(20 Points)

Übungen zur Theorie der Kondensierten Materie II SS 16

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1. Linked Cluster Theorem

The *linked cluster theorem* states that in computing the thermodynamic potential Ω only the connected diagrams of the perturbative expansion must be considered. In this exercise we will check this theorem on some concrete examples. Consider the problem of electrons interacting with phonons. The unperturbed Hamiltonian H_0 is given by

$$H_0 = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} (a^{\dagger}_{\boldsymbol{q}} a_{\boldsymbol{q}} + 1/2), \qquad (1)$$

where the c's refer to electrons and the a's refer to the phonons. Next we introduce the interaction H' between electrons and phonons:

$$H' = V^{-1/2} \sum_{\boldsymbol{p},\boldsymbol{q},\sigma} M_{\boldsymbol{q}} A_{\boldsymbol{q}} c^{\dagger}_{\boldsymbol{p}+\boldsymbol{q},\sigma} c_{\boldsymbol{p},\sigma}$$
(2)

$$A_{\boldsymbol{q}} = a_{\boldsymbol{q}} + a_{-\boldsymbol{q}}^{\dagger} \tag{3}$$

The thermodynamic potential Ω of this problem is then given by

$$e^{-\beta\Omega} = \sum_{n=0}^{\infty} e^{-\beta\Omega_0} W_n \tag{4}$$

$$W_n = \frac{1}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \dots \int_0^\beta d\tau_n \langle T_\tau \tilde{H}'(\tau_1) \tilde{H}'(\tau_2) \dots \tilde{H}'(\tau_n) \rangle_0$$
(5)

where Ω_0 is the thermodynamic potential of H_0 , the $\tilde{H}'(\tau_i)$ operators are in the interactionpicture and the average $\langle \ldots \rangle_0$ is taken with respect to H_0 .

- (a) Explain why the thermal expectation value $\langle A_{\boldsymbol{q}}^m \rangle_0 = 0$ for odd m and therefore $W_m = 0.$ (1 Pt.)
- (b) The phonon propagator is denoted by $D(q, \tau \tau')$ and is defined as

$$D(\boldsymbol{q},\tau-\tau') = -\langle T_{\tau}\tilde{A}_{\boldsymbol{q}}(\tau)\tilde{A}_{-\boldsymbol{q}}(\tau')\rangle, \qquad (6)$$

where the \tilde{A} are the A in interaction picture

$$\tilde{A} = e^{\tau H_0} A e^{-\tau H_0}.$$
(7)

Calculate the unperturbed $D^0(\boldsymbol{q}, \tau - \tau')$, i.e. using the H_0 Hamiltonian. You should obtain the result

$$D^{0}(\boldsymbol{q},\tau) = -\theta(\tau) \left[(n_{B}(\omega_{\boldsymbol{q}}) + 1)e^{-\tau\omega_{\boldsymbol{q}}} + n_{B}(\omega_{\boldsymbol{q}})e^{\tau\omega_{\boldsymbol{q}}} \right]$$
(8)

$$-\theta(-\tau)\left\lfloor n_B(\omega_{\boldsymbol{q}})e^{-\tau\omega_{\boldsymbol{q}}} + (n_B(\omega_{\boldsymbol{q}})+1)e^{\tau\omega_{\boldsymbol{q}}}\right\rfloor.$$
(9)

Finally transform this result to frequency space. You should obtain

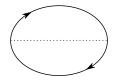
$$D^{0}(\boldsymbol{q}, i\omega_{n}) = -\frac{2\omega_{\boldsymbol{q}}}{\omega_{n}^{2} + \omega_{\boldsymbol{q}}^{2}}.$$
(10)

(5 Pts.)

(c) The lowest non-trivial term in the perturbative expansion of $e^{-\beta(\Omega-\Omega_0)}$ is

$$W_2 = \frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \ \langle T_\tau \tilde{H}'(\tau_1) \tilde{H}'(\tau_2) \rangle_0.$$
(11)

Use Wick's theorem to carry out the thermal average inside the integrals. Corresponding to these terms one can draw the Feynman diagrams. One diagram is (full lines = electrons, dashed = phonon):



Let us call the term corresponding to this bubble U_2 . Draw the other diagram. (3 Pts.)

(d) Consider now the next non-vanishing term in the perturbation series

$$W_4 = \frac{1}{4!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \ \langle T_\tau \tilde{H}'(\tau_1) \tilde{H}'(\tau_2) \tilde{H}'(\tau_3) \tilde{H}'(\tau_4) \rangle_0.$$
(12)

This already contains a large number of terms and diagrams are very helpful in organizing these. Think about possible contractions and draw at least 3 connected diagrams describing terms of this series. Also note that there are disconnected diagrams that are double copies of the diagram shown in part (c). Draw these disconnected diagrams. (2 Pts.)

(e) By considering possible contractions that lead to these disconnected diagrams, show that their total contribution to W_4 is

$$\frac{3}{4!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle T_\tau \tilde{H}'(\tau_1) \tilde{H}'(\tau_2) \rangle_0 \times \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \langle T_\tau \tilde{H}'(\tau_3) \tilde{H}'(\tau_4) \rangle_0 = \frac{1}{2} U_2^2.(13)$$
(2 Pts.)

(f) The next order in the perturbation series is

$$W_{6} = \frac{1}{6!} \int_{0}^{\beta} d\tau_{1} \dots \int_{0}^{\beta} d\tau_{6} \ \langle T_{\tau} \tilde{H}'(\tau_{1}) \tilde{H}'(\tau_{2}) \tilde{H}'(\tau_{3}) \tilde{H}'(\tau_{4}) \tilde{H}'(\tau_{5}) \tilde{H}'(\tau_{6}) \rangle_{0}.$$
(14)

This term will contain 3 copies of the bubble shown in problem (c). Explain why there are 15 such disconnected 3-bubble diagrams in W_6 . Show that therefore these diagrams contribute to W_6 a total of $\frac{1}{6}U_2^3$. (2 Pts.)

(g) Note that we found that diagrams which are just copies of U_2 contribute to $W_0 + W_2 + W_4 + W_6$ a total of

$$1 + \frac{1}{1!}U_2 + \frac{1}{2!}U_2^2 + \frac{1}{3!}U_2^3.$$
 (15)

This suggests that if we consider the perturbation theory to order 2n, i.e. W_{2n} , then the total contribution due to n copies of bubbles will just be $\frac{1}{n!}U_2^n$. Prove this by considering the combinatorics of the contractions that give rise to n bubble copies. (4 Pts.)

(h) Notice that the sum of the bubble plus copies equals $\sum_{n=0}^{\infty} \frac{1}{n!} U_2^n = \exp U_2$. Explain how this is a consequence of the linked cluster theorem. (1 Pt.)