Surface Hamiltonian of a higher-order topological insulator for $MoTe_2$

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Higher-order topological insulators are topological insulators with a dimensional difference between the bulk and zero energy state by more than one. This will lead to interesting physical situations such as a 3-dimensional system with a zero energy hinge mode or a 2-dimensional system with corner modes. Using the bulk Hamiltonian of the metal dichalcogenides $MoTe_2$ as the cornerstone, results of a 3-dimensional second-order topological insulator is given [1]. To find the properties of the surface, the surface Hamiltonian is also given to analytically calculate the location and circumstances of hinge states to arise. The finite Hamiltonian is given via the tight-binding method, with the system being a cuboid the size of 30 lattice sites for the x and y directions each while periodic in the z direction. The surface Hamiltonian of the system is calculated using a Dirac equation approximation in cylindrical coordinates [2]. For a specific set of parameters, the electron density of the system shows a concentration of the zero energy wavefunction at two opposing hinges. Geometry of the finite system is changed to show change of the corner states in regard to the collapse of the corner. The Z_4 index of the system is calculated using the parity eigenvalues [3], which will separate topological insulators and the second-order topological insulator.

References:

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