PHYS 525
Solutions to HW 5

(Dated: March 21, 2019)

PROBLEM 1

a) We first consider the eigenstates of the Hamiltonian

$$\mathcal{H}(\vec{k}) = \lambda\sigma_z\left(s_x \sin k_y - s_y \sin k_x\right) + \lambda_z \sigma_y \sin k_z + \sigma_x M_{\vec{k}} \tag{1}$$

$$M_{\vec{k}} = \epsilon - 2t\left(\cos k_x + \cos k_y\right) - 2t_z \cos k_z. \tag{2}$$

We have

$$\mathcal{H}^2(\vec{k}) = \left(\lambda^2(\sin^2 k_y + \sin^2 k_y) + M_{\vec{k}}^2\right)\mathbf{1}_{4\times 4}. \tag{3}$$

For $\lambda = 1$, the eigenstates are

$$\boxed{\varepsilon(\vec{k}) = \pm\sqrt{\sin^2 k_x + \sin^2 k_y + \lambda_z^2 \sin^2 k_z + M_{\vec{k}}^2}.} \tag{4}$$

Note that each band is doubly-degenerate.

Under the inversion $\mathcal{P}$ and time-reversal $\mathcal{T}$ operations, the Hamiltonian transforms as

$$\mathcal{P}: \quad \sigma_x \mathcal{H}(\vec{k})\sigma_x = -\sigma_z\left(s_x \sin k_y - s_y \sin k_x\right) - \lambda_z \sigma_y \sin k_z + \sigma_x M_{\vec{k}} \tag{5}$$

$$= \mathcal{H}(-\vec{k}) \tag{6}$$

$$\mathcal{T}: \quad s_y \mathcal{H}^*(\vec{k}) s_y = \sigma_z\left(-s_x \sin k_y + s_y \sin k_x\right) - \lambda_z \sigma_y \sin k_z + \sigma_x M_{\vec{k}} \tag{7}$$

$$= \mathcal{H}(-\vec{k}) \tag{8}$$

b) The occupied bands satisfy

$$\mathcal{H}(\vec{k})\Psi_\alpha^{(-)}(\vec{k}) = -|\varepsilon(\vec{k})|\Psi_\alpha^{(-)}, \tag{9}$$

where $\alpha \in 1, 2$ is an effective angular momentum index. The 8 TRIM $\vec{\Gamma}_{i=1\ldots 8}$ occur at $k_{x,y,z} = 0, \pi$. At these TRIM, $|\varepsilon(\vec{\Gamma}_i)| = |M_{\vec{\Gamma}_i}|$. Moreover, $\mathcal{H}(\vec{\Gamma}_i) = \sigma_x M_{\vec{\Gamma}_i}$. Therefore, we can write

$$\mathcal{H}(\vec{\Gamma}_i)\Psi_\alpha^{(-)}(\vec{\Gamma}_i) = \sigma_x M_{\vec{\Gamma}_i}\Psi_\alpha^{(-)} \tag{10}$$

$$= -|M_{\vec{\Gamma}_i}|\Psi_\alpha^{(-)}. \tag{11}$$

The eigenvalues under inversion are then

$$\boxed{\sigma_x \Psi_\alpha^{(-)} = -\mathrm{sgn}(M_{\vec{\Gamma}_i})\Psi_\alpha^{(-)}.} \tag{12}$$

We impose $t = t_z > 0$ and $\lambda_z = \lambda$. Refer to Fig. 1.

The ν_0 $\mathbb{Z}_2$ index is determined from

$$(-1)^{\nu_0} = \prod_{i=1}^{8} -\mathrm{sgn}(M_{\vec{\Gamma}_i}) \tag{13}$$

$$= \mathrm{sgn}\left[(-1)^8(\epsilon - 6t)(\epsilon + 6t)\left[(\epsilon - 2t)(\epsilon + 2t)\right]^3\right] \tag{14}$$

$$= \mathrm{sgn}\left[(|\epsilon| - 6t)(|\epsilon| - 2t)\right]. \tag{15}$$

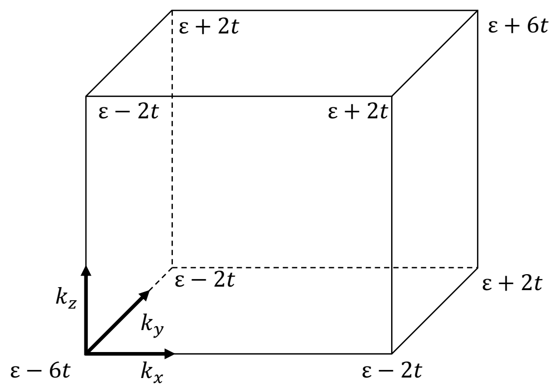

FIG. 1. $M_{\vec{\Gamma}_i}$ at TRIM for a).

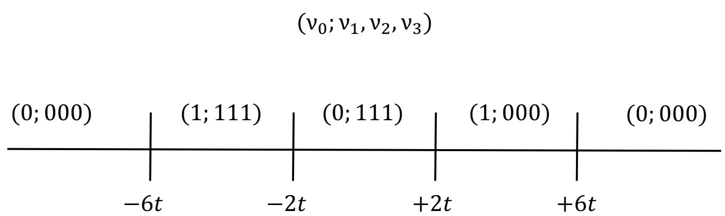

FIG. 2. Phase diagram for b).

$$\boxed{\nu_0 = \begin{cases} 0, & |\epsilon| < 2t \text{ or } |\epsilon| > 6t \\ 1, & \text{otherwise} \end{cases}} \tag{16}$$

For all other three indices $\nu_{i=1,2,3}$, we have the unique expression

$$(-1)^{\nu_i} = \prod_{i=j}^{4} -\text{sgn}(M_{\vec{\Gamma}_j}) \tag{17}$$

$$= \text{sgn}(-1)^4 \left[(\epsilon + 2t)^2(\epsilon - 2t)(\epsilon + 6t)\right] \tag{18}$$

$$= \text{sgn}\left[(\epsilon + 6t)(\epsilon - 2t)\right]. \tag{19}$$

Note that the products above correspond to the eigenvalues of the inversion at TRIM $\Gamma_{j,x}$ with x, y, z components set to π respectively.

$$\boxed{\nu_{i=1,2,3} \begin{cases} 0, & \epsilon < -6t \text{ or } \epsilon > 2t \\ 1, & \text{otherwise.} \end{cases}} \tag{20}$$

c)

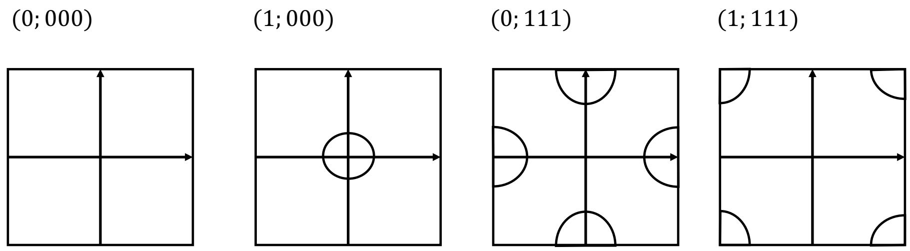

FIG. 3. Fermi surfaces for the $z = 0$ boundary.

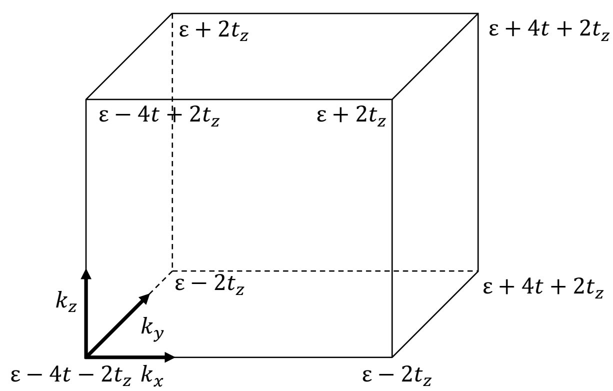

FIG. 4. $M_{\vec{\Gamma}_i}$ at TRIM for d).

d) Consider $t \neq t_z$ and refer to Fig. 4

$$(-1)^{\nu_1} = (-1)^{\nu_2} = (-1)^4 \mathrm{sgn}\left[(\epsilon + 2t_z)(\epsilon - 2t_z)(\epsilon + 4t - 2t_z)(\epsilon + 4t + 2t_z)\right] \tag{21}$$
$$= \mathrm{sgn}\left[(|\epsilon| - 2t_z)(|\epsilon + 4t| - 2t_z)\right] \tag{22}$$
$$(-1)^{\nu_3} = (-1)^4 \mathrm{sgn}\left[(\epsilon + 2t_z)^2(\epsilon + 4t + 2t_z)(\epsilon - 4t + 2t_z)\right] \tag{23}$$
$$= \mathrm{sgn}\left[|\epsilon + 2t_z| - 4t\right] \tag{24}$$
$$(-1)^{\nu_0} = (-1)^8 \mathrm{sgn}\left[(\epsilon + 2t_z)^2(\epsilon - 2t_z)^2(\epsilon + 4t + 2t_z)(\epsilon + 4t - 2t_z)(\epsilon - 4t + 2t_z)(\epsilon - 4t - 2t_z)\right] \tag{25}$$
$$= \mathrm{sgn}\left[(|\epsilon - 4t| - 2t_z)(|\epsilon + 4t| - 2t_z)\right] \tag{26}$$

The (1;110) phase occurs for a range of parameters indicated in Fig. 5 which also shows all other phases that are possible in the system when the condition $t_z = t$ is relaxed.

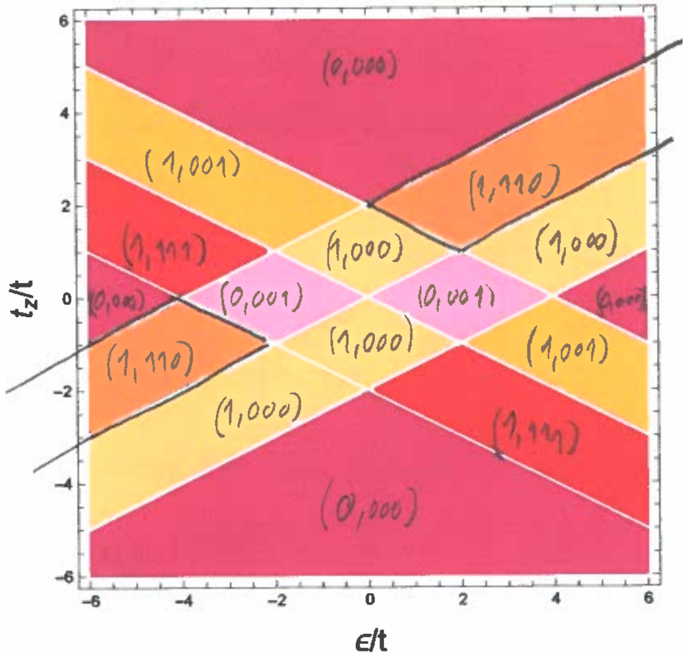

FIG. 5. Phase diagram for $t_z \neq t$. (Figure courtesy of Rafael Haenel).

PROBLEM 2

a) We know from the dispersion found in the previous problem ($\lambda = \lambda_z$) that for when $\epsilon = 6t$ the bulk gap can close when $k_{x,y,z} = 0$. Allowing $\epsilon(x, y, z) = 6t - \Delta(x, y, z)$, we can expand the Hamiltonian to linear order about this point:

$$\boxed{\mathcal{H}_{eff}(\vec{q}) = \sigma_z(s_x q_y - s_y q_x) + \sigma_y q_z - \Delta(x, y, z)\sigma_x}. \tag{27}$$

b) <u>$x = 0$ surface</u>:

Let $\Delta(x, y, z) = \Delta(x)$, with opposite signs on either side of the surface. Ignoring the dispersion along the surface ($q_y = q_z = 0$), we can solve the following Hamiltonian:

$$\mathcal{H}_{eff} = i\sigma_z s_y \partial_x - \Delta(x)\sigma_x. \tag{28}$$

This can be brought into an effective 1D form if we rotate $s_y \to s_z$. We look for zero-modes with the ansatz

$$\Psi_x = \begin{pmatrix} u_a \\ u_b \\ v_a \\ v_b \end{pmatrix} \phi(x). \tag{29}$$

The equations are

$$(iu_a\partial_x - v_a\Delta(x))\phi(x) = 0 \tag{30}$$
$$(iu_b\partial_x + v_b\Delta(x))\phi(x) = 0 \tag{31}$$
$$(iv_a\partial_x + u_a\Delta(x))\phi(x) = 0 \tag{32}$$
$$(iv_b\partial_x - u_b\Delta(x))\phi(x) = 0 \tag{33}$$

We can find two solutions when either (i) $u_b = v_b = 0, u_a = iv_a \neq 0$ **or (ii)** $u_b = iv_b \neq 0, u_a = v_a = 0$**.** In either case, $\phi(x) = Ce^{-\int_0^x dx'\Delta(x')}$.

<u>$z = 0$ surface</u>

Now we have $\Delta(x, y, z) = \Delta(z)$ with similar sign change about the surface and set $q_x = q_y = 0$:

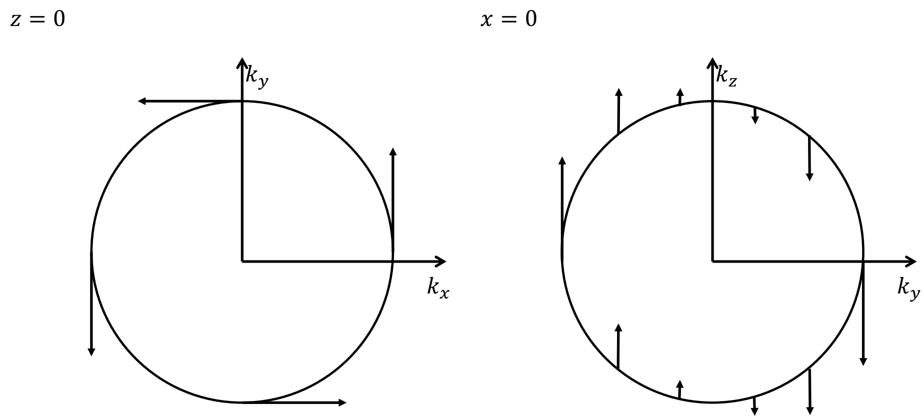

FIG. 6. Surface spectrum and spin orientation for one surface. The orientation is reversed for the other surface. In the $x = 0$ plane, the spin is oriented along $\hat{x}$.

$$\mathcal{H}_{eff} = -i\sigma_y\partial_z - \Delta(z)\sigma_x. \tag{34}$$

This reduces to

$$u_a(-\partial_z - \Delta(z))\phi(z) = 0 \tag{35}$$
$$u_b(-\partial_z - \Delta(z))\phi(z) = 0 \tag{36}$$
$$v_a(\partial_z - \Delta(z))\phi(z) = 0 \tag{37}$$
$$v_b(\partial_z - \Delta(z))\phi(z) = 0. \tag{38}$$

We can find solutions when either (i) $u_a = 1, u_b = v_a = v_b = 0$ **or (ii)** $u_b = 1, u_b = v_a = v_b = 0$**.**

Note that for the $x = 0$ case, we can find a vector in a mixed orbital-spin space which rotates like $\vec{s}$ as in the $z = 0$ case.

c)

PROBLEM 3

Consider the low-energy effective Hamiltonian of the previous problem:

$$\mathcal{H}_{eff}(\vec{q}) = \sigma_z(s_x q_y - s_y q_x) + \sigma_y q_z - \Delta(x, y, z)\sigma_x. \tag{39}$$

We can add a term $m\sigma_z s_z$ **that breaks time-reversal and that anti-commutes with** $\mathcal{H}_{eff}(\vec{q})$**.** The resulting spectrum is

$$\varepsilon(\vec{q}) = \pm\sqrt{|\vec{q}|^2 + \Delta^2(\vec{r}) + m^2}. \tag{40}$$

Thus, it is possible to pass from regions with $\Delta > 0$ to those with $\Delta < 0$ without closing the gap. In this case, there are no gapless surface states.