Model of TI Thin Film

Bulk Hamiltonian

$k \cdot p$ Hamiltonian from https://aip.scitation.org/doi/abs/10.1063/1.4790804

- Basis we used: $\{|P1_z^+, \uparrow>, |P2_z^-, \uparrow>, |P1_z^+, \downarrow>, |P2_z^-, \downarrow>\}$
- Origin Hamiltonian of 3D TI:

$$H(k) = \epsilon_0(k) + \begin{pmatrix} M(k) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -M(k) & A_2 k_- & 0 \\ 0 & A_2 k_+ & M(k) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -M(k) \end{pmatrix}$$

,where $\epsilon(k) = C + D_1 k_z^2 + D_2 k_\perp^2, M(k) = M - B_1 k_z^2 - B_2 k_\perp^2$

Discretization

- Discretized H in the z direction, with discretization length Δ. The diagonal term is:

$$h_{ii}(k) = \epsilon(k_x, k_y) + U(z_i) + \frac{2G_{zz}}{\Delta^2} + \begin{pmatrix} M(k_x, k_y) & 0 & 0 & A_2 k_- \\ 0 & -M(k_x, k_y) & A_2 k_- & 0 \\ 0 & A_2 k_+ & M(k_x, k_y) & 0 \\ A_2 k_+ & 0 & 0 & -M(k_x, k_y) \end{pmatrix}$$

and the coupling term between nearest layer:

$$t_{i,i+1} = -\frac{G_{zz}}{\Delta^2} - \frac{G_z}{2\Delta}$$
$$t_{i,i-1} = -\frac{G_{zz}}{\Delta^2} + \frac{G_z}{2\Delta}$$

,where

$$G_{zz} = \begin{pmatrix} D_1 - B_1 & 0 & 0 & 0 \\ 0 & D_1 + B_1 & 0 & 0 \\ 0 & 0 & D_1 - B_1 & 0 \\ 0 & 0 & 0 & D_1 + B_1 \end{pmatrix}$$

and

$$G_z = \begin{pmatrix} 0 & +iA_1 & 0 & 0 \\ +iA_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -iA_1 \\ 0 & 0 & -iA_1 & 0 \end{pmatrix}$$

- The total Schrodinger Equation is $H_{ij}(k_x, k_y)\psi_j = E\psi_i$, and the large Hamiltonian is

$$H(k_x, k_y) = \begin{pmatrix} h_{1,1} & t_{1,2} & 0 & 0 \\ t_{2,1} & h_{2,2} & t_{2,3} & 0 \\ 0 & t_{3,2} & \ddots & \ddots \\ 0 & 0 & \ddots & h_{N,N} \end{pmatrix}$$

Constants

	PRB 82,045122(2010)	Haizhou Lu	HJ Zhang 2009 First-Pinciple,Bulk
$A_1(\mathrm{eV}\cdot\mathrm{\AA})$	2.26	3.3	2.2
$A_2(\mathrm{eV}\cdot\mathrm{\AA})$	3.33	4.1	4.1
$C(\mathrm{eV})$	-0.0083	-0.0068	-0.0068
$D_1(\mathrm{eV}\cdot\mathrm{\AA}^2)$	5.74	1.2	1.3
$D_2(\mathrm{eV}\cdot\mathrm{\AA}^2)$	30.4	-30.1	19.6
$M(\mathrm{eV})$	0.28	0.28	0.28
$B_1(\mathrm{eV}\cdot\mathrm{\AA}^2)$	6.86	1.5	10
$B_2(\mathrm{eV}\cdot\mathrm{\AA}^2)$	44.5	-54.1	56.6