WANNIER BERRI : an advanced tool for interpolation of Berry curvature and related quantities. (aka Wannier19)

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Anomalous Hall and Nernst effects

Tee AHC tensor is given by:

$$\sigma^{\rm AHE}_{\alpha\beta}(0) = -\frac{e^2}{\hbar}\int\frac{d\mathbf{k}}{(2\pi)^3}\sum_n f_{n\mathbf{k}}\Omega_{n,\alpha\beta}(\mathbf{k}) \qquad (1)$$

in terms of Berry curvature:

$$\Omega_{n,\alpha\beta}(\mathbf{k}) = -2{\rm Im}\langle\nabla_{k_\alpha}u_{n\mathbf{k}}|\nabla_{k_\beta}u_{n\mathbf{k}}\rangle. \qquad (2)$$

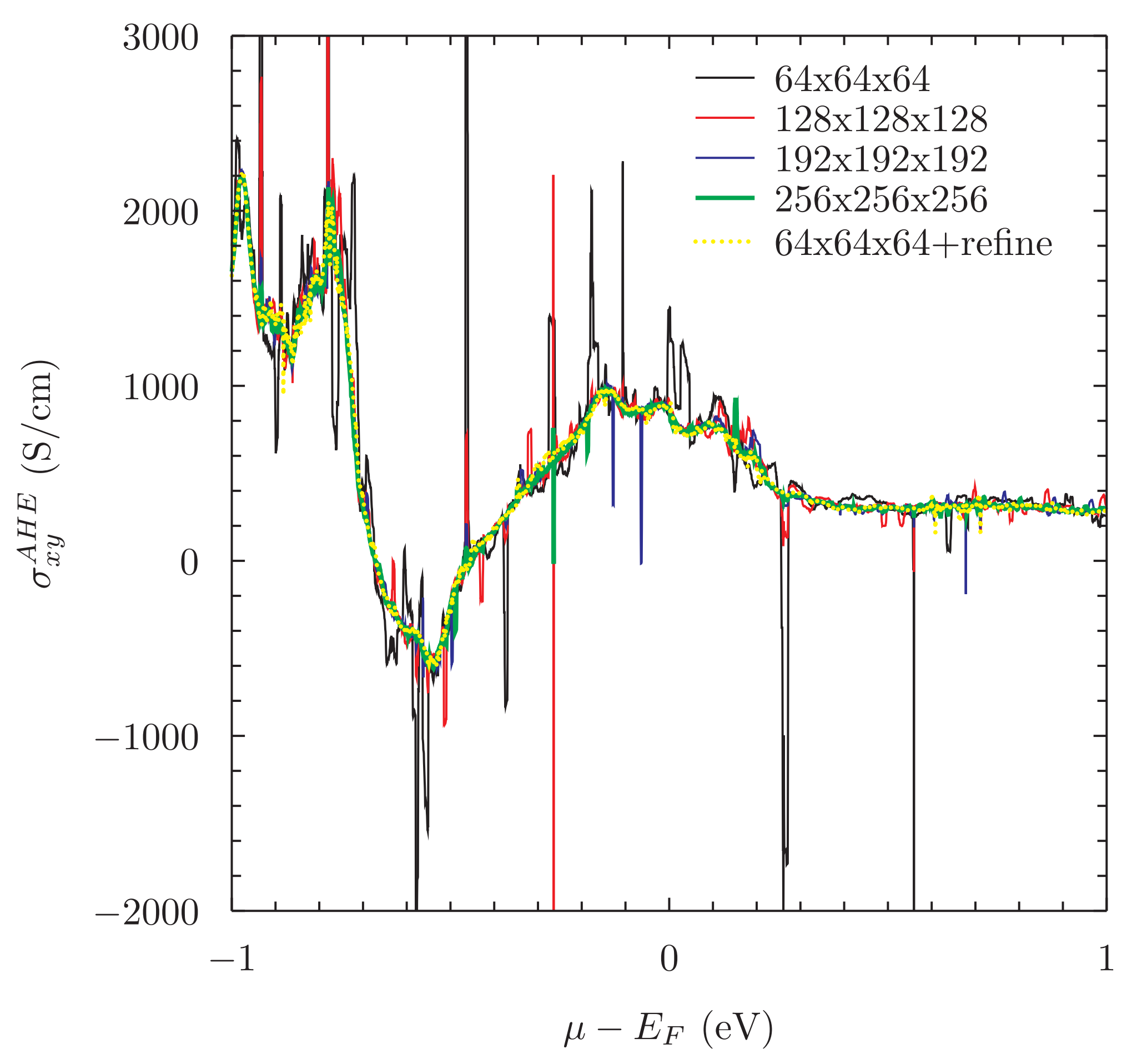
where $|u_{n\mathbf{k}}\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{n\mathbf{k}}\rangle$ is the cell-periodic Bloch function. to evaluate it one needs:

- a smooth gauge
- dense grid of **k**-points

That is where Wannier interpolation helps a lot.
Anomalous Nernst Effect is even harder

$$\alpha^{\rm ANE}_{xy} = -\frac{1}{e}\int d\varepsilon\frac{\partial f}{\partial\varepsilon}\sigma^{\rm AHE}_{xy}(\varepsilon)\frac{\varepsilon-\mu}{T} \qquad (3)$$

because at low T it is essentially the derivative of σ^{AHE}



Irudia 1: Example: AHC of bcc Fe as a function of chemical potential μ, for different interpolation grids, with and without recursive refinement

Overview

W-BERRI is an improved python implementation of postw90.x part of **Wannier90**. ("19-- because it was started in 2019.)

W-BERRI accepts the Wannier functions generated by Wannier90, or any tight-binding model. Than a BZ integral of any combination of velocities, Berry curvatures and other k-space quantities can be evaluated.

Wannier90 is **good**, because it

- is a well-established code
- known for ages
- has a broad community of developers
- has many implemented features
- ..... (many more)

W-BERRI is **better**, because it

- is faster
- Employs a mixture of fast and slow Fourier transforms
- uses recursive adaptive refinement for accurate evaluation around special points in BZ
- accounts for the symmetries, to integrate only the irreducible part of BZ and make the result symmetric.
- is written in object-oriented Python, which allows easier further development.
- has some more efficient algorithms, in particular
  - for multiple Fermi levels
  - minimal-distance replica selection method

Hosted on github

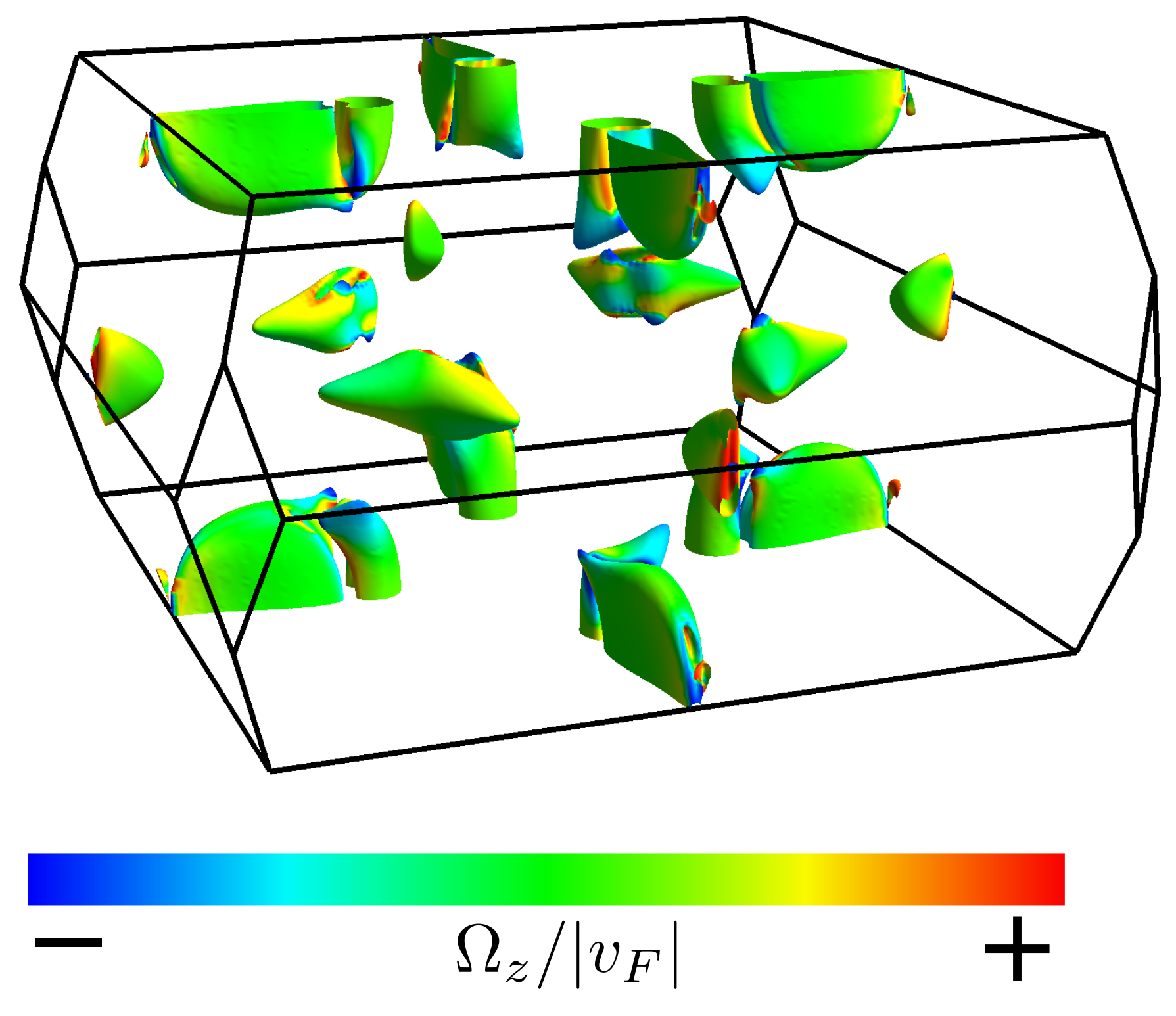
https://github.com/stepan-tsirkin/wannier-berri

Install with pip

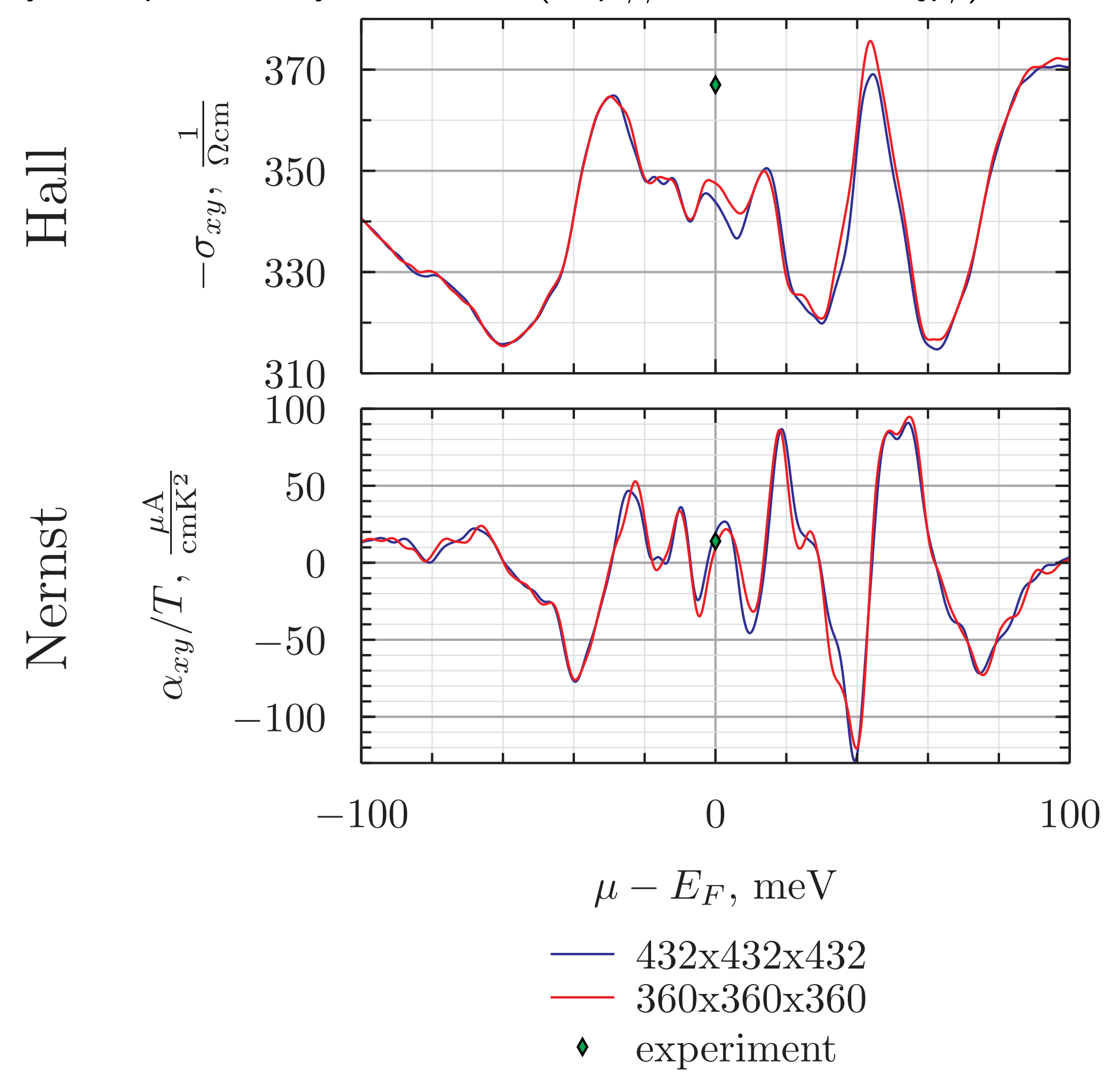
```
pip3 install wannierberri
```

First real-life use: AHE and ANE in magnetic Weyl Semimetal PrAlGe

"Magnetism and anomalous transport in the Weyl semimetal PrAlGe: possible route to axial gauge fields". D. Destraz, L. Das, S.S. Tsirkin, Y. Xu, *et al.* Accepted in **npj Quantum Materials**.



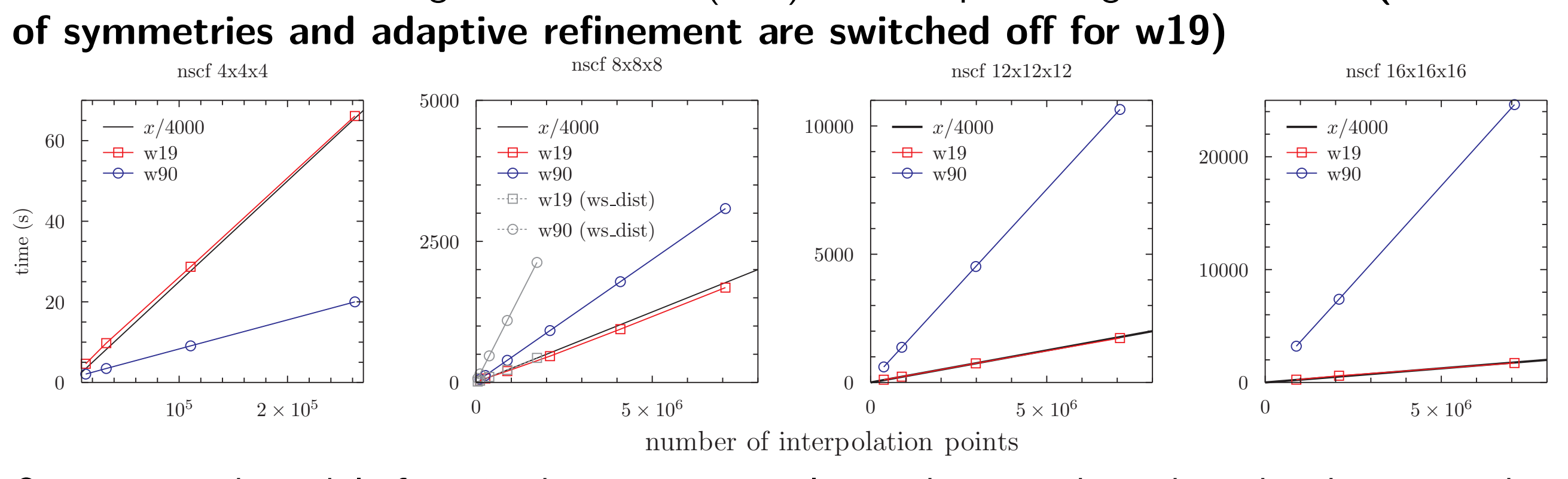
Irudia 2: Fermi surface of ReAlGe coloured by Berry curvature divided by Fermi velocity. Plot produced by FermiSurfer (http://fermisurfer.osdn.jp/)



Irudia 3: AHE and ANE calculated in PrAlGe in comparison with experiment

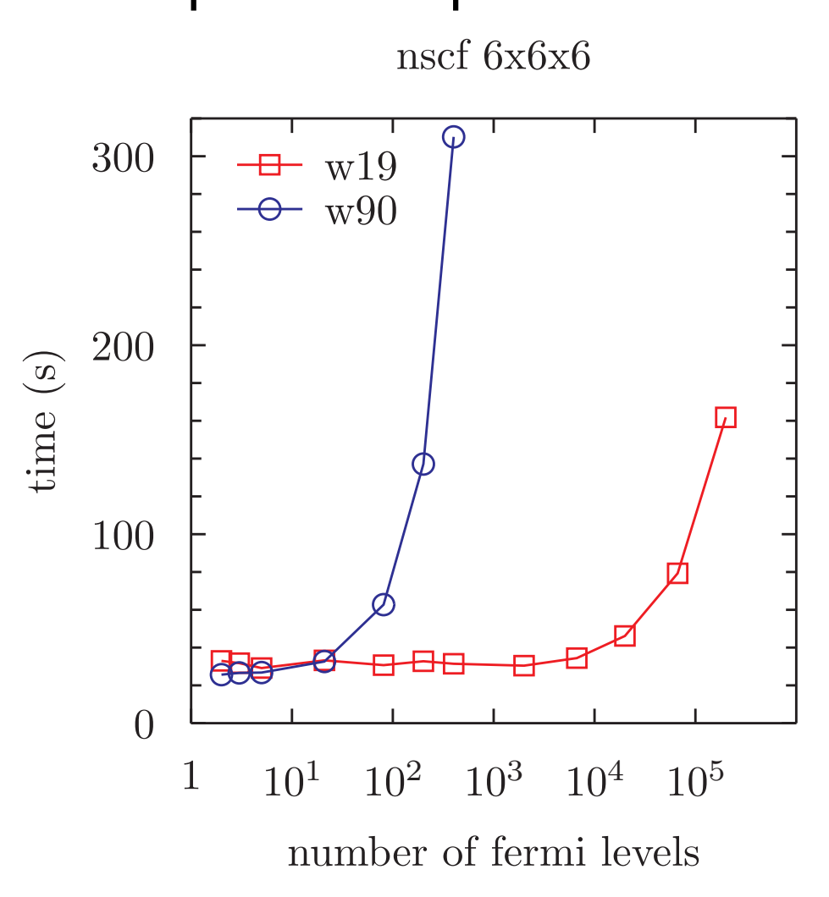
Computational time

Calculations were performed with WannierBerri and wannier90 on identical 40-core nodes of a cluster at UZH. Different grids of ab-initio (nscf) and interpolation grids were used. **(account of symmetries and adaptive refinement are switched off for w19)**



One can see that while for w19 the computational time does not depend on the ab-initio grid and the use of parameter "use_ws_distance". While for w90 they increase time a lot.

Also scanning multiple fermi levels has almost no cost in w19 up to 10^4 points:



Recursive adaptive refinement

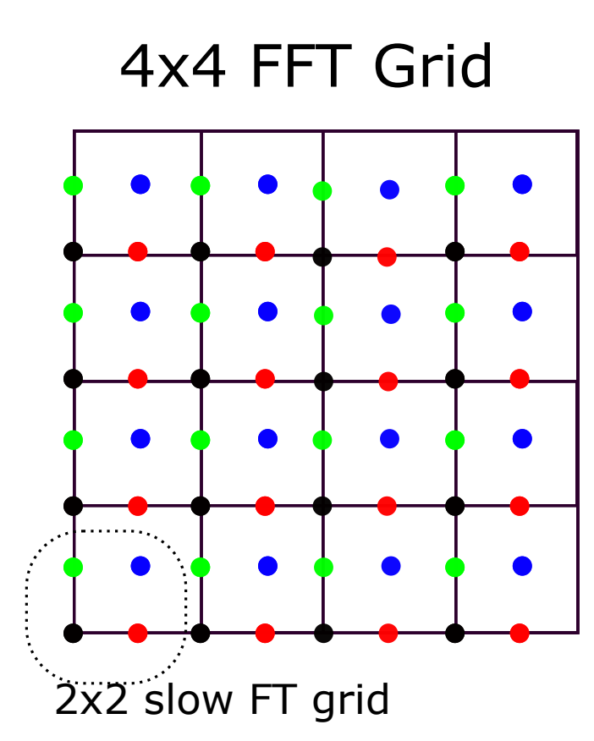
A few k-points are chosen that give the largest contribution to the integral, or to the jittering of the curve. — typically the points near (avoided) degeneracies. They are replaced by grids of 2x2x2 points surrounding it. The procedure is repeated recursively (new points can be refined again) to get a smoother curve.

Mixed Fourier Transform

n — size of *ab initio* grid
$N = m\times n$ — size of interpolation grid (m-integer)
we want to Fourier Transform a quantity A:
$A(R_1),\ldots,A(R_n)\rightarrow A(k_0),\ldots A(k_{N-1})$, where $k_i = 2\pi i/N$

For each $j = 0,\ldots,m-1$ we "slow FT"
$A(R_l)\rightarrow\tilde{A}^j(R_l) = A(R_l)\times e^{2\pi l\frac{j}{N}}$
and then do a FFT of $\tilde{A}^j(R_l)$, thus getting k-points $k_{i,j} = 2\pi(j+im)/N$

time scaling:
slow FT $\propto N\times n$
fast FT $\propto N\log N$
mixed FT $\propto N\log n$



Thus, FFT is better then SFT for large ab initio grids, while MFT is better in any case.

Advantages of mixed FT over FFT:

- easier parallelization
- allows to remove symmetry-equivalent "slow"k-point
- no need to store the whole interpolation grid (less memory needed)
- allows adaptive recursive refinement of most "important"points.

tutorial.py

```python
#!/usr/bin/env python3
import wannier19 as w19
import numpy as np

name="Fe"
NK=(96,96,96)  # a grid 96x96x96
Efermi=np.linspace(12.,13.,1001)  # range of Fermi levels
system=w19.System(tb_file='Fe_tb.dat',getAA=True)

# symmetries of the system to be accounted for :
SYM=w19.symmetry
generators=[SYM.Inversion,SYM.C4z,SYM.TimeReversal*SYM.C2x]

# tabulate quntities to be plotted by FermiSurfer
w19.tabulate(system,
             NK=NK,
             quantities=["V","berry"],
             symmetry_gen=generators,
             fout_name=name,
             numproc=4,
             Ef0=0,
             restart=False  )

# integrated quantities
w19.integrate(system,
            NK=NK,
            Efermi=Efermi,
            smearEf=10,
            quantities=["ahc","dos"],
            numproc=4,
            adpt_num_iter=10,
            fout_name=name,
            symmetry_gen=generators,
            restart=False  )
```

Acknowledgements

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