kdotpy – Calculating the electronic properties of topological insulators using k·p theory

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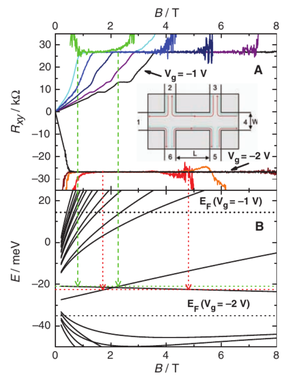
Background

In 2005, Laurens Molenkamp and his group successfully realized **topological-insulator physics** in a transport experiment on a (Hg,Cd)Te/HgTe/(Hg,Cd)Te heterostructure [1].



Analytical models describe the essential physics of these materials in a limited number of cases. Usually one needs more degrees of freedom, such as **k·p theory** [2]. This model provides an accurate description of the electronic structure, but it requires numerical evaluation.

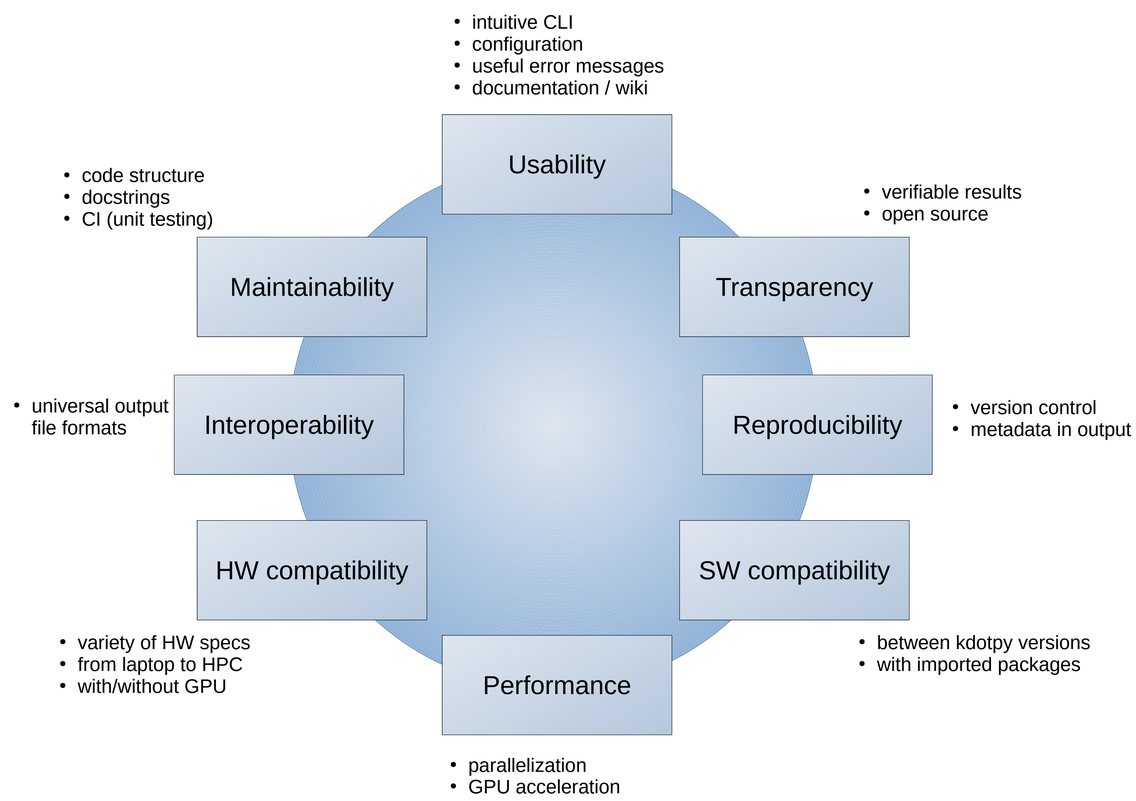
$$H = \begin{pmatrix} T & 0 & -\frac{1}{\sqrt{2}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{6}}Pk_- & 0 & -\frac{1}{\sqrt{3}}Pk_z & -\frac{1}{\sqrt{3}}Pk_- \\ 0 & T & 0 & -\frac{1}{\sqrt{6}}Pk_+ & \sqrt{\frac{2}{3}}Pk_z & \frac{1}{\sqrt{2}}Pk_- & -\frac{1}{\sqrt{3}}Pk_+ & \frac{1}{\sqrt{3}}Pk_z \\ -\frac{1}{\sqrt{2}}k_-P & 0 & U+V & -\bar{S}_- & R & 0 & \frac{1}{\sqrt{2}}\bar{S}_- & -\sqrt{2}R \\ \sqrt{\frac{2}{3}}k_zP & -\frac{1}{\sqrt{6}}k_-P & -\bar{S}_+^\dagger & U-V & C & R & \sqrt{2}V & -\sqrt{\frac{3}{2}}\bar{S}_- \\ \frac{1}{\sqrt{6}}k_+P & \sqrt{\frac{2}{3}}k_zP & R^\dagger & C^\dagger & U-V & \bar{S}_+ & -\sqrt{\frac{3}{2}}\bar{S}_+ & -\sqrt{2}V \\ 0 & \frac{1}{\sqrt{2}}k_+P & 0 & R^\dagger & \bar{S}_+ & U+V & \sqrt{2}R^\dagger & \frac{1}{\sqrt{2}}\bar{S}_+ \\ -\frac{1}{\sqrt{3}}k_zP & -\frac{1}{\sqrt{3}}k_-P & -\frac{1}{\sqrt{2}}\bar{S}_-^\dagger & \sqrt{2}V & -\sqrt{\frac{3}{2}}\bar{S}_+^\dagger & \sqrt{2}R & U-\Delta & C \\ -\frac{1}{\sqrt{3}}k_+P & \frac{1}{\sqrt{3}}k_zP & -\sqrt{2}R^\dagger & -\sqrt{\frac{3}{2}}\bar{S}_-^\dagger & -\sqrt{2}V & \frac{1}{\sqrt{2}}\bar{S}_+^\dagger & C^\dagger & U-\Delta \end{pmatrix}.$$

The model encodes the physics as a matrix Hamiltonian $H(k_x, k_y, k_z)$ [3]. The **band structure** is obtained as its eigenvalues and -vectors. This process, known as **diagonalization**, is the most important numerical step.

Physical observables are extracted from the band structure and can be matched with the experiments, e.g., magneto-transport and optical spectroscopy.

Historically, there was a **FORTRAN program** [4], but:
- it has not been maintained since > 15 years
- has a clumsy interface (input = output file)
- its code is not transparently structured
- there is very little documentation

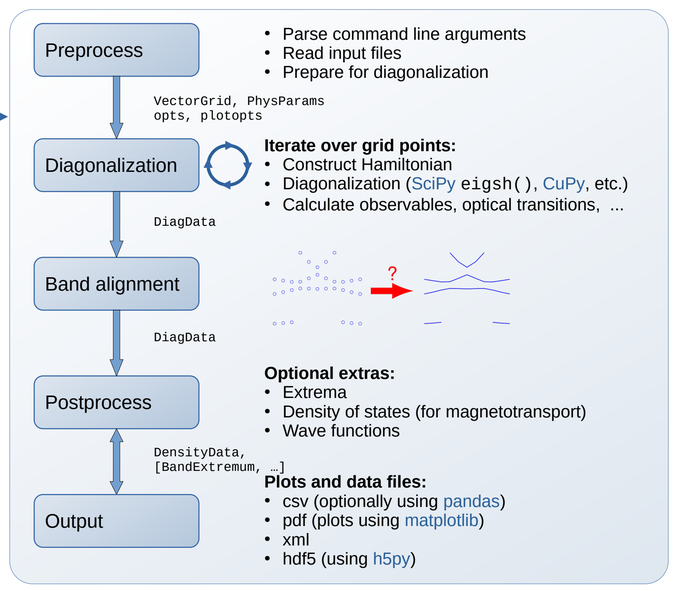
Design philosophies



The application

kdotpy is a python application for **k·p** band structure analysis of semiconductor heterostructures

- Python application (module)
- Command line interface
- **Calculation subprograms**:
  `kdotpy 1d`, `kdotpy 2d`, `kdotpy bulk`, `kdotpy ll`, `kdotpy bulk-ll`
- Replot subprograms:
  `kdotpy merge`, `kdotpy compare`
- Auxiliary subprograms:
  `kdotpy batch`, `kdotpy help`, `kdotpy config`



The project

- Managed and developed by *The kdotpy collaboration*
  kdotpy@uni-wuerzburg.de
- Used internally since ~ 6 years
- Currently in beta stage
  in preparation for publication
- Open source
  GNU GPL license

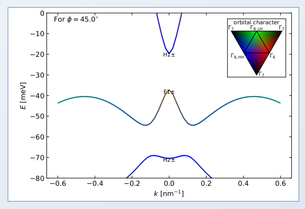
- Git repository
  2700 commits
  116 .py source files, 55000 lines of code
- Gitlab
  many constructive discussions in issue tracker
  `https://git.physik.uni-wuerzburg.de/kdotpy/kdotpy`
- Wiki
  documentation, background, tutorials
  `https://git.physik.uni-wuerzburg.de/kdotpy/kdotpy/-/wikis/home`
- Website
  (not online yet)
- Scientific article
  (work in progress)

Example use cases

1. Simple dispersion of a quantum well

```
$ kdotpy 2d 8o noax msubst CdZnTe 4% mlayer HgCdTe 68% HgTe
HgCdTe 68% llayer 10 7 10 zres 0.25 k -0.6 0.6 / 60 kphi 45
erange -80 0 split 0.01 obs orbitalrgb legend char out -7nm
outdir data-qw localminmax
```

```
dispersion-7nm.csv
dispersion-7nm.pdf
dispersion-7nm.byband.csv
extrema-7nm.csv
output-7nm.xml
```



- Analysis of band inversion
- ⇒ **Theory of topological insulators**
- Refs. [5,6,7]

2. Landau fan with Hall conductance

```
$ kdotpy ll 8o msubst CdZnTe 4% mlayer HgCdTe 68% HgTe
HgCdTe 68% llayer 10 7 10 zres 0.25 b 0 10 // 100 erange
-60 40 nll 20 neig 300 targetenergy -30 split 0.01 obs
llindex.jz legend char out -7nm-ll outdir data-qw-ll hall
cardens 0.001 config 'dos_quantity=p;dos_unit=cm'
```

```
bdependence-7nm-ll.csv
bdependence-7nm-ll.pdf
sigmah-vs-n-7nm-ll.csv
sigmah-vs-n-7nm-ll.pdf
output-7nm-ll.xml
(24 more files)
```


- Using ‘real’ observables
  - magnetic field B
  - carrier density n
  - Hall conductance σ_H, Hall resistance R_{xy}
- ⇒ **Magnetotransport experiments**
- Refs. [5,6,7,8]

3. Landau fan with optical transitions

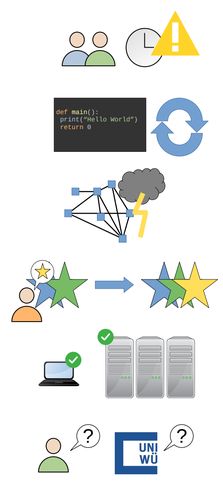
```
$ kdotpy ll 8o bia msubst CdTe mlayer HgCdTe 68% HgCdTe
4.0% HgCdTe 68% llayer 10 10.2 10 zres 0.2 b 0 15 // 60
erange -60 40 nll 10 neig 120 targetenergy 10 split 0.01
obs llindex.jz legend char out -trans outdir data-trans
hall cardens 0.0008 config 'dos_quantity=p;dos_unit=cm'
transitions
```

```
bdependence-transitions-trans.pdf
ellipticity-spectrum-trans.pdf
transitions-filtered-trans.csv
transitions-filtered-trans.pdf
output-trans.xml
(44 more files)
```


[10]

- Extract spectroscopic observables, e.g.,
  - ellipticity
  - relative absorption
  - refractive index
- ⇒ **Optical spectroscopy**
- Refs. [9,10]

Challenges



- Limited human resources
  Small team, people working on other projects too
- Not initially designed for publication
  Requires revisiting and updating existing code
- Dependency hell
  Complicated internal structure
- Changing demands
  New questions pop up continuously (e.g., when new experiments are done)
- Variety of different hardware (requirements)
  Workstation to HPC cluster; with/without GPU
- We’re not primarily software developers
  Difficult to find the right expertise within organization

References and acknowledgements

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[10] Fürst *et al.*, in preparation

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