1 (15 points)

1(a)

We perform a mean-field decoupling as shown in class of the interaction Hamiltonian,

$$-V_1 \sum_{\mathbf{r},a=\hat{\mathbf{x}},\hat{\mathbf{y}}} c^\dagger_{\mathbf{r}} c_{\mathbf{r}} c^\dagger_{\mathbf{r}+\mathbf{a}} c_{\mathbf{r}+\mathbf{a}} \longrightarrow V_1 \sum_{\mathbf{r},a} \langle c^\dagger_{\mathbf{r}} c^\dagger_{\mathbf{r}+\mathbf{a}} \rangle c_{\mathbf{r}} c_{\mathbf{r}+\mathbf{a}} + \langle c_{\mathbf{r}} c_{\mathbf{r}+\mathbf{a}} \rangle c^\dagger_{\mathbf{r}} c^\dagger_{\mathbf{r}+\mathbf{a}} + \text{const.} \tag{1}$$

After Fourier transforming, we get (for ease of notation we set $V = N^2 a = 1$)

$$V_1 \sum_{\mathbf{r},a} \langle c_{\mathbf{r}} c_{\mathbf{r}+\mathbf{a}} \rangle c^\dagger_{\mathbf{r}} c^\dagger_{\mathbf{r}+\mathbf{a}} = \sum_{\mathbf{q},\mathbf{a}} \underbrace{V_1 \sum_{\mathbf{k}'} e^{i\mathbf{k}'\mathbf{a}} \langle c_{\mathbf{k}'+\mathbf{q}} c_{-\mathbf{k}'} \rangle}_{\Delta_a(\mathbf{q})} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{a}} c^\dagger_{\mathbf{k}+\mathbf{q}} c^\dagger_{-\mathbf{k}} \,. \tag{2}$$

Assuming a spatially uniform gap, one has $\Delta_a(\mathbf{q}) = \Delta_a$ and we get

$$\sum_{\mathbf{k}a} \Delta_a e^{-i\mathbf{k}\mathbf{a}} c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} = \sum_{\mathbf{k}a} \Delta_a \left(\cos \mathbf{k}\cdot\mathbf{a} - i \sin \mathbf{k}\cdot\mathbf{a}\right) c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} = -i \sum_{\mathbf{k}a} \Delta_a \sin(\mathbf{k}\cdot\mathbf{a}) c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} \tag{3}$$

Here the cos-term averages to zero after momentum summation, since it is even in $\mathbf{k}$ and $c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}}$ is odd. The factor of $-i$ is an overall phase that can be "gauged away", that is absorbed in the definition of Δ_a, leaving us with the final expression

$$\sum_{\mathbf{k}} \left(\Delta_x \sin k_x + \Delta_y \sin k_y\right) c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} + \text{h.c.} \tag{4}$$

The full Hamiltonian is

$$\mathcal{H} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k}} \Big[\left(\Delta_x \sin k_x + \Delta_y \sin k_y\right) c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} + \text{h.c.}\Big] \tag{5}$$

with $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$.

1(b)

In part (a) we defined

$$\Delta_a = V_1 \sum_{\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{a}) \; \langle c_{\mathbf{k}} c_{-\mathbf{k}} \rangle. \tag{6}$$

Decomposing $\Delta_a = \Delta'_a + i\Delta''_a$ into its real and imaginary parts we can further express the real part in terms of the Nambu-Gorkov Green's function

$$\begin{aligned} \Delta'_a &= = V_1 \sum_{\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{a}) \; \frac{1}{2} \mathrm{Tr}\left[\sigma_x G_0(\mathbf{k}, t=0^-)\right] &(7)\\ &= \frac{V_1}{\beta} \sum_{\omega_n,\mathbf{k}} \sin(\mathbf{k}\cdot\mathbf{a}) \; \frac{1}{2} \mathrm{Tr}\left[\sigma_x G_0(\mathbf{k},\omega_n)\right]. &(8) \end{aligned}$$

Δ''_a satisfies the same equation with $\sigma_x \to \sigma_y$.

Inserting the expression for the Green's function

$$G_0(\mathbf{k},\omega_n) = \frac{1}{\beta}\frac{i\omega_n + \xi_\mathbf{k}\sigma_z + \Delta'_\mathbf{k}\sigma_x + \Delta''_\mathbf{k}\sigma_y}{(i\omega_n)^2 - E_\mathbf{k}^2} \tag{9}$$

where

$$\Delta_\mathbf{k} = \Delta_x \sin k_x + \Delta_y \sin k_y, \quad E_\mathbf{k}^2 = \xi_\mathbf{k}^2 + |\Delta_\mathbf{k}|^2, \tag{10}$$

and performing the Matsubara sum, we obtain

$$\Delta_a = -\frac{V_1}{\beta}\sum_{\omega_n \mathbf{k}} \frac{\sin(\mathbf{k}\cdot\mathbf{a})\ \Delta_\mathbf{k}}{\omega_n^2 + E_\mathbf{k}^2} = V_1 \sum_\mathbf{k} \frac{\sin(\mathbf{k}\cdot\mathbf{a})\ \Delta_\mathbf{k}}{2E_\mathbf{k}} \tanh\left(\beta E_\mathbf{k}/2\right). \tag{11}$$

This is a set of two coupled equations for Δ_x, Δ_y. They can be solved self-consistently by numerical iteration, or analytically in the limits where either T or Δ_a is small.

1(c)

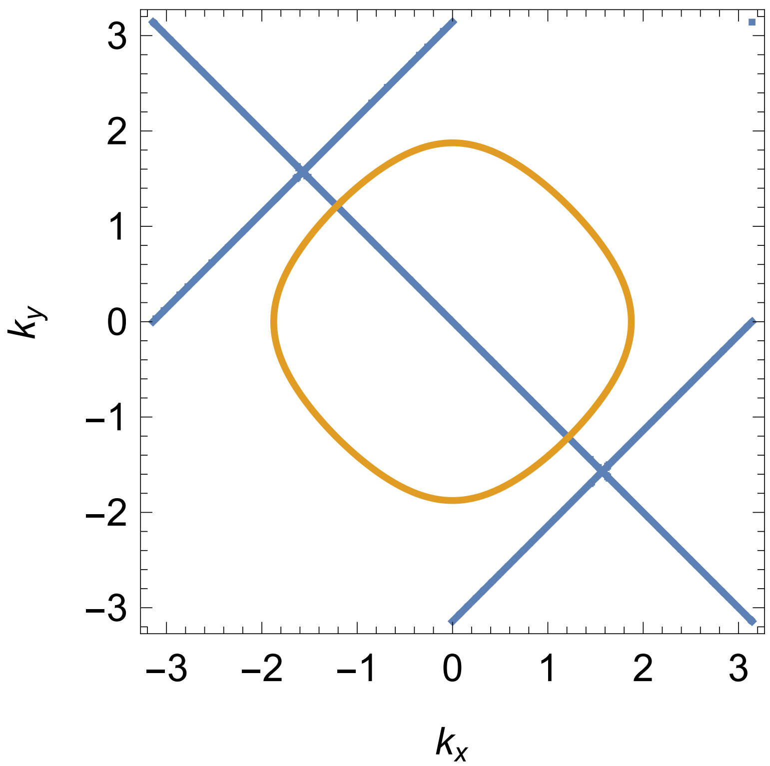
As usual the quasiparticle excitation spectrum is given by the poles of the Green's function

$$E_\mathbf{k} = \sqrt{\xi_\mathbf{k} + |\Delta_\mathbf{k}^2|} \tag{12}$$

where

$$\Delta_\mathbf{k} = \Delta_x \sin k_x + \Delta_y \sin k_y = \Delta\left(\sin k_x + e^{i\varphi}\sin k_y\right) \tag{13}$$

For $\varphi = 0$ we have $|\Delta_\mathbf{k}^2| = \Delta^2\left(\sin k_x + \sin k_y\right)^2 = \Delta^2\left(\sin^2 k_x + \sin^2 k_y + 2\sin k_x \sin k_y\right)$. We find that the gap vanishes at $k_x = -k_y$ and $k_x = k_y + \pi$ which is indicated by the blue lines in the figure below. The excitation energy vanishes when both $\xi_\mathbf{k} = 0$, i.e. at the Fermi surface shown as orange contour, and $\Delta_\mathbf{k} = 0$. Thus, $E_\mathbf{k}$ vanishes at the intersection of the blue and orange lines; the spectrum is generically gapless in this case.



For $\varphi = \pi/2$, we have $|\Delta_{\mathbf{k}}^2| = \Delta^2 \left(\sin^2 k_x + \sin^2 k_y\right)$ which vanishes at four points $\mathbf{k} = (0,0), (0,\pi), (\pi,0), (\pi,\pi)$ in the Brillouine zone. These do not generically intersect with the Fermi surface and the spectrum is fully gapped.

2 (10 points) Edge states of a topological superconductor: Analytical derivation

2(a)

We start with Eq. (4.3.14) of *Doniach and Sondheimer*. Note that for our 2×2 Hamiltonian, the Green's function G_0 and the perturbation U are 2×2 matrices and all multiplications are in fact matrix multiplications.

$$F(\mathbf{p};\mathbf{p}',\varepsilon) = G_0(\mathbf{p},\varepsilon)\delta_{\mathbf{p},\mathbf{p}'} + G_0(\mathbf{p},\varepsilon)\sum_{\mathbf{q}} U(\mathbf{p}-\mathbf{q})F(\mathbf{q};\mathbf{p}',\varepsilon) \tag{14}$$

The use of the F function with two momenta $\mathbf{p},\mathbf{p}'$ is necessary, since the presence of a line impurity $U_0\delta(x)$ breaks translational invariance of in the x-direction. Above equation can be solved by iteration, yielding

$$\begin{aligned}F(\mathbf{p};\mathbf{p}',\varepsilon) = {} & G_0(\mathbf{p},\varepsilon)\delta_{\mathbf{p},\mathbf{p}'} + G_0(\mathbf{p},\varepsilon)U(\mathbf{p}-\mathbf{p}')G_0(\mathbf{p}',\varepsilon) \\ & + G_0(\mathbf{p},\varepsilon)\sum_{\mathbf{q_1}} U(\mathbf{p}-\mathbf{q_1})G_0(\mathbf{q_1},\varepsilon)U(\mathbf{q_1}-\mathbf{p}')G_0(\mathbf{p}',\varepsilon) \\ & + G_0(\mathbf{p},\varepsilon)\sum_{\mathbf{q_1}} U(\mathbf{p}-\mathbf{q_1})G_0(\mathbf{q_1},\varepsilon)\sum_{\mathbf{q_2}} U(\mathbf{q_1}-\mathbf{q_2})G_0(\mathbf{q_2},\varepsilon)U(\mathbf{q_2}-\mathbf{p}')G_0(\mathbf{p}',\varepsilon) + \dots . \end{aligned}\tag{15}$$

Just like in the lecture we can repackage this iteration series inside the T-matrix. Then we obtain the form

$$F(\mathbf{p};\mathbf{p}',\varepsilon) = G_0(\mathbf{p},\varepsilon)\delta_{\mathbf{p},\mathbf{p}'} + G_0(\mathbf{p},\varepsilon)T(\mathbf{p};\mathbf{p}',\varepsilon)G_0(\mathbf{p}',\varepsilon) \tag{16}$$

where

$$\begin{aligned}T(\mathbf{p};\mathbf{p}',\varepsilon) = {} & U(\mathbf{p}-\mathbf{p}') + \sum_{\mathbf{q_1}} U(\mathbf{p}-\mathbf{q_1})G_0(\mathbf{q_1},\varepsilon)U(\mathbf{q_1}-\mathbf{p}') \\ & + \sum_{\mathbf{q_1}} U(\mathbf{p}-\mathbf{q_1})G_0(\mathbf{q_1},\varepsilon)\sum_{\mathbf{q_2}} U(\mathbf{q_1}-\mathbf{q_2})G_0(\mathbf{q_2},\varepsilon)U(\mathbf{q_2}-\mathbf{p}') + \dots . \end{aligned}\tag{17}$$

Above expression involves a series of convolutions. These simplify significantly, once we insert the actual form of the perturbation U which is given by

$$U(\mathbf{r}) = U_0\delta(x) = u_0\sigma_z\delta(x)\,, \tag{18}$$

where σ_z is the Pauli-z-matrix. In Fourier space, this becomes

$$U(\mathbf{q}) = \int dxdy e^{iq_x x + iq_y y} U\delta(x) = U_0\delta_{q_y,0}\,. \tag{19}$$

The $\delta_{q_y,0}$ function is reminiscent of the fact that our line impurity only breaks translational invariance along the x-direction. Along y, translational invariance is still presence. Moreover, the perturbation does not have any q_x-dependence due to its $\delta(x)$-localization in real space.

Inserting this expression into the T-matrix Eq. (**??**) yields

$$
\begin{aligned}
T(\mathbf{p};\mathbf{p}',\varepsilon) &= U_0\delta_{p_y,p'_y} + \sum_{q_{1x}} U_0 G_0(q_{1x}p_y,\varepsilon)U_0\delta_{p_y,p'_y} + \sum_{q_{1x}} U_0 G_0(q_{1x}p_y,\varepsilon)\sum_{q_{2x}} U_0 G_0(q_{2x}p_y,\varepsilon)U_0\delta_{p_y,p'_y} + \ldots \\
&= \left(\mathbb{1} + \sum_{q_x} U_0 G_0(q_x p_y,\varepsilon) + \left(\sum_{q_x} U_0 G_0(q_x p_y,\varepsilon)\right)^2 + \ldots\right) U_0\delta_{p_y,p'_y} \\
&= \left[\mathbb{1} - U_0\sum_{q_x} G_0(q_x p_y,\varepsilon)\right]^{-1} U_0\delta_{p_y,p'_y}\,.
\end{aligned}
\tag{20}
$$

We are now interested in the Green's function $G(x,p_y,\varepsilon) = F(xp_y;xp_y,\varepsilon)$ at position x and momentum k_y. Inserting Eq. (**??**) into Eq. (**??**), we arrive at the final result.

$$
\begin{aligned}
G(x,p_y,\varepsilon) = F(xp_y;xp_y,\varepsilon) &= \sum_{p_x p'_x} e^{ip_x x}e^{-ip'_x x}F(p_x p_y;p'_x p_y,\varepsilon) \\
&= \sum_{p_x} G_0(p_x p_y,\varepsilon) + \left[\sum_{p_x} e^{ip_x x}G_0(p_x p_y,\varepsilon)\right]\left[\mathbb{1} - U_0\sum_{q_x} G_0(q_x p_y,\varepsilon)\right]^{-1} U_0 \left[\sum_{p'_x} e^{-ip'_x x}G_0(p'_x p_y,\varepsilon)\right]
\end{aligned}
\tag{21}
$$

2(a) [10 bonus points]

Expression (**??**) is numerically evaluated in the solution python file. We are interested in the local Green's function at the boundary. The position of the boundary is determined by the line impurity at $x = 0$. Thus, we need to evaluate $G(xk_y,\varepsilon)$ at $x = 1$ or $x = -1$, i.e. left or right of the boundary.

Note that in the limit $u_0 \to \infty$, we have

$$
\left[\mathbb{1} - U_0\sum_{q_x} G_0(q_x p_y,\varepsilon)\right]^{-1} U_0 = -\left[\sum_{q_x} G_0(q_x p_y,\varepsilon)\right]^{-1}\,. \tag{22}
$$

The different terms in Eq. (**??**) are denoted as follows in the python code:

$$
\underbrace{G(x,p_y,\varepsilon)}_{\text{Gsurface}} = \underbrace{\sum_{p_x} G_0(p_x p_y,\varepsilon)}_{\text{Gbulk}} + \underbrace{\left[\sum_{p_x} e^{ip_x x}G_0(p_x p_y,\varepsilon)\right]}_{\text{G0x}}\underbrace{\left[-U_0\sum_{q_x} G_0(q_x p_y,\varepsilon)\right]^{-1}}_{\text{T}}\underbrace{\left[\sum_{p'_x} e^{-ip'_x x}G_0(p'_x p_y,\varepsilon)\right]}_{\text{G0x}_-} \tag{23}
$$

You can run your code or the solution and change the model parameters as well as the variable x.