Question-1.

- **Conclusion for Q1**

we see that

$$\left.\begin{aligned} m(K) &= m - 3\sqrt{3}\,t\sin\varphi \\ m(K') &= m + 3\sqrt{3}\,t\sin\varphi \end{aligned}\right] \text{eff mass terms}$$

now as we know from usual graphene / MoS_2 physics that gap closing changes the chern number of each valley.

Hence, we can make cases as:-

① $m > 3\sqrt{2}\sin\varphi \cdot t$: no Gap closing

$\Rightarrow \sigma_{xy} = 0$ [trivial as net $C = 0$ from both valleys]

② $-3\sqrt{2}t\sin\varphi < m < 3\sqrt{2}t\sin\varphi$ for $\varphi > 0$

At $m = 3\sqrt{2}t\sin\varphi$, gap closes at K & we have a net "non-zero" chern number

$\Delta\sigma_{xy} = -\frac{e^2}{h}$. The Gap at K' is open still

③ $m < -3\sqrt{2}t\sin\varphi$, $\varphi > 0$

→ Gap at K' closes & $C = 0$ again.

For $\varphi < 0$, the signs of chern numbers are inverted.

The resulting phase diagram is the one shown in Mathematica notebook.

Q2. Let's start with

$$\mathcal{H} = k_+^3 \sigma_- + k_-^3 \sigma_+ + m\sigma_z \quad \text{\& then we'll set } m \to 0$$

$$(\vec{\Omega}_-)_z = \frac{m}{\left[(k_+^3+k_-^3)^2 + [i(k_-^3 - k_+^3)]^2 + m^2\right]^{3/2}}$$

[Berry curvature of $\vec{d}\cdot\vec{\sigma}$ models = monopole in parameter space]

$$= \frac{m}{[4k_+^3 k_-^3 + m^2]^{3/2}}$$

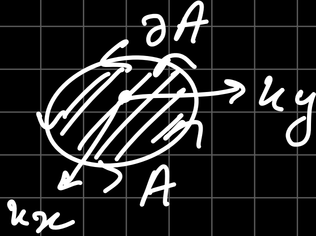
$$= \frac{m}{\left[4\{(\vec{k}\cdot\vec{k})_{2D}\}^3 + m^2\right]^{3/2}}$$

$\therefore$ In general for $\mathcal{H} = k_+^n \sigma_- + k_-^n \sigma_+ + m\sigma_z$,

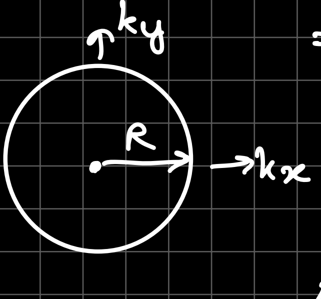
$$(\vec{\Omega}_-)_z = \frac{m}{\left[4(\vec{k}\cdot\vec{k})_{2D}^n + m^2\right]^{3/2}}$$

$$\therefore \quad \gamma = \int_{\vec{A}} \vec{\Omega}\cdot d\vec{S}_{xy}$$

where $\vec{A}$ is the area bounded by some path around the deg. pnt $k_x = k_y = 0$



$$= \lim_{m\to 0} \int_{\vec{A}} \frac{m \; dk_x\, dk_y}{\left[4(\vec{k}\cdot\vec{k})_{2D}^n + m^2\right]^{3/2}}$$



$$= \lim_{m\to 0} \int_{k=0}^{R} \frac{2m\pi \, k\, dk}{[4k^{2n} + m^2]^{3/2}}$$

(we change coordinates assuming that $\vec{A}$ is a circle of some radius $R>0$ for the time being)

$$= \lim_{m\to 0} \pi m \int_{t=0}^{t=\sqrt{R}} \frac{dt}{[4t^n + m^2]^{3/2}}$$

where $t = k^2$

now set $t = m^{2/n} y \Rightarrow y \in [0, m^{-2/n}\sqrt{R}]$

$$= \lim_{m \to 0} \pi \int_0^{m^{-2/n}\sqrt{R}} \frac{m^{1+2/n}\, dy}{m^3 [4y^n + 1]^{3/2}}$$

$$= \lim_{m \to 0} \pi\, m^{2-2/n} \int_0^{m^{-2/n}\sqrt{R}} \frac{dy}{[4y^n + 1]^{3/2}}$$

Now,

as $m \to 0$, $\frac{\sqrt{R}}{m^{2/n}}$ for $n \in \mathbb{N}$, $n \geq 3$ $\longrightarrow \infty \Rightarrow$ integral is indpt of m
n, fixed

as $m \to 0$, $m^{2-2/n}$, for $n \in \mathbb{N}$, $n \geq 3$, $\rightarrow 0$
n fixed

$$\therefore \lim_{m \to 0} \pi\, m^{2-2/n} \int_0^{m^{-2/n}\sqrt{R}} \frac{dy}{[4y^n + 1]^{3/2}}$$

for small m $\approx$ $\pi \lim_{m \to 0} m^{2-2/n} \int_0^{\infty} \frac{dy}{[4y^n + 1]^{3/2}}$

$\Rightarrow \gamma = 0$ for for $n = 3, 4, 5 \ldots$

(for $n = 1$, $\gamma = \pi \lim_{m \to 0} m^{2-2/1} \times$(some #)
$\neq 0$
hence this is consistent)

Q 3.

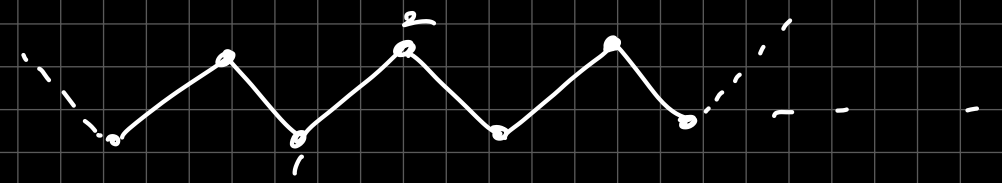
(a) $V_{lattice} = \frac{K}{2} \sum_n (u_{n+1} - u_n)^2$

$u_{n+1} - u_n = u_0 (-1)^n [(-1) - 1] = (-2) u_0 (-1)^n$

$\therefore V_{lattice} = \frac{K}{2} \sum_{n=1}^{N} 2^2 u_0^2 (-1)^{2n}$, where N = Total # of sites

$= 2 K u_0^2 N$ (periodic BC $\therefore$ N is taken, not $N-1$)

(b)



$\mathcal{H}(k) = t_0 e^{-ika} + t_0 e^{ika} = 2t \cos ka \rightarrow 1$ site basis

for a two site basis

$$\mathcal{H}(k) = \begin{pmatrix} 0 & t_0 + t_0 e^{-ik \cdot (2a)} \\ t_0 + t_0 e^{ik(2a)} & 0 \end{pmatrix}$$

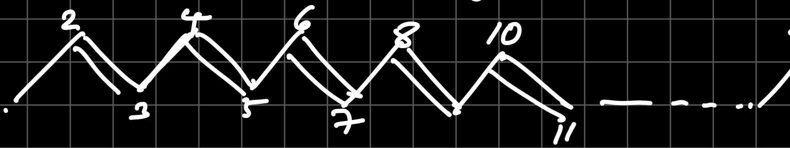
eigenvalues $\Rightarrow \pm 2 t_0 \cos ka$

see the Mathematica file for the rest of the answer.

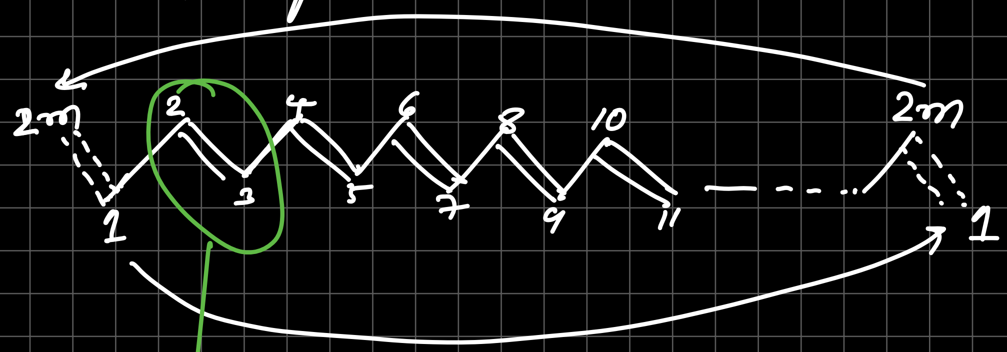
(c) $t_{n+1,n} = t_0 - \alpha (u_{n+1} - u_n)$

$= t_0 + 2\alpha u_0 (-1)^n$ for $u_n = (-1)^n u_0$

so the chain looks something like this



→ under periodic BC



unit cell ⇒ Picking this unit cell with

$$\backslash\backslash \equiv t_0 + 2\alpha u_0$$

$$\backslash \equiv t_0 - 2\alpha u_0$$

Constructing a 2x2 hamiltonian we have

$$\mathcal{H}(k) = \begin{pmatrix} 0 & (t_0 + 2\alpha u_0) + (t_0 - 2\alpha u_0)e^{-ik \times 2a} \\ (t_0 + 2\alpha u_0) + (t - 2\alpha u_0)e^{ik \times 2a} & 0 \end{pmatrix}$$

$$E_{\pm} = \pm\sqrt{2(t^2 + 4u^2\alpha^2 + (t^2 - 4u^2\alpha^2).\cos 2ak}$$

See mathematica file for further sol^n.

(d) $E = E_{lattice} + E_{e\ominus}$

from (a), $E_{lattice} = 2 \times u_0^2 N = 2K N \times \left(\frac{t_0 z}{2\alpha}\right)^2$

where $z = \frac{2\alpha u_0}{t_0}$ $\quad = \frac{K N t_0^2 z^2}{2\alpha^2}$

$$E_{e\ominus} = \underset{\substack{\uparrow \\ \text{spin deg}}}{2} \times \sum_{k=-\pi/2a}^{\pi/2a} E_-(k) = \frac{Na}{(2\pi)} \sum_{k=-\pi/2a}^{k=\pi/2a} E_-(k)\left(\frac{2\pi}{Na}\right) \times 2$$

$$= \frac{Na}{2\pi} \int_{k=-\pi/2a}^{k=\pi/2a} E_-(k)\, dk \times 2$$

$$= \left(-\frac{Na}{\pi}\right) \int_{-\pi/2a}^{\pi/2a} \sqrt{2(t^2+4u^2\alpha^2 + (t^2-4u^2\alpha^2)\cdot\cos 2ak}\; dk$$

$$= \left(-\frac{Na}{\pi}\right) \times 2 \int_{0}^{\pi/2a} \sqrt{2(t_0^2+4u^2\alpha^2 + (t_0^2-4u^2\alpha^2)\cos 2ak}\; dk$$

$$k \rightarrow ka$$

$$= \left(-\frac{2Nt_0}{\pi}\right) \int_{0}^{\pi/2} \sqrt{2(1+z^2+(1-z^2)\cos 2k)}\; dk$$

$$= \left(-\frac{2Nt_0}{\pi}\right) \int_{0}^{\pi/2} \sqrt{2\times\left[2-(1-z^2)(1-\cos 2k)\right]}\; dk$$

$\cos 2\theta = \cos^2\theta - \sin^2\theta = 1 - 2\sin^2\theta$

$$= \left(-\frac{2Nt_0}{\pi}\right) \int_{0}^{\pi/2} 2\sqrt{(1-(1-z^2)\sin^2 k)}\; dk$$

$$= \left(-\frac{4Nt_0}{\pi}\right) E(1-z^2)$$

$$\therefore E_{net} = \underbrace{-\frac{4Nt_0}{\pi} E(1-z^2)}_{E_{el}} + \underbrace{\frac{NKt_0^2 z^2}{2\alpha^2}}_{E_{lattice}}$$

(e) $E(1-z^2) = 1 + \frac{1}{2}\left[\ln\left(\frac{4}{|z|}\right) - \frac{1}{2}\right] z^2 + \cdots$

$$E_0 = -\frac{4Nt_0}{\pi} \left\{ -\frac{2Nt_0}{\pi}\left[\ln\left(\frac{4}{|z|}\right) - \frac{1}{2}\right] z^2 + \frac{NKt_0 z^2}{2\alpha^2} \right\}$$

$$E_{0\,perch} = \frac{-4t_0}{\pi} - \frac{4t_0}{\pi}\left[\frac{1}{2}\ln\left(\frac{4}{|z|}\right) - \frac{1}{4}\right]z^2 + \frac{\kappa t_0 z^2}{2\alpha^2}$$

Plot & rest of the answer is in the mathematica notebook.