Abstract Submitted for the MAR15 Meeting of The American Physical Society

An Efficient numerical method to calculate the conductivity tensor for disordered topological matter¹ JOSE H. GARCIA, Universidade Federal do Rio de Janeiro, LUCIAN COVACI, Universiteit Antwerpen, TATIANA G. RAP-POPORT, Universidade Federal do Rio de Janeiro — We propose a new efficient numerical approach to calculate the conductivity tensor in solids. We use a realspace implementation of the Kubo formalism where both diagonal and off-diagonal conductivities are treated in the same footing. We adopt a formulation of the Kubo theory that is known as Bastin formula and expand the Green's functions involved in terms of Chebyshev polynomials using the kernel polynomial method. Within this method, all the computational effort is on the calculation of the expansion coefficients. It also has the advantage of obtaining both conductivities in a single calculation step and for various values of temperature and chemical potential, capturing the topology of the band-structure. Our numerical technique is very general and is suitable for the calculation of transport properties of disordered systems. We analyze how the method's accuracy varies with the number of moments used in the expansion and illustrate our approach by calculating the transverse conductivity of different topological systems.

¹T.G.R, J.H.G and L.C. acknowledge Brazilian agencies CNPq, FAPERJ and INCT de Nanoestruturas de Carbono, Flemish Science Foundation for financial support.

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Date submitted: 13 Nov 2014

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