Advanced Condensed Matter Theory — SS10

Exercise 9

<u>9.1. Explicit Solution for the Coupling Factor J_{μ} in the Anisotropic s-d Model</u>

We have seen from the lecture that the two relevant coupling constants in the anisotropic Kondo model, denoted J_{\parallel} and J_{\perp} , obeys the following scaling equations

$$\frac{\mathrm{d}J_{\perp}}{\mathrm{d}\ln D} = -2\rho_0 J_{\parallel} J_{\perp} \tag{1}$$

$$\frac{\mathrm{d}J_{\parallel}}{\mathrm{d}\ln D} = -2\rho_0 J_{\perp}^2 \tag{2}$$

where D is the bandwidth of the conduction electrons, as defined in the lecture, and ρ_0 is a flat band (constant) density of states.

a) Derive the additional condition

$$J_{\parallel}^2 - J_{\perp}^2 = C \tag{3}$$

where the constant C can take on values of C > 0 or C < 0.

b) Substituting (3) into (2), you obtain a decoupled differential equation for J_{\parallel} only, which can be solved via separation of variables. An example of this was done for the *isotropic* s-d model already in the lecture. Solve the resulting differential equation. *Hint:* Differentiate between the cases C > 0 and C < 0. For the case of C < 0 write

C = -|C|.

9.2. Magnon-Magnon Interaction and Self-Energy

In the previous exercise sheet we have worked with the *spin-wave approximation* of the Holstein-Primakoff transformation for the description of spin waves in antiferromagnetism. In this approximation we only have our creation and annihilation operators in bilinear form, i.e., it does not include interactions between magnons. In this exercise we would like to see how magnon-magnon interaction is taken into account by going beyond the spin-wave approximation. We start with the simplest Heisenberg Hamiltonian which includes magnon-magnon interactions:

$$\mathcal{H} = \sum_{\mathbf{q}} 2S \left\{ J(0) - J(\mathbf{q}) \right\} \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}} - \frac{1}{N} \sum_{\mathbf{q}_{1} \mathbf{q}_{2} \mathbf{q}_{3} \mathbf{q}_{4}} \hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}}^{\dagger} \hat{a}_{\mathbf{q}_{3}} \hat{a}_{\mathbf{q}_{4}} \delta_{\mathbf{q}_{1} + \mathbf{q}_{2}, \mathbf{q}_{3} + \mathbf{q}_{4}} \left\{ J(\mathbf{q}_{1} - \mathbf{q}_{3}) - J(\mathbf{q}_{3}) \right\}$$
(4)

where the creation and annihilation operators $[\hat{a}_{\mathbf{q}}, \hat{a}_{\mathbf{q}}^{\dagger}] = \delta_{\mathbf{q},\mathbf{q}'}$ are bosonic operators, and $J(\mathbf{q}) = J \sum_{\mathbf{r}} \exp(i\mathbf{q} \cdot \mathbf{r}) = r J \gamma_{\mathbf{q}}$. In addition J(0) = r J. Here the summation over \mathbf{r} is over nearest neighbours, J is the strength of the nearest neighbour ferromagnetic interaction, r is the number of nearest neighbours, and $\gamma_{\mathbf{q}} = \frac{1}{r} \sum_{\mathbf{r}} \exp(i\mathbf{q} \cdot \mathbf{r})$, where $\gamma_{\mathbf{q}} = \gamma_{-\mathbf{q}}$.

a) We begin with the usual definition of a Green's function

$$G_{\mathbf{q},\mathbf{q}'}(t) = -i\theta(t) \left\langle \left[\hat{a}_{\mathbf{q}}(t), \hat{a}_{\mathbf{q}'}^{\dagger} \right] \right\rangle$$

with the resulting equation of motion in frequency space

$$\hbar\omega G_{\mathbf{q},\mathbf{q}'}(\omega) = \hbar \left\langle \left[\hat{a}_{\mathbf{q}}, \hat{a}_{\mathbf{q}'}^{\dagger} \right] \right\rangle + \left\langle \left\langle \left[\hat{a}_{\mathbf{q}}, \mathcal{H} \right]; \hat{a}_{\mathbf{q}'}^{\dagger} \right\rangle \right\rangle$$
(5)

where the notation $\langle \langle \hat{B}; \hat{B}^{\dagger} \rangle \rangle \equiv G(\omega)$. Show that the higher-order Green's function

$$\langle \langle [\hat{a}_{\mathbf{q}}, \mathcal{H}]; \hat{a}_{\mathbf{q}'}^{\dagger} \rangle \rangle = 2r J S (1 - \gamma_{\mathbf{q}}) G_{\mathbf{q}, \mathbf{q}'}(\omega) - \frac{r J}{N} \sum_{\mathbf{q}_{1} \mathbf{q}_{2} \mathbf{q}_{3}} \delta_{\mathbf{q} + \mathbf{q}_{1}, \mathbf{q}_{2} + \mathbf{q}_{3}} \left\{ \gamma_{\mathbf{q} - \mathbf{q}_{2}} - 2\gamma_{\mathbf{q}_{2}} + \gamma_{\mathbf{q}_{1} - \mathbf{q}_{2}} \right\} \left\langle \langle \hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}; \hat{a}_{\mathbf{q}'}^{\dagger} \rangle \rangle \quad (6)$$

b) Neglect the 2nd term in (6). Show that you obtain the Green's function for the 1-magnon (linear) approximation

$$G_{\mathbf{q},\mathbf{q}'}(\omega) = \hbar \delta_{\mathbf{q}\mathbf{q}'} \left\{ \hbar \omega - 2rJS(1-\gamma_{\mathbf{q}}) \right\}^{-1}$$

c) Define the following vectors:

$$\mathbf{q}_2 = \frac{1}{2}\mathbf{K} + \mathbf{Q}$$
 and $\mathbf{q}_3 = \frac{1}{2}\mathbf{K} - \mathbf{Q}$

and call the higher order Green's function $\langle\langle \hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}; \hat{a}_{\mathbf{q}}^{\dagger} \rangle\rangle \equiv A_{\mathbf{K}}(\mathbf{Q})$, where we suppress for the moment dependence on \mathbf{q} and \mathbf{q}_{1} . Using the identity for translationally invariant systems

$$\sum_{\mathbf{Q}} \gamma_{\mathbf{Q}-\mathbf{q}'} A_{\mathbf{K}}(\mathbf{Q}) = \gamma_{\mathbf{q}'} \sum_{\mathbf{Q}} \gamma_{\mathbf{Q}} A_{\mathbf{K}}(\mathbf{Q})$$

show that the second term in (6)

$$-\frac{rJ}{N}\sum_{\mathbf{q}_{1}\mathbf{q}_{2}\mathbf{q}_{3}}\delta_{\mathbf{q}+\mathbf{q}_{1},\mathbf{q}_{2}+\mathbf{q}_{3}}\left\{\gamma_{\mathbf{q}-\mathbf{q}_{2}}-2\gamma_{\mathbf{q}_{2}}+\gamma_{\mathbf{q}_{1}-\mathbf{q}_{2}}\right\}A_{\mathbf{K}}(\mathbf{Q}) =$$
$$=\frac{2rJ}{N}\sum_{\mathbf{K},\mathbf{q}_{1}}\delta_{\mathbf{q}+\mathbf{q}_{1},\mathbf{K}}\left\{\gamma_{\mathbf{K}/2}-\gamma_{\mathbf{q}-\mathbf{K}/2}\right\}\sum_{\mathbf{Q}}\gamma_{\mathbf{Q}}A_{\mathbf{K}}(\mathbf{Q}) \quad (7)$$

and we see that the important quantity to be determined is $\sum_{\mathbf{Q}} \gamma_{\mathbf{Q}} A_{\mathbf{K}}(\mathbf{Q})$

d) We would like to derive an equation of motion for $A_{\mathbf{K}}(\mathbf{Q})$. According to the template in (5) one would expect an equation of the following form:

$$\hbar\omega A_{\mathbf{K}}(\mathbf{Q}) = \hbar \left\langle \left[\hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \hat{a}_{\mathbf{q}}^{\dagger} \right] \right\rangle + \left\langle \left\langle \left[\hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \mathcal{H} \right]; \hat{a}_{\mathbf{q}}^{\dagger} \right\rangle \right\rangle$$

$$(8)$$

where the Hamiltonian \mathcal{H} is given in (4). The evaluation of the 2nd term in (8) can be simplified via several approximations.

i) Show that the following higher order Green's function, which appears in the second term in (8)

$$\langle \langle \left[\hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \hat{a}_{\mathbf{p}_{1}}^{\dagger} \hat{a}_{\mathbf{p}_{2}}^{\dagger} \hat{a}_{\mathbf{p}_{3}} \hat{a}_{\mathbf{p}_{4}} \right]; \hat{a}_{\mathbf{q}}^{\dagger} \rangle \rangle = \\ = \langle \langle \hat{a}_{\mathbf{q}_{1}}^{\dagger} \left[\hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \hat{a}_{\mathbf{p}_{1}}^{\dagger} \hat{a}_{\mathbf{p}_{2}}^{\dagger} \right] \hat{a}_{\mathbf{p}_{3}} \hat{a}_{\mathbf{p}_{4}}; \hat{a}_{\mathbf{q}}^{\dagger} \rangle \rangle + \langle \langle \hat{a}_{\mathbf{p}_{2}}^{\dagger} \hat{a}_{\mathbf{p}_{3}}^{\dagger} \left[\hat{a}_{\mathbf{q}_{1}}^{\dagger}, \hat{a}_{\mathbf{p}_{3}} \hat{a}_{\mathbf{p}_{4}} \right] \hat{a}_{\mathbf{q}_{2}}; \hat{a}_{\mathbf{q}}^{\dagger} \rangle \rangle$$

$$(9)$$

We neglect the second term in (9) and approximate the first term as

$$\langle\langle \hat{a}_{\mathbf{q}_{1}}^{\dagger} [\hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \hat{a}_{\mathbf{p}_{1}}^{\dagger} \hat{a}_{\mathbf{p}_{2}}^{\dagger}] \hat{a}_{\mathbf{p}_{3}} \hat{a}_{\mathbf{p}_{4}}; \hat{a}_{\mathbf{q}}^{\dagger} \rangle\rangle \approx \langle [\hat{a}_{\mathbf{q}_{2}} \hat{a}_{\mathbf{q}_{3}}, \hat{a}_{\mathbf{p}_{1}}^{\dagger} \hat{a}_{\mathbf{p}_{2}}^{\dagger}] \rangle \langle\langle \hat{a}_{\mathbf{q}_{1}}^{\dagger} \hat{a}_{\mathbf{p}_{3}} \hat{a}_{\mathbf{p}_{4}}; \hat{a}_{\mathbf{q}}^{\dagger} \rangle\rangle$$

ii) We want to approximate the expression $\langle [\hat{a}_{\mathbf{q}2} \hat{a}_{\mathbf{q}3}, \hat{a}_{\mathbf{p}1}^{\dagger} \hat{a}_{\mathbf{p}2}^{\dagger}] \rangle$. Using the fact that $\langle \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}'} \rangle = \delta_{\mathbf{q}\mathbf{q}'} \langle \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}} \rangle = \delta_{\mathbf{q}\mathbf{q}'} n_{\mathbf{q}}$ show that, at temperature T = 0

$$\langle [\hat{a}_{\mathbf{q}_2} \hat{a}_{\mathbf{q}_3}, \hat{a}_{\mathbf{p}_1}^{\dagger} \hat{a}_{\mathbf{p}_2}^{\dagger}] \rangle = \delta_{\mathbf{p}_1 \mathbf{q}_2} \delta_{\mathbf{p}_2 \mathbf{q}_3} + \delta_{\mathbf{p}_1 \mathbf{q}_3} \delta_{\mathbf{p}_2 \mathbf{q}_2}$$

Hint: At T = 0 the occupation number of the magnons vanishes.

e) Putting everything together show that the equation of motion for $A_{\mathbf{K}}(\mathbf{Q})$ reads as

$$\{\hbar\omega - E(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)\} A_{\mathbf{K}}(\mathbf{Q}) = \hbar \langle [\hat{a}_{\mathbf{q}_1}^{\dagger} \hat{a}_{\mathbf{q}_2} \hat{a}_{\mathbf{q}_3}, \hat{a}_{\mathbf{q}}^{\dagger}] \rangle + \frac{2rJ}{N} \{\gamma_{\mathbf{K}/2} - \gamma_{\mathbf{Q}}\} \sum_{\mathbf{Q}'} \gamma_{\mathbf{Q}'} A_{\mathbf{K}}(\mathbf{Q}') \quad (10)$$

where $E(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \equiv \hbar(\omega_{\mathbf{q}_2} + \omega_{\mathbf{q}_3} - \omega_{\mathbf{q}_1})$ and $\hbar\omega_{\mathbf{q}} = 2rJS(1 - \gamma_{\mathbf{q}}).$

f) By first evaluating the 1st term on the right-hand side of (10), keeping in mind that $\langle \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}'} \rangle = \delta_{\mathbf{q}\mathbf{q}'} \langle \hat{a}_{\mathbf{q}}^{\dagger} \hat{a}_{\mathbf{q}} \rangle$, we can solve (10) for $\sum_{\mathbf{Q}} \gamma_{\mathbf{Q}} A_{\mathbf{K}}(\mathbf{Q})$. We can do this by multiplying through (10) by $\gamma_{\mathbf{Q}}$ and summing over \mathbf{Q} . Show that the solution is

$$\{1 - W_{\mathbf{q}_1}(\mathbf{K}, \omega)\} \sum_{\mathbf{Q}} \gamma_{\mathbf{Q}} A_{\mathbf{K}}(\mathbf{Q}) = 2n_{\mathbf{q}_1} \gamma_{\mathbf{q}-\mathbf{K}/2} \delta_{\mathbf{q}+\mathbf{q}_1, \mathbf{K}} / (\omega - \omega_{\mathbf{q}})$$
(11)

where

$$W_{\mathbf{q}_1}(\mathbf{K},\omega) \equiv \frac{2rJ}{N} \sum_{\mathbf{Q}} \gamma_{\mathbf{Q}}(\gamma_{\mathbf{K}/2} - \gamma_{\mathbf{Q}}) \left\{ \hbar\omega - E(\mathbf{q}_1, \frac{1}{2}\mathbf{K} + \mathbf{Q}, \frac{1}{2}\mathbf{K} - \mathbf{Q}) \right\}^{-1}$$

g) The final step involves the recognization of the fact that the factor in (11) $\{\omega - \omega_{\mathbf{q}}\}^{-1} \equiv G_{\mathbf{qq}}(\omega)$. Going back to our original equation of motion for $G_{\mathbf{qq}}(\omega)$ (Eq. (5)) and by substituting our result (11) in the right hand side of (7) show that we can write (5) in the form

$$\{\hbar\omega - \hbar\omega_{\mathbf{q}} - \Sigma_{\mathbf{q}}(\omega)\} G_{\mathbf{q}\mathbf{q}}(\omega) = \hbar$$
(12)

where the self energy resulting from magnon-magnon interactions is given by

$$\Sigma_{\mathbf{q}}(\omega) = \frac{4rJ}{N} \sum_{\mathbf{p},\mathbf{K}} n_{\mathbf{p}} \delta_{\mathbf{p}+\mathbf{q},\mathbf{K}} \gamma_{\mathbf{q}-\mathbf{K}/2} \left\{ \gamma_{\mathbf{K}/2} - \gamma_{\mathbf{q}-\mathbf{K}/2} \right\} \left\{ 1 - W_{\mathbf{p}}(\mathbf{K},\omega) \right\}^{-1}$$
(13)