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## kdotpy: Calculating the electronic properties of topological insulators using k p theory

The exotic properties of topological insulators were theoretically predicted and experimentally realized around 2005. While for some parameters (material composition, dimensions of the device) it is possible to use simplified, analytically solvable models to describe the physics, this is not generally the case.

In order to simulate the devices fabricated and measured at the Institute for Topological Insulators and Experimentelle Physik III in Würzburg, we use band structure calculations based on k $\cdot$ p theory. In its simplest form, the problem boils down to diagonalization (finding the eigenvalues and eigenvectors) of an  $8 \times 8$  matrix that depends on momentum variables.

However, the geometry of the devices, typically a layer stack of several different materials, dictates spatial confinement in one or two dimensions. In the confined dimensions, the momentum has to be converted to a discretized lattice of real-space coordinates. The matrix size grows to  $\sim 10^3 \times 10^3$  for one and  $\sim 10^5 \times 10^5$  for two confinement directions. Diagonalization of such large matrices is a computationally demanding problem that requires sparse algorithms to be solved.

Our Python application kdotpy provides the infrastructure to tackle these problems. The core of kdotpy is the construction of the large Hamiltonian matrices in a sparse format and the application of a suitable diagonalization solver. The user can choose the solver, depending on the nature of the problem and the available hardware: The default solver in kdotpy is the sparse solver 'eigsh' from SciPy (based on ARPACK), but kdotpy also provides an interface to GPU accelerated solvers using CuPy. Very large problems that require large amounts of memory (about 10 GB per data point and above) can be run on the HPC cluster. If needed, the problem can be split up into smaller ones, and the data put together afterwards using a tool included with kdotpy.

Moreover, kdotpy provides functions to "post-process" the diagonalization results and convert them to a form that allows for a direct comparison with the measurements on the devices. In particular, we provide a conversion between energy and carrier-density dependence, relevant for magnetotransport experiments for example, and we calculate optical transitions for comparison to spectroscopic measurements. The output is provided in the form of images, data files in CSV format, and an XML-based serialized data format designed to be maximally compatible between versions and to be suitable for long-term data storage.

## Slot length

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