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Bulk-boundary correspondence from the inter-cellular Zak phase
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— The Zak phase γ, the generalization of the Berry phase to Bloch wave functions in solids, is often used to characterize inversion-symmetric 1D topological insulators; however, since its value can depend on the choice of real-space origin and unit cell, only the difference between the Zak phase of two regions is believed to be relevant. Here, we show that one can extract an origin-independent part of γ, the so-called inter-cellular Zak phase γ^{inter}, which can be used as a bulk quantity to predict the number of surface modes as follows: a neutral finite 1D tight-binding system has $n_s = \gamma^{\text{inter}}/\pi \pmod 2$ number of in-gap surface modes below the Fermi level if there exists a commensurate bulk unit cell that respects inversion symmetry. We demonstrate this by first verifying that $\pm e\gamma^{\text{inter}}/2\pi \pmod e$ is equal to the extra charge accumulation in the surface region for a general 1D insulator, while the remnant part of γ, the intra-cellular Zak phase γ^{intra}, corresponds to the electronic part of the dipole moment of the bulk's unit cell. Second, we show that the extra charge accumulation can be related to the number of surface modes when the unit cell is inversion symmetric.

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