Computing topological invariants without inversion symmetry

ALEXEY SOLUYANOV, DAVID VANDERBILT, Rutgers University — We consider the problem of calculating the weak and strong topological indices in noncentrosymmetric time-reversal (T) invariant insulators. In 2D we use a gauge corresponding to hybrid Wannier functions that are maximally localized in one dimension. Although this gauge is not smoothly defined on the two-torus,\(^1\) it respects the T symmetry of the system and allows for a definition of the \(Z_2\) invariant in terms of time-reversal polarization.\(^2\) In 3D we apply the 2D approach to T-invariant planes. We illustrate the method with first-principles calculations on GeTe and HgTe under [100] and [111] strain. Our approach is different from the one suggested previously by Fukui and Hatsugai\(^3\) and should be easier to implement in \textit{ab initio} code packages. Time permitting, we will also discuss methods for decomposing the band space into T-paired Chern subspaces, and for carrying out a general construction of a Wannier representation for \(Z_2\) insulators.

\(^1\)A. A. Soluyanov and D. Vanderbilt, arXiv:1009.1415