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The Shockley-model description of the edge states in topological insulators VICTOR YAKOVENKO, SERGEY PERSHOGUBA, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, Maryland 20742-4111 — We show that the edge states in topological insulators can be understood based on the well-known Shockley model, a 1D tight-binding model with two atoms per elementary cell connected via alternating tunneling amplitudes. We generalize the model to a 3D Shockley-like model corresponding to the sequence of layers connected via the tunneling amplitudes dependent on the in-plane momentum $\mathbf{p} = (\mathbf{p_x}, \mathbf{p_y})$. The Hamiltonian of the model is a 2×2 matrix with the complex off-diagonal matrix element $t(k, \mathbf{p})$ dependent on both $\mathbf{p}$ and the out-of-plane momentum k. The equation $t(k, \mathbf{p}) = \mathbf{0}$ defines vortex lines in the 3D momentum space. We show that the projection of the vortex lines on the 2D momentum space defines a boundary between the regions of $\mathbf{p}$ where the edge states exist or do not exist. The vorticity of the vortex lines determines the crystal sublattice on which the edge states are localized. We illustrate how our approach works for the well-established topological insulator model by Fu, Kane, and Mele. We find that different configurations of the vortex contours are responsible for the topological insulator phases with even or odd numbers of the surface Dirac cones. We discuss how real materials, such as Bi_2Se_3, can be described by this model.

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