

Classification of band topology from Wannier functions and tight-binding

J. Zhang, Dept. of Physics, Imperial College London, UK

Topological insulators present an obstruction to the description of connected bands by Wannier functions in real space. Starting with a set of Wannier functions, the electronic dispersion can be obtained using tight binding (TB) methods. In the case of gapped systems under such description, there is no obvious ways of distinguishing if the connected valence/conduction bands have trivial or non-trivial topology.

Symmetry techniques are developed to identify connected bands with trivial topology, leaving others as symmetry indicated as having non-trivial topology. A key aspect of the symmetry analysis requires the recognition of the **orientability** of the Brillouin zone (BZ) (torus). The BZ of the honeycomb lattice is illustrated in Fig.1. Such orientation changes under some space group operations. The presence of such operations in the space group forbids topological invariants, such as Chern numbers, in connected bands with an invariant band description induced from Wannier functions. This gives rise to the basic selection rule on the topological invariants in connected bands with invariant band description. Connected bands without an invariant band description under TB are symmetry-indicated as having non-trivial topology. The hierarchy of connected band in terms of Wannier function description is shown in Fig.2

Under the TB model, the obstruction to real-space Wannier function description manifests as a lack of invariant band description of the connected bands. The configuration of band connectivity of connected bands with trivial/non-trivial topology is established from Wannier functions using the projection operator technique and provides the corresponding classification of band topology.

The TQC criteria of classifying topological phases are modified from “having atomic limit” to “having an invariant band description induced from Wannier functions”. In turn, Wannier functions, single or multi-centred, can only be defined from Fourier transform of connected bands with trivial topology.

The analysis is illustrated with the honeycomb lattice (graphene). Earlier work was reported in PCSI49.

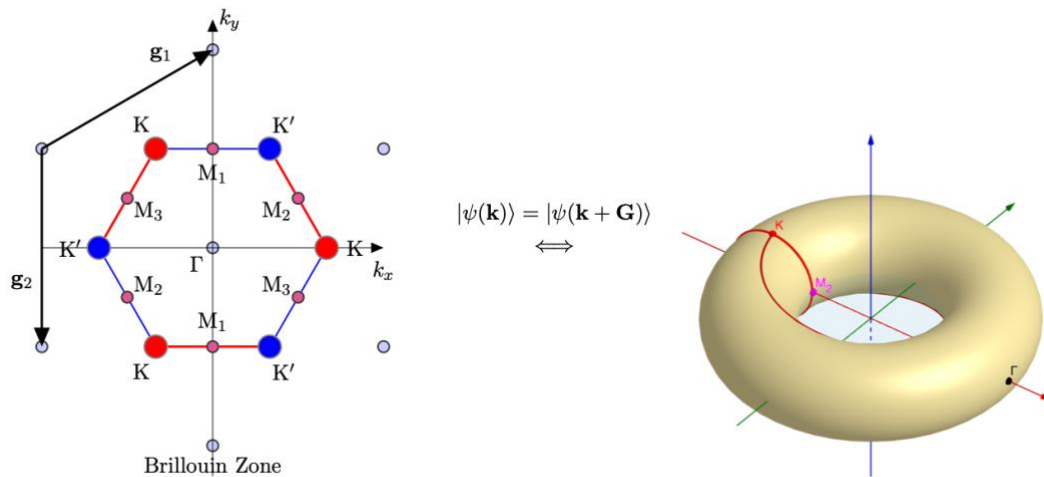


Figure 1: Brillouin zone of graphene ($\mathcal{G} = 80(L)$). (a) First Brillouin zone. (b) BZ torus. Segments of Wilson loop path are illustrated.

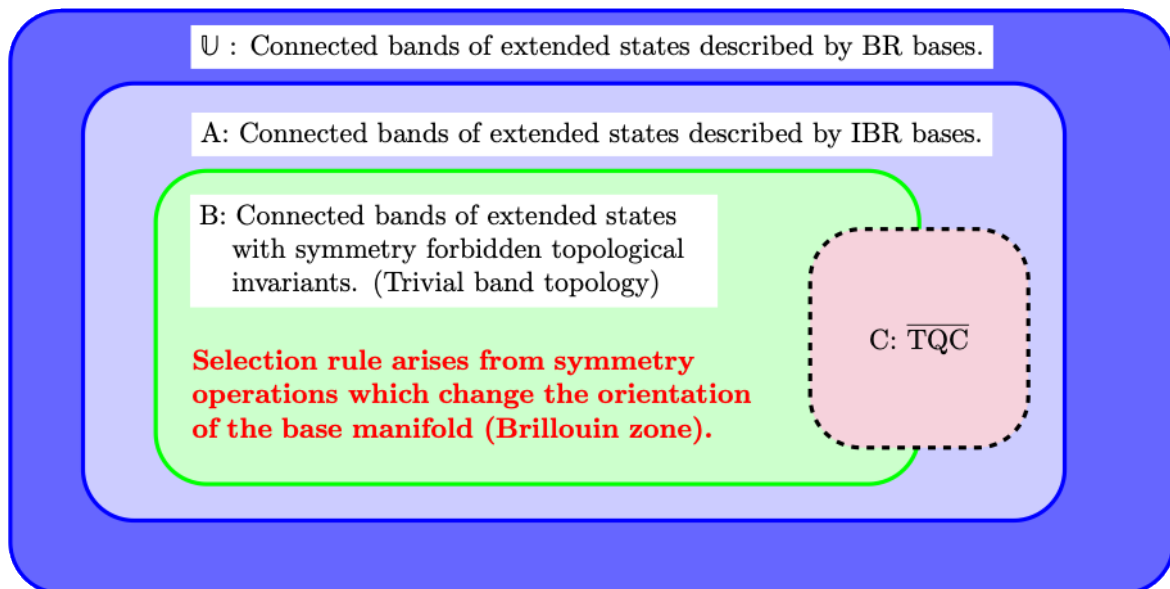


Fig.2 Partition of electronic dispersion of connected band under band representation description.