TFY4210/FY8302
Solutions to the exam
May 2023

1a Let us first rewrite the Hamiltonian in terms of the number operators $n_{i\sigma} \equiv c^{\dagger}_{i\sigma} c_{i\sigma}$:

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

<u>Shortcut</u>: The <u>total</u> 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:

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

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

Next, let us consider hopping terms. This is most easily done using the inverse Fourier transformation:

$$c_{i\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{k} c_{k\sigma}^{\dagger} e^{ik\cdot r_i},$$

$$c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{k'} c_{k'\sigma} e^{-ik'\cdot r_j}.$$

Thus we get:

$$\sum_{\langle ij\rangle} c_{i\sigma}^{\dagger} c_{j\sigma} = \sum_{kk'} c_{k\sigma}^{\dagger} c_{k'\sigma} \times \frac{1}{N} \sum_{\langle ij\rangle} e^{i(k\cdot r_i - k'\cdot r_j)}.$$

Like in class, we now let:

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

where $\delta \equiv r_j - r_i$ is a nearest-neighbor vector.

We can then write:

$$\begin{aligned}
&k \cdot r_i - k' \cdot r_j \\
&= k \cdot r_i - k' \cdot (r_i + \delta) \\
&= (k - k') \cdot r_i - k' \cdot \delta
\end{aligned}$$

As a consequence:

$$\begin{aligned}
&\frac{1}{N} \sum_{\langle ij \rangle} e^{i(k \cdot r_i - k' \cdot r_j)} \\
&= \underbrace{\frac{1}{N} \sum_i e^{i(k-k') \cdot r_i}}_{\delta_{kk'}} \underbrace{\sum_\delta e^{-ik' \cdot \delta}}_{\gamma_{k'}}
\end{aligned}$$

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

$$\delta \in \{+e_x, -e_x, +e_y, -e_y\}$$

$$k' = k_x' e_x + k_y' e_y$$

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:

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

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

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

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

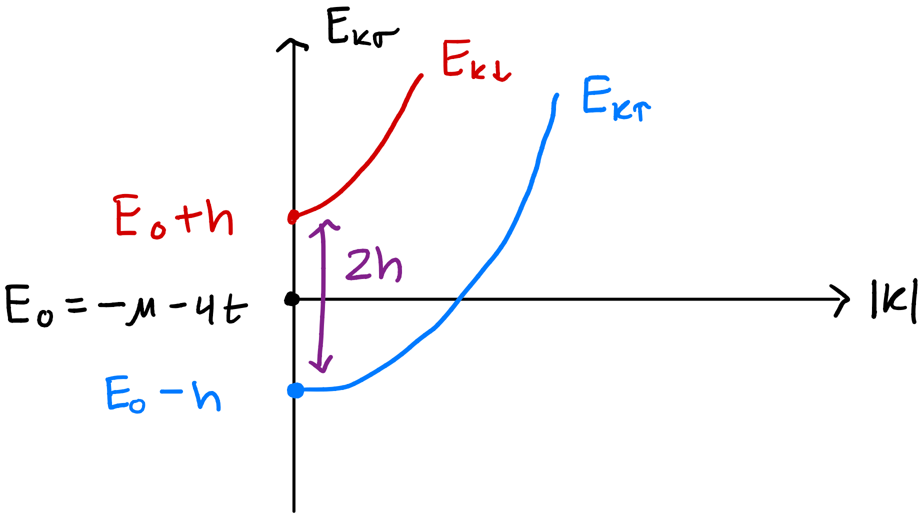
$$E_{k\sigma} \approx -\mu - 4t - 2h\sigma + tk^2.$$

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 $E_{k\sigma}$ follow the Fermi-Dirac distribution:

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

Here, T is the system temperature.

1^d

We basically have to rewrite the Hamiltonian in the form:

$$\mathcal{H} = \sum_{ij\sigma\sigma'} c^{+}_{i\sigma} H_{i\sigma, j\sigma'} c_{j\sigma'}$$

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:

$$H_{i\sigma, j\sigma'} = H_{x_i + Ly_i, \sigma, x_j + Ly_j, \sigma'}$$

$$= -\mu \delta_{\sigma\sigma'} \delta_{x_i x_j} \delta_{y_i y_j}$$

$$- t \delta_{\sigma\sigma'} \Big[\delta_{x_i x_j} (\delta_{y_i, y_j+1} + \delta_{y_i, y_j-1}) + \delta_{y_i y_j} (\delta_{x_i, x_j+1} + \delta_{x_i, x_j-1}) \Big]$$

$$- h \delta_{x_i x_j} \delta_{y_i y_j} (\delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}).$$

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.

1e

- In 1d, 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 $\{E_n\}$.

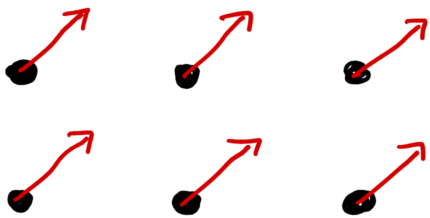
- Numerically, we cannot evaluate $D(E)$ for <u>every</u> energy E, but only a discrete subset $\{E_m\}$. To see the δ spikes, they need a finite width in that case.

  Based on the appendix, we can use:

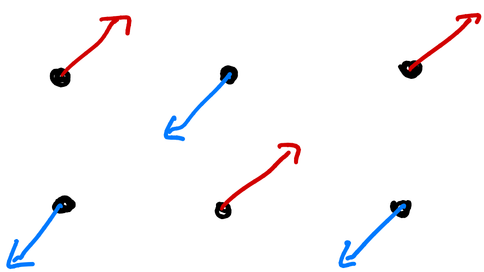
$$\delta(x) \approx \frac{1}{\pi} \frac{\eta}{\eta^2+x^2},$$

  where we choose a <u>finite</u> value for η instead of letting $\eta \to 0$.

2a When $J>0$, energy is minimized when S_i and S_j are parallel. This creates <u>ferromagnetism</u>:



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



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

2b 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:

$$S_i \cdot S_j = S_{ix} S_{jx} + S_{iy} S_{jy} + S_{iz} S_{jz}$$

$$= \frac{1}{4}\left(\cancel{S_{i+} S_{j+}} + S_{i+} S_{j-} + S_{i-} S_{j+} + \cancel{S_{i-} S_{j-}}\right)$$

$$- \frac{1}{4}\left(\cancel{S_{i+} S_{j+}} - S_{i+} S_{j-} - S_{i-} S_{j+} + \cancel{S_{i-} S_{j-}}\right)$$

$$+ S_{iz} S_{jz}$$

$$= \frac{1}{2}\left(S_{i+} S_{j-} + S_{i-} S_{j+}\right) + S_{iz} S_{jz}$$

$$\approx S\left(a_i a_j^\dagger + a_i^\dagger a_j\right) + S^2 - S\left(a_i^\dagger a_i + a_j^\dagger a_j\right),$$

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:

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

Simplifications:

- $\sum_{\langle ij \rangle} S^2 = 4\mathcal{N}S^2$ for a square lattice, where $\mathcal{N}$ 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:

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

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:

$$\sum_i c^\dagger_{i\sigma} c_{i\sigma} = \sum_k c^\dagger_{k\sigma} c_{k\sigma}$$

$$\sum_{\langle ij\rangle} c^\dagger_{i\sigma} c_{j\sigma} = \sum_k c^\dagger_{k\sigma} c_{k\sigma} \times 2(\cos k_x + \cos k_y).$$

Replacing $c_{i\sigma} \to a_i$ and $c^\dagger_{k\sigma} \to a_q$, 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:

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

$$= -4NJS^2 + 8JS \sum_q a_q^\dagger a_q - 4JS \sum_q (\cos q_x + \cos q_y) a_q^\dagger a_q$$

$$\equiv E_0 + \sum_q E_q n_q,$$

where we find:

$$E_0 \equiv -4NJS^2$$

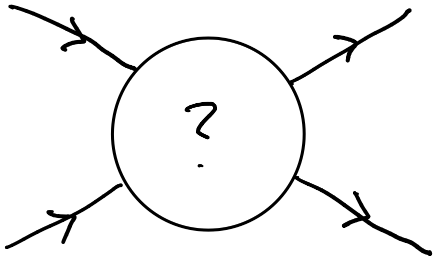
$$E_q \equiv 4JS\,(2 - \cos q_x - \cos q_y).$$

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

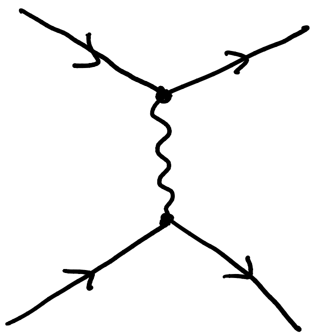
$$\langle n_q \rangle = \frac{1}{\exp(E_q/T) - 1}$$

where T is the system temperature.

3a We want to draw all diagrams of this class:

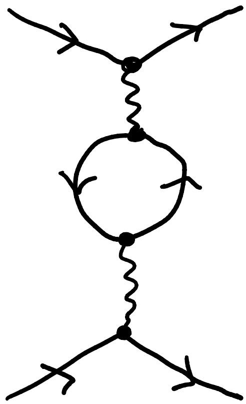


To order $\mathcal{O}(g^2)$ we have:

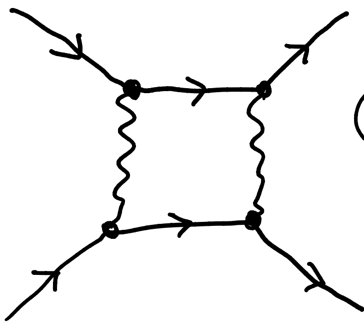


(phonon-mediated electron-electron interaction)

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

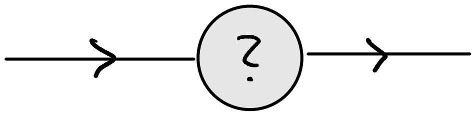


(The same, but with one "bubble" correction)

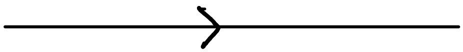


(Electrons exchange two phonons)

3b We want all diagrams like this:

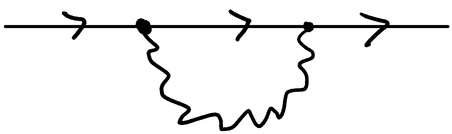


To order $\mathcal{O}(1)$ we have:



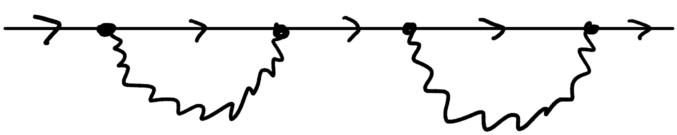
(non-interacting propagator)

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

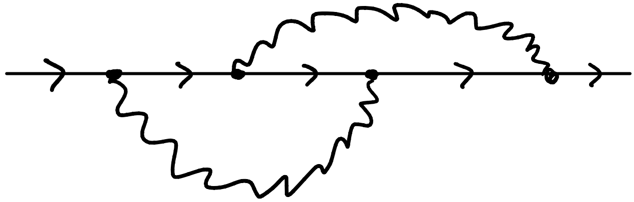


(electron emits then absorbs phonon)

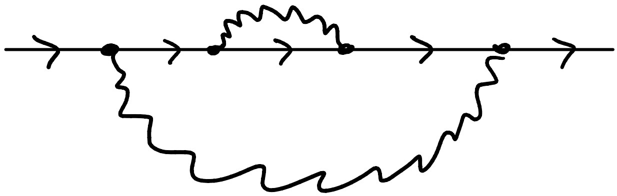
To order $\mathcal{O}(g^4)$ we also get:



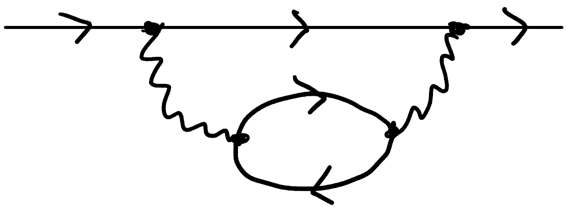
(two emissions and absorptions)



(same, but reordered)



(same, but reordered)



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

3c The Dyson equation is:

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

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

[to order $\Theta(\Sigma^2)$]

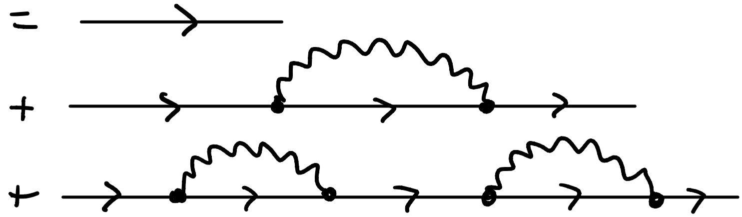
The simplest example of an amputated one-particle irreducible diagram is:

$\Sigma_2 =$ 

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

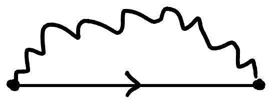
Dyson's equation with this Σ is:

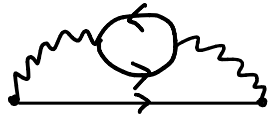
$$G = G_0 + G_0 \Sigma_2 G_0 + G_0 \Sigma_2 G_0 \Sigma_2 G_0$$

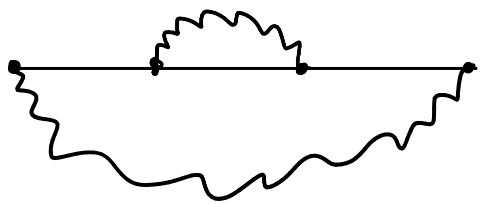


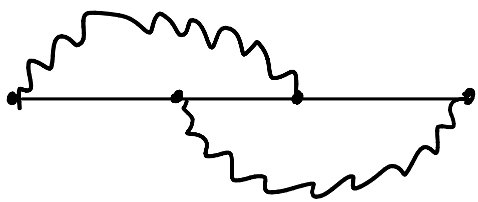
This illustrates that the one-particle <u>reducible</u> diagrams "with legs" are generated by Dyson's equation when Σ contains one-particle <u>irreducible</u> diagrams "without legs". The same pattern repeats at all orders in g and Σ. Thus, it is sufficient to include irreducible diagrams in Σ and let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

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

$\Sigma =$  $\mathcal{O}(g^2)$

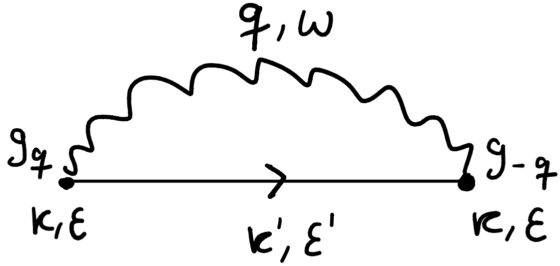
$+$  $\mathcal{O}(g^4)$

$+$  $\mathcal{O}(g^4)$

$+$  $\mathcal{O}(g^4)$

$+ \cdots$

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



- Propagators: $D_0(q,\omega)\, G_0(k', \varepsilon')$
- Vertices: $g_q\, g_{-q} = |g_q|^2$
- Energy and momentum conservation:

$$k' = k - q, \qquad \varepsilon' = \varepsilon - \omega$$

- Overall prefactor: $i^1(-2)^0 = i$
- Integrate remaining energy ω, momentum q. Include a factor $1/2\pi$.

Thus, we get:

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

To order $\Theta(g^2)$, 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 $r \to \infty$, 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:

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

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

There are two such terms:

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

$$=-\theta(\varepsilon_{k-q}-\varepsilon_F)\cdot\frac{1}{\omega-\underbrace{\omega_q}_{\equiv\alpha_1}+i0^+}\cdot\frac{1}{\omega-\underbrace{(\varepsilon-\varepsilon_{k-q})}_{\equiv\beta_1}-i0^+}$$

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

$$=+\theta(\varepsilon_F-\varepsilon_{k-q})\cdot\frac{1}{\omega-\underbrace{(-\omega_q)}_{\equiv\alpha_2}-i0^+}\cdot\frac{1}{\omega-\underbrace{(\varepsilon-\varepsilon_{k-q})}_{\equiv\beta_2}+i0^+}$$

Using the appendix integral identities, the integrals of the above are:

$$-\theta(\varepsilon_{k-q}-\varepsilon_F)\cdot\frac{2\pi i}{\beta_1-\alpha_1}=-\frac{2\pi i\ \theta(\varepsilon_{k-q}-\varepsilon_F)}{\varepsilon-\varepsilon_{k-q}-\omega_q}$$

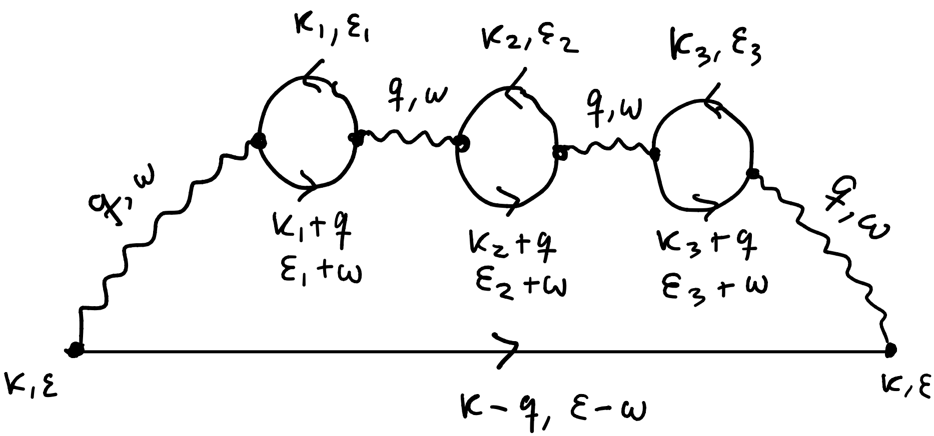
$$+\theta(\varepsilon_F-\varepsilon_{k-q})\cdot\frac{2\pi i}{\alpha_2-\beta_2}=+\frac{2\pi i\ \theta(\varepsilon_F-\varepsilon_{k-q})}{-\varepsilon+\varepsilon_{k-q}-\omega_q}$$

The integral had an overall prefactor $\frac{i}{2\pi}=-\frac{1}{2\pi i}$. Thus:

$$I=\frac{\theta(\varepsilon_{k-q}-\varepsilon_F)}{\varepsilon-\varepsilon_{k-q}-\omega_q}+\frac{\theta(\varepsilon_F-\varepsilon_{k-q})}{\varepsilon-\varepsilon_{k-q}+\omega_q}.$$

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 <u>every</u> 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 choce different energy and momentum variables, the details may differ.