

**1. (20 points)** Topological classification of  $\text{Bi}_2\text{Se}_3$  via parity eigenvalues.

The effective theory of the archetypal 3D topological insulator  $\text{Bi}_2\text{Se}_3$  is given by the following Bloch Hamiltonian on the simple cubic lattice,

$$\mathcal{H}(\mathbf{k}) = \lambda\sigma_z(s_x \sin k_y - s_y \sin k_x) + \lambda_z\sigma_y \sin k_z + \sigma_x M_{\mathbf{k}}.$$

Here  $M_{\mathbf{k}} = \epsilon - 2t(\cos k_x + \cos k_y) - 2t_z \cos k_z$  and  $\mathbf{s}, \boldsymbol{\sigma}$  represent the Pauli matrices in spin and orbital space, respectively.  $\lambda, \lambda_z, \epsilon$  and  $t, t_z$  are model parameters, reflecting the layered structure of  $\text{Bi}_2\text{Se}_3$ . Hereafter, we take  $\lambda = 1$  and measure the remaining parameters in units of  $\lambda$ .

a) Find the spectrum of  $\mathcal{H}(\mathbf{k})$ . Show that  $\mathcal{H}(\mathbf{k})$  respects both  $\mathcal{T}$  and  $\mathcal{P}$ . (The inversion operation here involves exchange of the two orbitals on the same site implemented by  $\sigma_x$ ).

b) Use the Fu-Kane parity criterion to classify the topological phases of  $\mathcal{H}(\mathbf{k})$  when the two negative-energy bands are filled. Consider the case when  $t = t_z > 0$  and  $\lambda_z = \lambda$ . Sketch the phase diagram as a function of  $\epsilon$ . Please label clearly the phase transitions and assign the  $Z_2$  indices  $(\nu_0; \nu_1\nu_2\nu_3)$  to the phases as appropriate.

c) Sketch the representative Fermi contours for the  $z = 0$  surface in the above phases.

d) Now relax the condition  $t = t_z$ . For what values of  $\epsilon$  and  $t_z$  will the system be in the (1;110) phase? Sketch the representative Fermi contours for the  $x = 0$  surface in this phase.

**2. (15 points)**  $\text{Bi}_2\text{Se}_3$  surface states.

Consider the above Hamiltonian with parameters appropriate for the (1;000) topological phase but close to the transition to the trivial (0;000) phase. To keep things simple focus again on the case when  $t = t_z > 0$  and  $\lambda_z = \lambda$ .

a) Formulate the effective low-energy theory for the electrons *in the bulk* for this situation.

b) Show explicitly that this theory implies a single gapless surface state on the boundary between the TI and the trivial phase. Find the low-energy Hamiltonian for this surface state appropriate for the boundary in the  $z = 0$  plane and in the  $x = 0$  plane.

c) Sketch the spectrum of the surface states for the two planes and indicate the spin orientation.

**3. (Bonus problem, 5 points)**  $\mathcal{T}$ -breaking in  $\text{Bi}_2\text{Se}_3$ .

Show that by allowing terms in the above-defined  $\mathcal{H}(\mathbf{k})$  that break time reversal the distinction between various topological phases disappears. *Hint:* This is easiest done by finding a  $\mathcal{T}$ -breaking term that anticommutes with  $\mathcal{H}(\mathbf{k})$ .