)
.15	efcut. energy range of chemical potential around efermi that is used for integrals (Eqs.(p12-p15))
800. 50.	Tmax, temperature grid
-1	Energyrange of bands given individual DOS output sig_xxx and dos_xxx (xxx is band number). Negative: no individual DOS.
HISTO	scheme to obtain DOS. HISTO/TETRA: histogram/tetrahedron[2] samp

Table 1.1: Input file for CoSb₃. The Equations refer to the paper[1].

1.2.2 Output files. BOLTZ option

The traces of the conductivity tensors are written as a function of μ and T in the file called case.trace. You must write your own program/script to extract the information you need. The last columns were added after the paper was accepted and are the electronic specific heat c

$$c(T; \mu) = \int n(\varepsilon)(\varepsilon - \mu) \left[\frac{\partial f_{\mu}(T; \varepsilon)}{\partial T} \right] d\varepsilon \quad (1.1)$$

column	1	2	3	4	5	6	7	8	9	10
quantity	μ	T	N	$n(\mu)$	S	σ/τ	R_H	κ^0	c	χ
unit	Ry	K	e/uc	e/uc	V/K	1/(Ω m s)	m ³ /C	W/(m K s)	J/(mol K)	m ³ /mol

Table 1.2: Output in case.trace

and the magnetic susceptibility

$$\chi(T; \mu) = \mu_0 \mu_B^2 \int n(\varepsilon) \left[-\frac{\partial f_\mu(T; \varepsilon)}{\partial \varepsilon} \right] d\varepsilon \quad (1.2)$$

The program outputs the individual components of the conductivity tensors (files case.condtens and case.halltens). The first three columns are like in the case.trace file.

In case.condtens next nine columns are the σ/τ components (3x3 tensor). These are followed by the nine Seebeck components and finally the nine κ^0 components.

In case.halltens 27 columns follow (The Hall tensor is 3x3x3 tensor)

The coordinate-system used is defined so that the x axis is parallel to the crystallographic a-axis (of the conventional cell). The y-axis lies in the crystallographic ab plane and is orthogonal to the x-axis and the z-axis is orthogonal to the x and y axes. If you want a different coordinate system you must work out the appropriate transformation yourself (a good reference is "J.F. Nye, Physical Properties of Crystals"). The axes setup is done in the subroutine latgen2.f.

1.3 Frequently Asked Question

How many k-points should I use for a transport calculation.

This of-course depends on your system, but generally “a lot”. A rule of thumb is that your convergence tests should *start* at $16 \times 10^6 / V_{puc}$, where V_{puc} is the volume of the primitive unit cell. Please note that you do not need to redo the full scf cycle with the dense k-mesh

I have calculated my energy files in parallel how do I include them in BoltzTraP

The utility

```
gather_energy.pl <case>
```

will stick your case.energy(so)* into one case.energy(so) file that can be fed into BoltzTraP

How can I calculate the conductivity.

One can only calculate the conductivity if one knows τ . The distribution includes a calculation for Al for which Ashcroft and Mermin[3] list $\rho = 2.45 \mu\Omega\text{cm} = 2.45 \times 10^{-8} \Omega\text{m}$ (page 8). If you look in Table 1.2 you’ll see that BoltzTraP outputs σ/τ . At 270 K one obtains $\sigma/\tau \approx 3.17 \times 10^{21} (\Omega\text{m})^{-1}$. Using $\tau = 0.8 \times 10^{-14}$ s (page 9) one get for the resistivity $\rho = 1/(3.17 \times 10^{21} \cdot 0.8 \times 10^{-14}) = 3.9 \times 10^{-8} \Omega\text{m}$ which is a nice agreement considering the large uncertainty in τ (Ashcroft and Mermin use free electron bands)

Bibliography

- [1] Madsen, G. K. H.; Singh, D. J. *Comput. Phys. Commun.* **2006**, *175*, 67-71.
- [2] Blöchl, P.; Jepsen, O.; Andersen, O. K. *Phys. Rev. B* **1994**, *49*, 16223-16233.
- [3] Ashcroft, N. W.; Mermin, N. D. *Solid State Physics*. Saunders College Publishing, Orlando, Florida, 1976.