Berry phases and curvatures, hybrid Wannier centers, and topological insulators

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In recent years there has been a dramatic growth of interest in the description of certain properties of crystalline materials in terms of Berry phases or Berry curvatures associated with their electronic bandstructures. These properties include electric polarization, anomalous Hall conductivity, orbital magnetization, and orbital magnetoelectric coupling. The field has exploded further in recent years with the theoretical prediction and experimental discovery of topological insulators (TIs), a class of insulators in which the electronic bands have a non-trivial topology in the Brillouin zone, and the realization that these topological properties are also closely related to Berry phases and curvatures.

In this pedagogical talk, I will begin by introducing the concepts of Berry phases and Berry curvatures, and explain how these are related to the properties listed above. As a common theme, I will introduce the concept of hybrid Wannier functions, which by definition are localized in one real-space dimension of an N-dimensional crystal and remain Bloch-like in the orthogonal (N-1) k-space dimensions. I will attach special emphasis to the Wannier charge centers (WCCs), which express the real-space location of the Wannier center in the (N-1)-dimensional k-space, arguing that they provide a powerful tool for revealing topological properties. For example, I will show how the "flow" of these WCCs can help us to visualize the differences between different kinds of TI states. This allows a natural formulation of the Chern invariant of the 2D quantum anomalous Hall (QAH) state or the Z2 invariant of the quantum spin Hall state, and provides an insightful visualization of the difference between normal, weak topological, and strong topological insulators in 3D. Illustrations will be given for tight-binding models in 2D and 3D, as well as for real materials such as the much-studied 3D strong topological insulator Bi_2Se_3.

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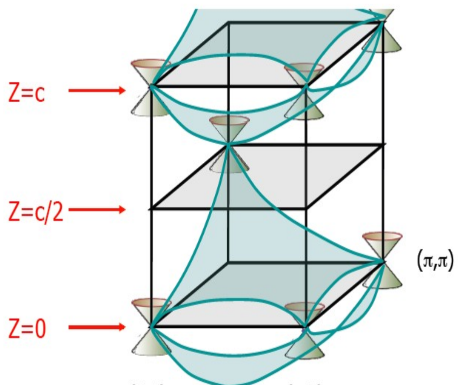

Fig. 1. Sketch of Wannier charge center (WCC) sheets for a 3D strong topological insulator having inversion symmetry.