# Efficient real space simulations of topological transport properties of graphene systems

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## Abstract

A new numerical development significantly reduces the computational cost of the Kernel Polynomial Method (KPM) for Kubo transport calculations. Widely used for Density of States (DOS) calculations, its adoption for transport calculations has been hindered by high computational complexity and memory cost. While the complexity issues have been addressed by the FastCheb method [1], the question remained about whether a similar improvement could be achieved for its memory cost. By leveraging properties of the Fourier expansion that underlies the method, we managed to drastically reduce the number of spectral components needed to resolve the Kubo-Bastin equation close to the charge neutrality point – where the most relevant physical features are typically located. Real space KPM simulations are particularly well-suited for studying large systems with periodic symmetry breaking features, such as spatial disorder and moiré patterns. In this work, we apply the novel approach to compute Fermi sea transport properties in large graphene systems, such as Anomalous Hall and spin Hall conductivities induced in graphene by a Kane-Mele spin-orbit coupling term, the conductivity of a quasicrystalline bilayer graphene rotated close to 30°, and the conductance of a disordered magic-angle twisted bilayer graphene.

## References

[1] Fast Fourier-Chebyshev Approach to Real-Space Simulations of the Kubo Formula Santiago Giménez de Castro, João M. Viana Parente Lopes, Aires Ferreira, and D. A. Bahamon Phys. Rev. Lett. 132, 076302

## Figures

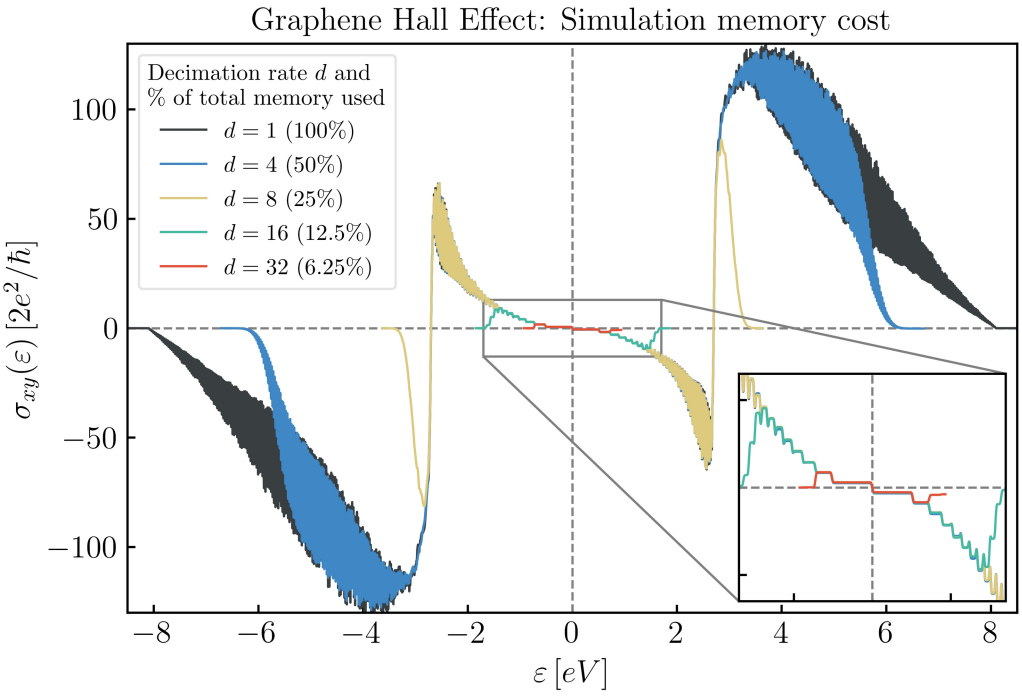


**Figure 1:** Simulations with increasing decimation rate *d* show how it is possible to study the Hall conductivity of Graphene at lower computational cost while maintaining accuracy close to the charge neutrality point.