Bismuth antiphase domain wall: A three-dimensional manifestation of the Su-Schrieffer-Heeger model

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The Su, Schrieffer, and Heeger (SSH) model[1], describing the soliton excitations in polyacetylene due to the formation of antiphase domain walls (DW) from the alternating bond pattern, has served as a paradigmatic example of one-dimensional (1D) chiral topological insulators. While the SSH model has been realized in photonic and plasmonic systems, there have been limited analogues in three-dimensional (3D) electronic systems, especially regarding the formation of antiphase DWs. Here, we propose that pristine bulk Bi, in which the dimerization of (111) atomic layers renders alternating covalent and van der Waals bonding within and between successive (111) bilayers, respectively, serves as a 3D analogue of the SSH model. First, we confirm that the two dimerized Bi structures belong to different Zak phases[2] of 0 and π by considering the parity eigenvalues and Wannier charge centers, while the previously reported bulk topological phases of Bi remain invariant under the dimerization reversal. Next, we demonstrate the existence of topologically non-trivial (111) and trivial (11-2) DWs in which the number of in-gap DW states (ignoring spin) is odd and even respectively, and show how this controls the interlinking of the Zak phases of the two adjacent domains. Finally, we derive general criteria specifying when a DW of arbitrary orientation exhibits a π Zak phase based on the flip of parity eigenvalues.

References

[1] W.P. Su, J.R. Schrieffer, and A.J. Heeger, Phys. Rev. Lett. **42** (1979) 1698-1701.
[2] J. Zak, Phys. Rev. Lett. **62** (1989) 2747-2750.

Figures

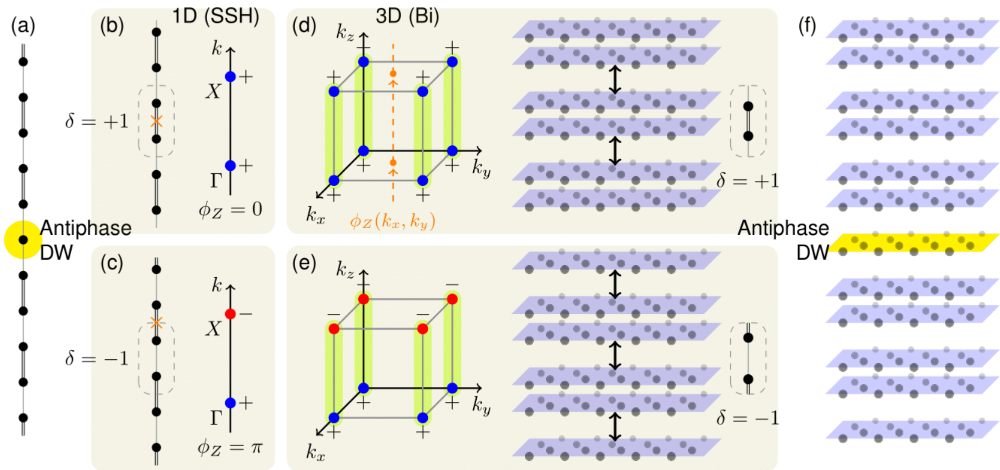

Figure 1: Schematic view of the SSH model and comparison with the 3D analogue. (a) Antiphase DW of the SSH model. (b, c) Two dimerized phases (δ=±1) and corresponding parity eigenvalues, whose product determines the Zak phase (Φ_Z). (d, e) 3D analogue of the SSH model where the Zak phase also depends on the dimerization. (f) Antiphase DW as the 3D analogue of the SSH model.