Signal processing techniques for real-space conductance simulations of TBG

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Abstract

The Kernel Polynomial Method (KPM) has long been established as tool for real-space calculations of quantum properties. Its favourable scaling in terms of both resolution and system size make it an outstanding option for obtaining the DOS of a system. Unfortunately, that performance is not mirrored for transport calculations, such as the evaluation of the Kubo formula. In those cases, simulation cost scales quadratically with respect to the resolution. Here, this issue is tackled thanks to an analogy between the underlying Chebyshev vector sequence and a digital signal, which allows to take advantage of signal processing techniques in order to achieve numerical improvements. Most notably, the Fast Fourier Transform algorithm (FFT) was used to massively undercut the computational cost of the Kubo formula evaluation, yielding an method we denominated Fast Fourier-Chebyshev (FastCheb). Because the computational time grows linearly with an increase in resolution, a vast new range of resolutions is now under reach. Using the FastCheb, we unveil features never before seen of the conductance spectrum of a large TBG nanoribbon in real space.

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

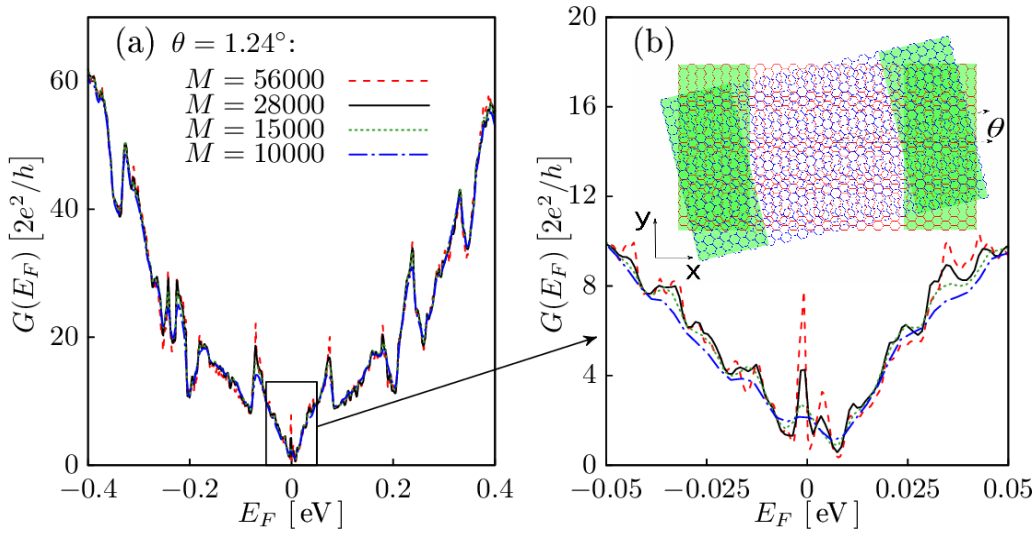

Figure 1: Panoramic and detailed views of linear conductance curves for a TBG device with a total of 2.3×10^6 orbitals, and a twist angle of 1.24°. The data series correspond to increasing values of M, which directly increases resolution.