Tkwant: a software package for time-dependent quantum transport

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Tkwant[1,2] is a Python package for simulating the dynamics of nanoelectronic devices which are driven out-of-equilibrium by external perturbations.
It is an extension of the Kwant[3] package and focusses on similar problems, involving semiconductors, graphene, topological materials, superconductors, metals and magnets, that can be described by tight-binding Hamiltonians. The simulated device typically consists of a scattering region of arbitrary dimension and shape, which is coupled to a number of semi-infinite electrodes in thermal equilibrium (Fig. 1).The problem is genuinely many-body even in the absence of interactions and is treated within the non-equilibrium Keldysh formalism. The code has been designed to be modular and easy to use (Fig. 2). Tkwant is free software distributed under a BSD license.

References

[1] T. Kloss, J. Weston, B. Gaury, B. Rossignol, C. Groth and X. Waintal, Tkwant: a software package for time-dependent quantum transport, *New J. Phys.* **23** 023025 (2021).
[2] https://tkwant.kwant-project.org/
[3] https://kwant-project.org/

Figures

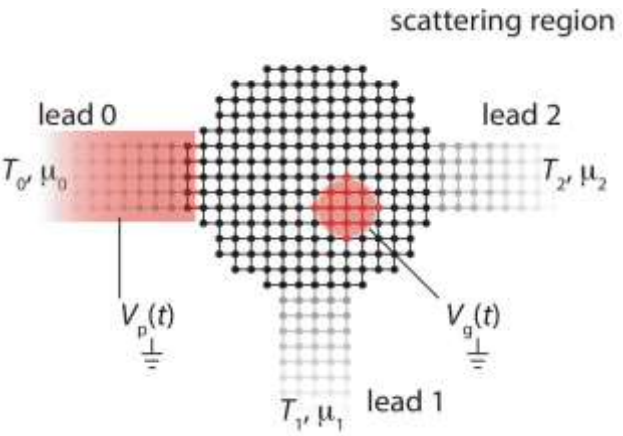

Figure 1: The system typically consists of a central scattering region which is connected to several leads.

```
import tkwant
import kwant

syst = make_system()

current_operator = kwant.operator.Current(syst)

state = tkwant.manybody.State(syst, tmax=1000)

for time in range(1000):
    state.evolve(time)
    current = state.evaluate(current_operator)
```

Figure 2: Using Tkwant is simple and consists in writing a small Python script that comes close to physical intuition.