Problem 3

(a) We start from the Hubbard Hamiltonian

$$H = -\sum t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

The Fourier-transformed Hamiltonian reads (see lecture notes on many-particle theory)

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow}.$$

With the BCS mean-field approximation we get

$$\begin{aligned} H \cong \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \Big(&\langle c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} \rangle c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} \langle c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \rangle \\ &- \langle c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} \rangle \langle c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \rangle \Big). \end{aligned}$$

The term $\langle c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} \rangle \langle c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \rangle$ gives a constant, which we neglect. Furthermore, we use $\langle c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow} \rangle = \delta_{-\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$, which gives

$$\begin{aligned} H_{\text{BCS}} &= \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{U}{\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'} \Big(\langle c^\dagger_{-\mathbf{k}'\uparrow} c^\dagger_{\mathbf{k}'\downarrow} \rangle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^\dagger_{-\mathbf{k}'\uparrow} c^\dagger_{\mathbf{k}'\downarrow} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \Big) \\ &= \sum_{\mathbf{k}} \Big(\xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} - \Delta^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - \Delta c^\dagger_{-\mathbf{k}'\uparrow} c^\dagger_{\mathbf{k}'\downarrow} \Big). \end{aligned}$$

(b) Inserting the Bogoliubov transformation into the BCS Hamiltonian, we obtain

$$\begin{aligned} H_{\text{BCS}} = \sum_{\mathbf{k}} \Big[&\xi_{\mathbf{k}} (u^*_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}\uparrow} + v^*_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow})(u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow}) \\ &+ \xi_{\mathbf{k}} (-v^*_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + u^*_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow})(-v_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}) \\ &- \Delta^* (-v_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow})(u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow}) \\ &- \Delta (u^*_{\mathbf{k}} \gamma^\dagger_{\mathbf{k}\uparrow} + v^*_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow})(-v^*_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + u^*_{\mathbf{k}} \gamma^\dagger_{-\mathbf{k}\downarrow}) \\ = &\gamma^\dagger_{\mathbf{k}\uparrow} \gamma^\dagger_{-\mathbf{k}\downarrow} (2\xi_{\mathbf{k}} u^*_k v_{\mathbf{k}} + \Delta^* v^2_{\mathbf{k}} - \Delta u^{*2}_{\mathbf{k}}) \\ &+ \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} (-2\xi_{\mathbf{k}} u_{\mathbf{k}} v^*_k + \Delta v^{*2}_{\mathbf{k}} - \Delta^* u^2_{\mathbf{k}}) \\ &+ \gamma^\dagger_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} (\xi_{\mathbf{k}} (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) + \Delta^* v_{\mathbf{k}} u_{\mathbf{k}} + \Delta v^*_{\mathbf{k}} u^*_{\mathbf{k}}) \\ &+ \gamma^\dagger_{\mathbf{k}\downarrow} \gamma_{\mathbf{k}\downarrow} (\xi_{\mathbf{k}} (|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) + \Delta^* v_{\mathbf{k}} u_{\mathbf{k}} + \Delta v^*_{\mathbf{k}} u^*_{\mathbf{k}}) \Big]. \end{aligned}$$

(c) We know that

$$\{c^\dagger_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}.$$

For the γ operators, we have

$$\begin{aligned} \gamma_{\mathbf{k}\uparrow} &= u^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}, \\ \gamma^\dagger_{-\mathbf{k}\downarrow} &= v^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} + u_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow}. \end{aligned}$$

Then,

$$\Big\{ \gamma^\dagger_{\mathbf{k}\uparrow}, \gamma_{\mathbf{k}\uparrow} \Big\} = \Big\{ u_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} - v^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow}, u^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow} \Big\} = |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2.$$

Thus if $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ holds the fermionic anticommutation relation for the γ follows.

Note that the equation is satisfied for

$$|u_{\mathbf{k}}| = \cos\alpha = \cos\frac{\theta}{2} \quad \text{and} \quad |v_{\mathbf{k}}| = \sin\alpha = \sin\frac{\theta}{2},$$

where the notation with half angles will prove useful later.

(d) H_{BCS} is diagonal if

$$2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}^* + \Delta v_{\mathbf{k}}^{*2} - \Delta^* u_{\mathbf{k}}^2 = 0. \tag{1}$$

We write the complex gap amplitude as $\Delta = |\Delta| e^{i\phi}$. The solutions for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ then take the form

$$u_{\mathbf{k}} = e^{i\phi/2}\cos\frac{\theta}{2} \quad \text{and} \quad v_{\mathbf{k}} = e^{i\phi/2}\sin\frac{\theta}{2}.$$

Equation (1) then becomes

$$\xi_{\mathbf{k}}\sin\theta - |\Delta|\cos\theta = 0.$$

The solutions read

$$\cos\theta = \frac{\xi_{\mathbf{k}}}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}} \quad \text{and} \quad \sin\theta = \frac{|\Delta|}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}}$$

as well as

$$\cos\theta = -\frac{\xi_{\mathbf{k}}}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}} \quad \text{and} \quad \sin\theta = -\frac{|\Delta|}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}}.$$

These two solutions only differ in an overall sign of all γ operators, which is irrelevant. We take the first solution, for which we obtain

$$|u_{\mathbf{k}}|^2 = \cos^2\frac{\theta}{2} = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}}\right)$$

and

$$|v_{\mathbf{k}}|^2 = \sin^2\frac{\theta}{2} = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{|\Delta|^2 + \xi_{\mathbf{k}}^2}}\right).$$

(e) Insertion into the BCS Hamiltonian gives

$$\begin{aligned} H_{\mathrm{BCS}} &= \sum_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma} \left[\xi_{\mathbf{k}}(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2) + \Delta^* v_{\mathbf{k}} u_{\mathbf{k}} + \Delta v_{\mathbf{k}}^* u_{\mathbf{k}}^*\right] \\ &= \sum_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma} (\xi_{\mathbf{k}}\cos\theta + |\Delta|\sin\theta) \equiv \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \gamma_{\mathbf{k}\sigma}^\dagger \gamma_{\mathbf{k}\sigma} \end{aligned}$$

so that the dispersion is $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$