The Kernel Polynomial Method in Kwant, Open-Source Software for Nanoscale Simulations

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Nanoscale simulations in condensed-matter, and realistic nanoscale devices are generally limited in size by computational requirements. Here, we present the kernel polynomial method (KPM) that has a linear scaling with the system size [1], which allows efficient calculations of physical properties over large systems. The KPM module is embedded into Kwant [2], an open-source software package, which offers an accessible entry point for quantum simulations.

The most basic application of the KPM module is to obtain the density of states of a closed system. Furthermore, with the KPM, the spectral density of any operator can also be obtained in linear time.

Later on, we will show the usage of the KPM in obtaining the Kubo conductivity. The implementation is based on the Kubo-Bastin formula [3], that allows the simulation of the conductivity tensor for non-zero temperatures. The KPM expansion of the conductivity tensor can be generalized to calculating the correlation matrix between any two operators. This greatly expands the field of possible applications to other observables, such as the optical conductivity.

Finally, we will show an example of using the KPM to calculate topological invariants [5], by expanding the projector on the ground state, and evaluating a local real-space expression of the Chern number for two-dimensional systems, and the winding number for one-dimensional and three-dimensional systems.

These examples show the versatility of the KPM module, that together with the linear scaling of spectral densities, makes it a very efficient tool for simulating devices at the nanoscale.

References

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