Symmetry constraints on topological invariants

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Abstract

Classification of topologically trivial/non-trivial crystalline insulators are based on the homology of Berry connection on the Bloch (vector) bundle with the Brillouin zone as the base manifold. Specifically, the trivial phase correspond to zero generalized Berry phase defined as

$$\phi_B = -i \ln \det \left[W(\mathbf{k}_0, C) \right] = -i \sum_n \oint_{\mathbf{k}_0}^{\mathbf{k}_0} \langle \psi_n(\mathbf{k}) \mid \nabla_{\mathbf{k}} \mid \psi_n(\mathbf{k}) \rangle \cdot \mathrm{d}\mathbf{k} \tag{1}$$

where W is the Wilson matrix, $|\psi_n(\mathbf{k})\rangle$ are the energy eigenstate of band n and path C is any closed path in the BZ. Whilst the transformation properties of $|\psi_n(\mathbf{k})\rangle$ may be well defined at given $\mathbf{k}$, it is generally a function of $\mathbf{k}$ and makes symmetry analysis of ϕ_B (path integral in BZ does not form a representation of the space group) difficult. There are symmetry analysis such as symmetry indicator method but they lack the group theoretical justification analogous to selection rules or Wigner-Eckart theorem. In this contribution, it is shown that ϕ_B can be evaluated using the band representation basis under the tight binding model and Stokes theorem.

$$i\phi_B = \sum_n \oint_{\mathbf{k}_0}^{\mathbf{k}_0} \langle \psi_n(\mathbf{k}) \mid \nabla_{\mathbf{k}} \mid \psi_n(\mathbf{k}) \rangle \cdot \mathrm{d}\mathbf{k} = \sum_j \oint_{\mathbf{k}_0}^{\mathbf{k}_0} \langle \phi_j(\mathbf{k}) \mid \nabla_{\mathbf{k}} \mid \phi_j(\mathbf{k}) \rangle \cdot \mathrm{d}\mathbf{k}. \tag{2}$$

where $|\phi_j(\mathbf{k})\rangle$ are the tight binding basis or elementary band representations with Slater-Koster choice of phase. The transformation properties of these EBRs contains no explicit $\mathbf{k}$ dependence and right hand side of Eq.(2) form a representation of the space group (The operation of space group takes the closed path to others in the BZ belonging to a closed set. These set of Berry phases along different paths within the set form the representation). Then symmetry argument may be applied with standard techniques such as selection rules and projection operators. As a closed path in the BZ is frequently not contained in the representation domain, it is important to consider the full group method, often neglected in preference to analysis within the representation domain of the BZ.

The base manifold of BZ are 2-torus (T^2, 2 dimensional lattice, layer group) or 3-torus (T^3, 3-dimensional lattice, space group). It is not simply connected

and one needs to inquivalent un-contractable closed path, as in homotopy analysis involving the fundamental group. The operation of symmetry group naturally takes closed path between such inequivalent set. Symmetry analysis shows the ϕ_B is generally not forbidden by symmetry of layer/space group. However, presence of some symmetry (e.g. inversion) may leads to specific selection rules that forces the Berry phase to be zero.

For a set of physically connected bands with symmetry at high symmetry points identical to direct sum of the EBRs, they have the same transformation properties as the set of EBRs and may be represented as such with appropriate interactions. The same symmetry analysis then may be applied. For close path containing the Γ point, what forms a representation of the group is not necessarily restricted to the whole close path, but half of a close path given that Γ point is invariant. Graphene is used as an example to illustrate both the trivial (sp_2 bands) and non-trivial (p_z band with spin).

The general conclusions are that not all ocuppied EBRs are symmetry forbidden from having non-zero Berry phase and occurrence of trivial phase are the exceptions. The symmetry indicator method at identifying trivial phase may include non-trivial phases.