First-Principles Calculation of Topological Invariants

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The discovery of topological insulators opened a new direction in band theory. The topology of a time-reversal symmetric insulating bulk band structure was shown to have a one-to-one correspondence to the presence of robust metallic edge or surface states in 2D (quantum spin Hall) or 3D (strong topological) insulators. We address the question of how to compute the topological indices of time-reversal symmetric insulators by means of a standard band structure calculation. In particular, we use an analysis based on hybrid Wannier functions, i.e., states that are localized in one direction in real space but remain Bloch-like in the other directions. Tracking the positions of the charge centers of these functions as a function of k allows one to obtain the topological invariants of the band structure in question [1]. The method is discussed from the point of its actual implementation in ab initio codes.

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[1] A. A. Soluyanov and D. Vanderbilt, Phys. Rev. B **83**, 235401 (2011).

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