

TFY4210/FY8302

Solutions to the exam

May 2023

1^a

Let us first rewrite the Hamiltonian in terms of the number operators $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$:

$$\mathcal{H} = -\mu \sum_{i\sigma} n_{i\sigma} - h \sum_i (n_{i\uparrow} - n_{i\downarrow}) - t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma}.$$

Shortcut: The total number of electrons with a given spin σ is equal in every basis:

$$N_\sigma = \sum_i n_{i\sigma} = \sum_k n_{k\sigma}$$

This can be used to rewrite the number operator terms trivially:

$$\mathcal{H}L = -\mu \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} - \hbar \sum_{\mathbf{k}} (n_{\mathbf{k}\uparrow} - n_{\mathbf{k}\downarrow}) \\ - t \sum_{\langle ij \rangle \sigma} C_{i\sigma}^{\dagger} C_{j\sigma}.$$

If you didn't think of this shortcut, the Fourier transformation of $\sum_i C_{i\sigma}^{\dagger} C_{i\sigma}$ is easily done using the equation $\frac{1}{N} \sum_i e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_i} = \delta_{\mathbf{k}, \mathbf{k}'}$ provided in the appendix.

Next, let us consider hopping terms.

This is most easily done using the inverse Fourier transformation:

$$C_{i\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} C_{\mathbf{k}\sigma}^{\dagger} e^{i\mathbf{k} \cdot \mathbf{r}_i},$$

$$C_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} C_{\mathbf{k}'\sigma} e^{-i\mathbf{k}' \cdot \mathbf{r}_j}.$$

Thus we get:

$$\begin{aligned} \sum_{\langle ij \rangle} C_{i\sigma}^{\dagger} C_{j\sigma} &= \sum_{\mathbf{k}\mathbf{k}'} C_{\mathbf{k}\sigma}^{\dagger} C_{\mathbf{k}'\sigma} \\ &\times \frac{1}{N} \sum_{\langle ij \rangle} e^{i(\mathbf{k} \cdot \mathbf{r}_i - \mathbf{k}' \cdot \mathbf{r}_j)}. \end{aligned}$$

Like in class, we now let:

$$\sum_{\langle ij \rangle} = \sum_i \sum_{\delta},$$

where $\delta \equiv \mathbf{r}_j - \mathbf{r}_i$ is a nearest-neighbor vector.

We can then write:

$$\begin{aligned} & \mathbf{k} \cdot \mathbf{r}_i - \mathbf{k}' \cdot \mathbf{r}_j \\ &= \mathbf{k} \cdot \mathbf{r}_i - \mathbf{k}' \cdot (\mathbf{r}_i + \boldsymbol{\delta}) \\ &= (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_i - \mathbf{k}' \cdot \boldsymbol{\delta} \end{aligned}$$

As a consequence:

$$\begin{aligned} & \frac{1}{N} \sum_{\langle i,j \rangle} e^{i(\mathbf{k} \cdot \mathbf{r}_i - \mathbf{k}' \cdot \mathbf{r}_j)} \\ &= \underbrace{\frac{1}{N} \sum_i e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_i}}_{\delta_{\mathbf{k}\mathbf{k}'}} \underbrace{\sum_{\boldsymbol{\delta}} e^{-i\mathbf{k}' \cdot \boldsymbol{\delta}}}_{\gamma_{\mathbf{k}'}} \end{aligned}$$

To evaluate $\gamma_{\mathbf{k}'}$, use that for a square lattice with $a = 1$:

$$\begin{aligned} \boldsymbol{\delta} &\in \{+\mathbf{e}_x, -\mathbf{e}_x, +\mathbf{e}_y, -\mathbf{e}_y\} \\ \mathbf{k}' &= k'_x \mathbf{e}_x + k'_y \mathbf{e}_y \end{aligned}$$

Thus, we must have $\gamma_{k'} = 2(\cos k_x' + \cos k_y')$.

Putting together these results:

$$-t \sum_{\langle ij \rangle \sigma} C_{i\sigma}^\dagger C_{j\sigma} = -2t \sum_{k\sigma} C_{k\sigma}^\dagger C_{k\sigma} \times (\cos k_x + \cos k_y).$$

For the Hamiltonian:

$$\mathcal{H} = -\mu \sum_{k\sigma} n_{k\sigma} - h \sum_k (n_{k\uparrow} - n_{k\downarrow}) - 2t \sum_{k\sigma} n_{k\sigma} (\cos k_x + \cos k_y).$$

This can be written $\mathcal{H} = \sum_{k\sigma} E_{k\sigma} n_{k\sigma}$ with:

$$E_{k\sigma} \equiv -\mu - 2h\sigma - 2t(\cos k_x + \cos k_y).$$

Here, I let $\sigma = +1/2$ and $\sigma = -1/2$ be the numerical values of $\sigma \in \{\uparrow, \downarrow\}$.

(Using $\sigma = \pm 1$ as numerical values also accepted.)

1^b

To order $\mathcal{O}(k^2)$ we have:

$$\cos k_x \approx 1 - \frac{1}{2}k_x^2$$

$$\cos k_y \approx 1 - \frac{1}{2}k_y^2$$

$$\therefore \cos k_x + \cos k_y \approx 2 - \frac{1}{2}k^2,$$

where $k^2 = k_x^2 + k_y^2$. Thus we find:

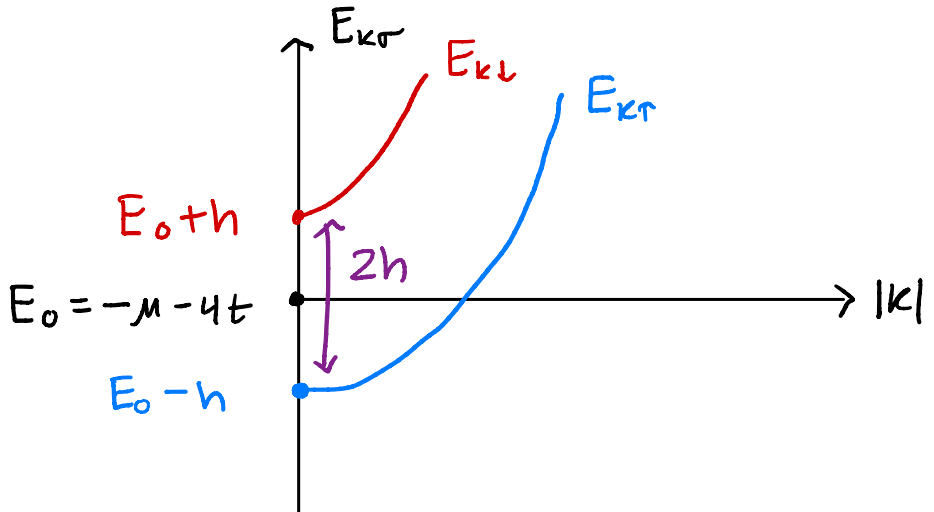
$$E_{k\sigma} \approx -\mu - 4t - 2\hbar\sigma + tk^2.$$

This takes the form

$$E_{k\sigma} = E_{0\sigma} + \frac{k^2}{2m^*},$$

where $m^* = 2/t$ is the effective electron mass. (Sanity check: Higher hopping $t \Rightarrow$ more mobile electrons $\Rightarrow$ lower effective mass. This fits.)

The two curves look like:



The exchange splitting h is the energy difference between spin-up and spin-down electron bands. It is a signature of magnetism: Electrons can lower their energies by flipping their spins from $\downarrow$ to $\uparrow$.

1^c

Particles with energy eigenvalues E_{kr} follow the Fermi-Dirac distribution:

$$\langle n_{kr} \rangle = \frac{1}{\exp(E_{kr}/T) + 1}$$

Here, T is the system temperature.

1^d

We basically have to rewrite the Hamiltonian in the form:

$$\mathcal{H} = \sum_{ij\sigma\sigma'} C_{i\sigma}^\dagger H_{i\sigma,j\sigma'} C_{j\sigma'}$$

in order to determine $H_{i\sigma,j\sigma'}$.

The hint in the problem is that we can write (as in homework problems):

$$i = x_i + L y_i,$$

where $x_i, y_i \in \{0, 1, \dots, L-1\}$. This maps lattice coordinates (x_i, y_i) to indices i .

You can verify that this matrix reproduces the original Hamiltonian:

$$\begin{aligned}
 H_{i\sigma, j\sigma'} &= H_{x_i + 2y_i, \sigma, x_j + 2y_j, \sigma'} \\
 &= -J \delta_{\sigma\sigma'} \delta_{x_i x_j} \delta_{y_i y_j} \\
 &\quad - t \delta_{\sigma\sigma'} \left[\delta_{x_i x_j} (\delta_{y_i, y_j+1} + \delta_{y_i, y_j-1}) \right. \\
 &\quad \quad \left. + \delta_{y_i y_j} (\delta_{x_i, x_j+1} + \delta_{x_i, x_j-1}) \right] \\
 &\quad - \hbar \delta_{x_i x_j} \delta_{y_i y_j} (\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}).
 \end{aligned}$$

The logic is that $\delta_{ij} = \delta_{x_i x_j} \delta_{y_i y_j}$ factors represent on-site terms, while e.g. $\delta_{x_i x_j} \delta_{y_i, y_j+1}$ would be a nearest-neighbor interaction along the y direction.

1^e

- In 1^d , we expressed the Hamiltonian $\mathcal{H}$ in terms of a matrix H . Since $\mathcal{H}$ and H have the same eigenvalues, we can numerically diagonalize H to obtain the eigenvalues $\{E_n\}$.

- Numerically, we cannot evaluate $D(E)$ for every energy E , but only a discrete subset $\{E_m\}$. To see the δ spikes, they need a finite width in that case.

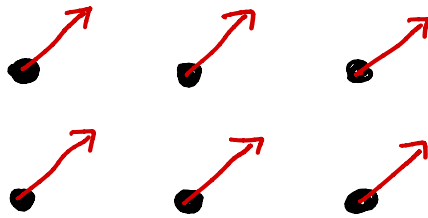
Based on the appendix, we can use:

$$\delta(x) \approx \frac{1}{\pi} \frac{\eta}{\eta^2 + x^2},$$

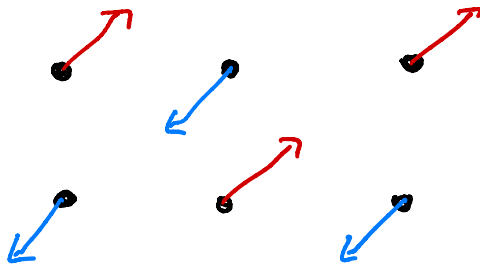
where we choose a finite value for η instead of letting $\eta \rightarrow 0$.

2^a

When $J > 0$, energy is minimized when S_i and S_j are parallel. This creates ferromagnetism:



When $J < 0$, energy is minimized for antiparallel configurations. This causes antiferromagnetism (Néel state):



Quantum-mechanically, the antiferromagnetic ground state changes due to quantum fluctuations even at zero temperature.

2^b The $J > 0$ case is the ferromagnetic case. Let us take the z axis to be the quantization axis, so the classical ground state is $S_{iz} = S$.

From the appendix, we get:

$$S_{i+} = \sqrt{2S - a_i^\dagger a_i} a_i \approx \sqrt{2S} a_i$$

$$S_{i-} = a_i^\dagger \sqrt{2S - a_i^\dagger a_i} \approx \sqrt{2S} a_i^\dagger$$

$$S_{iz} = S - a_i^\dagger a_i$$

The appendix also provides:

$$S_x \pm i S_y = S_\pm$$

which implies that:

$$S_x = \frac{1}{2}(S_+ + S_-)$$

$$S_y = \frac{1}{2i}(S_+ - S_-)$$

Let us use these to write dot products:

$$\begin{aligned}
 S_i \cdot S_j &= S_{ix} S_{jx} + S_{iy} S_{jy} + S_{iz} S_{jz} \\
 &= \frac{1}{4} (\cancel{S_{i+} S_{j+}} + S_{i+} S_{j-} + S_{i-} S_{j+} + \cancel{S_{i-} S_{j-}}) \\
 &\quad - \frac{1}{4} (\cancel{S_{i+} S_{j+}} - S_{i+} S_{j-} - S_{i-} S_{j+} + \cancel{S_{i-} S_{j-}}) \\
 &\quad + S_{iz} S_{jz} \\
 &= \frac{1}{2} (S_{i+} S_{j-} + S_{i-} S_{j+}) + S_{iz} S_{jz} \\
 &\approx S(a_i^\dagger a_j^\dagger + a_i^\dagger a_j) + S^2 - S(a_i^\dagger a_i + a_j^\dagger a_j),
 \end{aligned}$$

where we have neglected higher-order terms in a and $a^\dagger$. We now use:

$$[a_i, a_j^\dagger] = a_i a_j^\dagger - a_j^\dagger a_i = \delta_{ij} = 0$$

(we only sum over $i \neq j$.)

Thus we have:

$$\mathcal{H} = -J \sum'_{\langle ij \rangle} [S^2 + S(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j)].$$

Simplifications:

- $\sum_{\langle ij \rangle} S^2 = 4N S^2$ for a square lattice, where N is the number of lattice sites, 4 is the number of nearest neighbors per site.
- $a_i^\dagger a_i$ and $a_j^\dagger a_j$ contribute equally, since we sum over all sites.
- $a_i^\dagger a_j$ and $a_j^\dagger a_i$ similarly give the same contribution.
- $\sum_{\langle ij \rangle} a_i^\dagger a_i = 4 \sum_i a_i^\dagger a_i$ since the index j is not in the summand.

Thus, we arrive at:

$$\mathcal{H} = -4NJS^2 + 8JS \sum_i a_i^\dagger a_i - 2JS \sum_{\langle ij \rangle} a_i^\dagger a_j.$$

2c Shortcut: There is no fundamental difference between Fourier-transforming a fermionic and bosonic operator, especially when both are defined on the same lattice (2D square).

In problem 1, we established:

$$\sum_i C_{i\sigma}^\dagger C_{i\sigma} = \sum_{\mathbf{k}} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma}$$

$$\sum_{\langle ij \rangle} C_{i\sigma}^\dagger C_{j\sigma} = \sum_{\mathbf{k}} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} \times 2(\cos k_x + \cos k_y).$$

Replacing $C_{i\sigma} \rightarrow a_i$ and $C_{\mathbf{k}\sigma}^\dagger \rightarrow a_{\mathbf{k}}^\dagger$, the mathematics is the same.

(If you didn't notice, it's of course also fine to re-derive these transforms.)

This leads us to the result:

$$\mathcal{H} = -4N\hbar S^2 + 8\hbar S \sum_i a_i^\dagger a_i \\ - 2\hbar S \sum_{\langle ij \rangle} a_i^\dagger a_j$$

$$= -4N\hbar S^2$$

$$+ 8\hbar S \sum_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$$

$$- 4\hbar S \sum_{\mathbf{q}} (\cos q_x + \cos q_y) a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$$

$$\equiv E_0 + \sum_{\mathbf{q}} E_{\mathbf{q}} n_{\mathbf{q}},$$

where we find:

$$E_0 \equiv -4N\hbar S^2$$

$$E_{\mathbf{q}} \equiv 4\hbar S (2 - \cos q_x - \cos q_y).$$

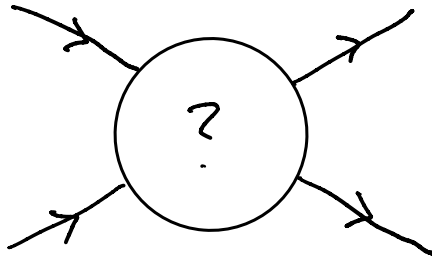
2d Magnons described by $a_q, a_q^\dagger$ are bosons. These follow Bose-Einstein Statistics. Thus, we can write:

$$\langle n_q \rangle = \frac{1}{\exp(E_q/T) - 1}$$

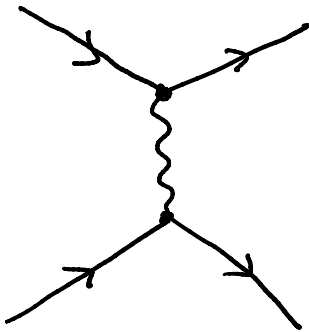
Where T is the system temperature.

3^a

We want to draw all diagrams of this class:

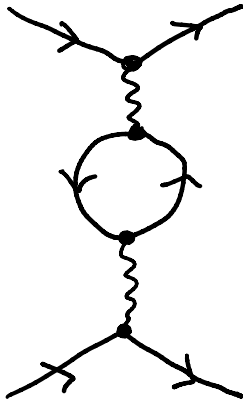


To order $\mathcal{O}(g^2)$ we have:

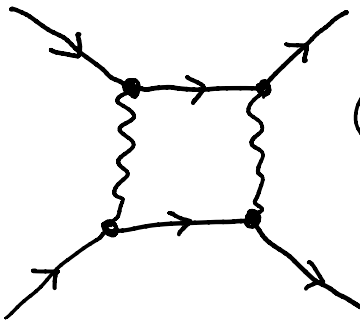


(photon-mediated
electron-electron
interaction)

To order $\mathcal{O}(g^4)$, we also get:



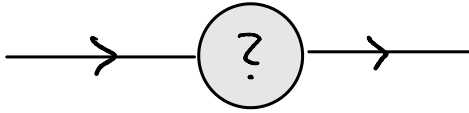
(The same, but with one "bubble" correction)



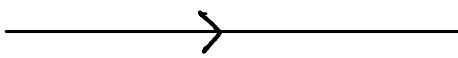
(Electrons exchange two phonons)

3^b

We want all diagrams like this:



To order $\mathcal{O}(1)$ we have:



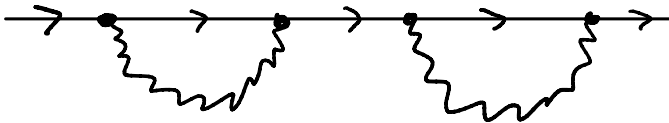
(non-interacting propagator)

To order $\mathcal{O}(g^2)$ we also get:

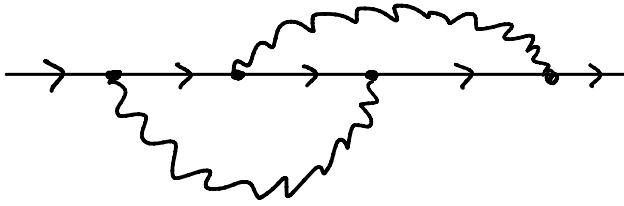


(electron emits then absorbs photon)

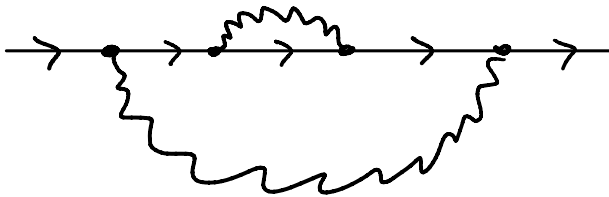
To order $\mathcal{O}(g^4)$ we also get:



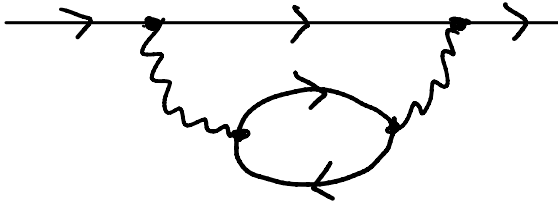
(two emissions and absorptions)



(same, but reordered)



(same, but reordered)



(electron emits a phonon, which fluctuates into an electron-hole pair, and is then absorbed)

3^c

The Dyson equation is:

$$G = G_0 (1 - \Sigma G_0)^{-1}$$

$$\approx G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0$$

$$[\text{to order } \mathcal{O}(\Sigma^2)]$$

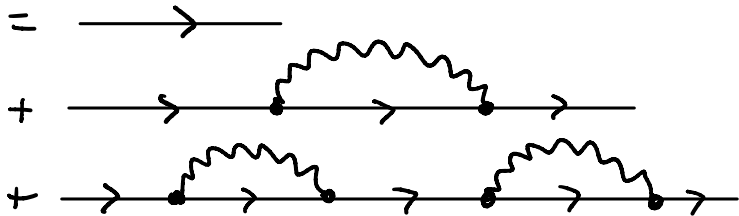
The simplest example of an amputated one-particle irreducible diagram is:



(The $\mathcal{O}(g^2)$ contribution)

Dyson's equation with this Σ is:

$$G = G_0 + G_0 \Sigma_2 G_0 + G_0 \Sigma_2 G_0 \Sigma_2 G_0$$

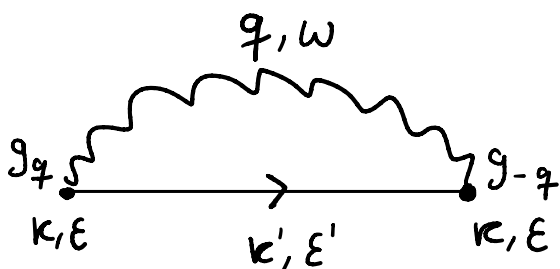


This illustrates that the one-particle reducible diagrams "with legs" are generated by Dyson's equation when Σ contains one-particle irreducible diagrams "without legs". The same pattern repeats at all orders in g and Σ . Thus, it is sufficient to include irreducible diagrams in Σ and let Dyson's equation handle the rest.

3^d Only the one-particle irreducible amputated diagrams contribute. Thus:

$$\begin{aligned}
 \Sigma &= \text{[Diagram 1]} && \mathcal{O}(g^2) \\
 &+ \text{[Diagram 2]} && \mathcal{O}(g^4) \\
 &+ \text{[Diagram 3]} && \mathcal{O}(g^4) \\
 &+ \text{[Diagram 4]} && \mathcal{O}(g^4) \\
 &+ \dots
 \end{aligned}$$

Let us now apply the Feynman rules in the appendix to the first one.



- Propagators: $D_0(q, \omega) G_0(k', \epsilon')$

- Vertices: $g_q g_{-q} = |g_q|^2$

- Energy and momentum conservation:

$$k' = k - q, \quad \epsilon' = \epsilon - \omega$$

- Overall prefactor: $i^1 (-2)^0 = i$

- Integrate remaining energy ω , momentum q .
Include a factor $1/2\pi$.

Thus, we get:

$$\frac{i}{2\pi} \int d\omega \sum_q |g_q|^2 D_0(q, \omega) G_0(k - q, \epsilon - \omega)$$

To order $\mathcal{O}(g^2)$, we can then

write $\Sigma(k, \varepsilon) = \sum_q |g_q|^2 I(\varepsilon, k, q)$ where:

$$I = \frac{i}{2\pi} \int_{-\infty}^{+\infty} d\omega D_0(q, \omega) G_0(k-q, \varepsilon-\omega)$$

The appendix specifies that we can assume the integrand goes to zero at complex infinity. Thus, we can close the contour in the upper complex half-plane using the contour $\Gamma(r)$ where $r \rightarrow \infty$, as defined in the appendix.

Thus, we now have:

$$I = \frac{i}{2\pi} \oint_{\Gamma(\infty)} d\omega D_0(q, \omega) G_0(k-q, \varepsilon-\omega)$$

Let's now use the definitions of D_0 and G_0 from the appendix:

$$\begin{aligned}
 & D_0(q, \omega) G_0(k-q, \varepsilon - \omega) \\
 &= \left\{ \frac{1}{\omega - \omega_q + i0^+} - \frac{1}{\omega + \omega_q - i0^+} \right\} \\
 &\times \left\{ \frac{\Theta(\varepsilon_{k-q} - \varepsilon_F)}{\varepsilon - \omega - \varepsilon_{k-q} + i0^+} + \frac{\Theta(\varepsilon_F - \varepsilon_{k-q})}{\varepsilon - \omega - \varepsilon_{k-q} - i0^+} \right\}.
 \end{aligned}$$

According to the residue integral identities in the appendix, only products of fractions of the form $\frac{1}{\omega - \alpha + i0^+} \frac{1}{\omega - \beta - i0^+}$ give finite contributions.

There are two such terms:

$$(i) \quad \frac{1}{\omega - \omega_q + i0^+} \cdot \frac{\Theta(\varepsilon_{k-q} - \varepsilon_F)}{\varepsilon - \omega - \varepsilon_{k-q} + i0^+}$$

$$\begin{aligned}
 &= -\Theta(\varepsilon_{k-q} - \varepsilon_F) \cdot \frac{1}{\omega - \omega_q + i0^+} \cdot \frac{1}{\omega - (\varepsilon - \varepsilon_{k-q}) - i0^+} \\
 &\quad \equiv \alpha_1 \qquad \qquad \qquad \equiv \beta_1
 \end{aligned}$$

$$\begin{aligned}
 (ii) &= -\frac{1}{\omega + \omega_q - i0^+} \cdot \frac{\theta(\epsilon_F - \epsilon_{k-q})}{\epsilon - \omega - \epsilon_{k-q} - i0^+} \\
 &= +\theta(\epsilon_F - \epsilon_{k-q}) \cdot \frac{1}{\omega - \underbrace{(-\omega_q)}_{\equiv \alpha_2} - i0^+} \cdot \frac{1}{\omega - \underbrace{(\epsilon - \epsilon_{k-q})}_{\equiv \beta_2} + i0^+}
 \end{aligned}$$

Using the appendix integral identities,

the integrals of the above are:

$$-\theta(\epsilon_{k-q} - \epsilon_F) \cdot \frac{2\pi i}{\beta_1 - \alpha_1} = -\frac{2\pi i \theta(\epsilon_{k-q} - \epsilon_F)}{\epsilon - \epsilon_{k-q} - \omega_q}$$

$$+ \theta(\epsilon_F - \epsilon_{k-q}) \cdot \frac{2\pi i}{\alpha_2 - \beta_2} = +\frac{2\pi i \theta(\epsilon_F - \epsilon_{k-q})}{-\epsilon + \epsilon_{k-q} - \omega_q}$$

The integral had an overall

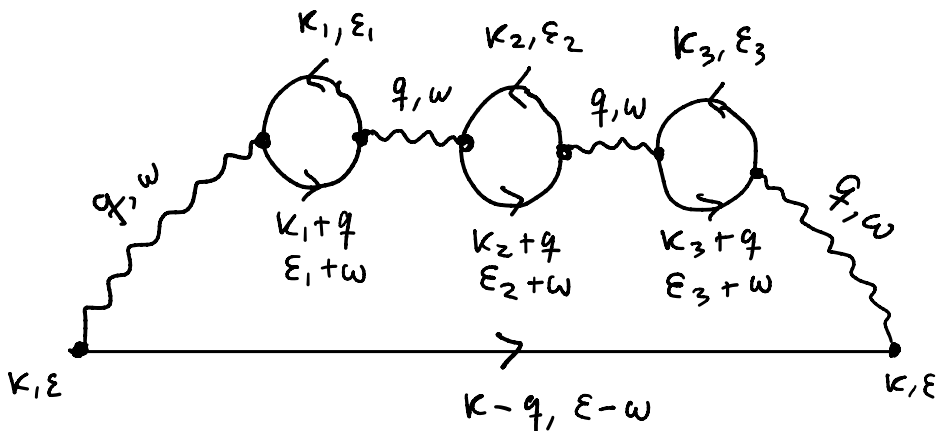
prefactor $\frac{i}{2\pi} = -\frac{1}{2\pi i}$. Thus:

$$I = \frac{\theta(\epsilon_{k-q} - \epsilon_F)}{\epsilon - \epsilon_{k-q} - \omega_q} + \frac{\theta(\epsilon_F - \epsilon_{k-q})}{\epsilon - \epsilon_{k-q} + \omega_q}.$$

This is the solution to the problem.

3e

We again consult the Feynman rules in the appendix. Note that a lot of work can be saved if we choose smart variable names, which already account for momentum and energy conservation. (Note that every phonon propagator has the same momentum and energy due to conservation at vertices.)



The Feynman rules give us:

$$\frac{i^4 (-2)^3}{(2\pi)^4} \int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\varepsilon_1 \int_{-\infty}^{+\infty} d\varepsilon_2 \int_{-\infty}^{+\infty} d\varepsilon_3 \sum_{k_1 k_2 k_3 q} |g_q|^8$$

$$\times D_0(q, \omega) D_0(q, \omega) D_0(q, \omega) D_0(q, \omega)$$

$$\times G_0(k_1, \varepsilon_1) G_0(k_1 + q, \varepsilon_1 + \omega)$$

$$\times G_0(k_2, \varepsilon_2) G_0(k_2 + q, \varepsilon_2 + \omega)$$

$$\times G_0(k_3, \varepsilon_3) G_0(k_3 + q, \varepsilon_3 + \omega)$$

$$\times G_0(k - q, \varepsilon - \omega).$$

Note that there are many correct ways to write the answer. If you choose different energy and momentum variables, the details may differ.