Wannier Charge Center Sheets in Topologically Non-trivial 3D Band Insulators

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The electronic ground state in a periodic crystalline insulator can be described by hybrid Wannier functions $|W_{nl_z}(k_x,k_y)\rangle$ which are maximally localized in one direction and Bloch-like in the other two. The sheets of Wannier charge centers (WCCs), defined as $\bar{z}_n(k_x,k_y) = \langle W_{n0}(k_x,k_y)|\hat{z}|W_{n0}(k_x,k_y)\rangle$, have distinct behaviors in different topological phases. In a 3D time-reversal (TR) invariant insulator, pairs of WCC sheets touch at the TR-invariant points in the 2D Brillouin zone. The Z_2 topological invariants $[\nu_0,\nu_1,\nu_2,\nu_3]$ can be determined by the way in which these TR-invariant points are connected by the WCC sheets. In a topologically trivial insulator, pairs of WCC sheets are well separated from each other, which means the four ν_μ are all positive. In a topological non-trivial insulator, however, a WCC sheet touches two different WCC sheets at different TR-invariant points. In a weak topological insulator, which can be thought of as a stack of 2D spin-Hall insulators, it is always possible to find a direction along which the WCC sheets pair up as in a trivial insulator, while they have a non-trivial behavior along the other two directions. The strong Z_2 index ν_0 is positive in this case, while at least one of ν_i is negative. In a strong topological insulator, ν_0 is negative and the WCC sheets have a topologically non-trivial behavior in any chosen direction. This distinct behavior is illustrated for different topological phases in the 3-D Kane-Mele model,[1,2] which is a four-band tight-binding model of s states on a diamond lattice with spin-orbit interaction. By varying the relative strength of a nearest-neighbor bond in one direction, the system can be switched between trivial, weak, and strong topological insulating phases. We also present the WCC sheets computed from first principles for the occupied states of the strong Z_2 insulator Bi_2Se_3 and trivial insulator Sb_2Se_3, again confirming that this approach correctly identifies the topological phases.

[1] L. Fu, C.L. Kane, and E Mele, Phys. Rev. Lett **98**, 106803 (2007).

[2] A. Essin, J. Moore, D. Vanderbilt, Phys. Rev. Lett. **102**, 146805 (2009).