Topological surface states scattering from first principles

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Materials with topologically protected surface states are gaining growing attention due to their potential for device applications, which is rooted in the fact that the current carried by such states is expected to be largely "protected" from scattering. For example, while the conducting properties of graphene usually deteriorate significantly if defects are present, the conductance of topological surfaces is expected to be largely independent on the amount of defects. Our aim is to quantitatively study the scattering properties of such systems in presence of different types of perturbations. Specifically, we study the scattering properties of topologically protected states on the Sb(111) and Bi_2Se_3(111) surfaces by using the ab initio electron transport code SMEAGOL [1]. We consider different types of defects, such as adatoms and extended barriers. In the presence of a strong surface perturbation in the form of a step separating surface terraces we obtain standing-wave states resulting from the superposition of spin-polarized surface states. By Fourier analysis, we identify the underlying two dimensional scattering processes and the spin texture [2]. We find evidence of resonant transmission across the surface barrier at quantum well state energies and evaluate their lifetimes. Our results are in good agreement with experimental findings [3,4].

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