NTNU – Trondheim
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Department of Physics

Examination paper for TFY4210 Quantum theory of many-particle systems

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Approved calculator

Rottmann: Matematisk Formelsamling

Rottmann: Matematische Formelsammlung

Barnett & Cronin: Mathematical Formulae

Other information:

The exam has 3 problems. In many cases it is possible to solve later subproblems even if an earlier subproblem was not solved. Some formulas can be found on the last two pages. The problems were developed by John Ove Fjærestad. (You can find the Norwegian version of the exam after the English version.)

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Date Signature

A white box (☐) at the start of a line signifies the beginning of new text that is not part of the preceding question.

We set $\hbar = 1$. The lattice spacings in Problems 1 and 2 are also set to 1.

Problem 1

Consider a Heisenberg ferromagnet on a square lattice. The Hamiltonian is

$$H_{\text{Heis}} = -J \sum_{\langle i,j \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j, \tag{1}$$

where $J > 0$ and the sum is over all pairs of nearest-neighbour spins. This model has ferromagnetic order in the ground state.

(a) Explain what is meant by a broken continuous symmetry. You may discuss this question in the context of the model (1).

☐ Using spin-wave theory, it can be shown (you should not show it) that (1) can be expressed as

$$H_{\text{Heis}} = E_0 + \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \tag{2}$$

where $E_0 = -2NJS^2$ and $\omega_{\boldsymbol{k}} = 2JS(2 - \cos k_x - \cos k_y)$. Here N is the number of sites and S is the total spin quantum number of each spin. Now we modify the Hamiltonian by adding a spin-anisotropy term

$$H_D = D \sum_j \left[(\hat{S}^x_j)^2 + (\hat{S}^y_j)^2 \right], \tag{3}$$

where $D \geq 0$ and the sum is over all sites. Thus the total Hamiltonian becomes $H_{\text{tot}} = H_{\text{Heis}} + H_D$.

(b) Discuss whether/how you expect the inclusion of H_D to affect the conditions for ferromagnetic order. Use spin-wave theory (in which terms describing interactions between magnons are neglected) to show that H_D can be written in the form

$$H_D = C + \Delta \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}, \tag{4}$$

and give expressions for the parameters C and Δ.

□ It follows from the above that H_{tot} can be written in the form

$$H_{\text{tot}} = E_0^{\text{tot}} + \sum_{\boldsymbol{k}} \omega^{\text{tot}}_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \tag{5}$$

where $E_0^{\text{tot}} = E_0 + C$ and $\omega^{\text{tot}}_{\boldsymbol{k}} \equiv \omega_{\boldsymbol{k}} + \Delta$.

(c) Give a physical interpretation of the parameter Δ. Discuss its variation with $D \geq 0$ in light of symmetry properties of H_{tot}.

□ Let $|G\rangle$ be the ground state of (5) defined by $a_{\boldsymbol{k}}|G\rangle = 0$ for all $\boldsymbol{k}$. Now consider the state $U|G\rangle$ where U is an operator that rotates *all* spins in the same way. To be specific, consider an *infinitesimal* rotation by an angle $d\theta$ around the x axis.

(d) Based on physical reasoning, for which value(s) of $D \geq 0$ do you expect also $U|G\rangle$ to be a ground state of H_{tot}? Also analyze the problem by calculating $H_{\text{tot}}(U|G\rangle)$ (with H_{tot} given by (5)) and interpreting the result. [Hint: First show that the total generator involved is the sum of the generators for the individual spins. Approximate the relevant Holstein-Primakoff expressions in the same way as usual.]

Problem 2

Consider a 1-dimensional lattice with N sites. On each lattice site j (where $j = 1, 2, \ldots, N$) there is a spin with $S = 1/2$, represented by the spin operator $\hat{\boldsymbol{S}}_j = (\hat{S}^x_j, \hat{S}^y_j, \hat{S}^z_j)$. The spins interact with their nearest neighbours as given by the following Hamiltonian:

$$H = -\sum_{j=1}^{N} \left[\frac{J_\perp}{2} (\hat{S}^+_j \hat{S}^-_{j+1} + \text{h.c.}) + J_z \hat{S}^z_j \hat{S}^z_{j+1} \right], \tag{6}$$

where $\hat{S}^\pm_j \equiv \hat{S}^x_j \pm i S^y_j$ are the standard ladder operators, $J_\perp > 0$, and J_z is so far arbitrary. Periodic boundary conditions are imposed on the spins, i.e. $\hat{\boldsymbol{S}}_{N+1} = \hat{\boldsymbol{S}}_1$.

We will analyze this spin model by making use of the Jordan-Wigner transformation to map it onto a spinless fermion model. The transformation is given by

$$\hat{S}^+_j = \hat{O}_j c^\dagger_j, \tag{7}$$

$$\hat{S}^-_j = \hat{O}_j c_j, \tag{8}$$

$$\hat{S}^z_j = \hat{n}_j - \frac{1}{2}, \tag{9}$$

where $\hat{O}_j = \prod_{i=1}^{j-1}(1 - 2\hat{n}_i)$ and $\hat{n}_j = c^\dagger_j c_j$. Here the operator $c^\dagger_j$ (c_j) creates (annihilates) a spinless fermion at site j. These operators satisfy standard fermionic anticommutation relations, i.e.,

$$\{c_j, c^\dagger_{j'}\} = \delta_{j,j'}, \tag{10}$$

$$\{c_j, c_{j'}\} = \{c^\dagger_j, c^\dagger_{j'}\} = 0. \tag{11}$$

According to Eq. (9), an up-spin (down-spin) on site j corresponds to the presence (absence) of a fermion on that site.

(a) Use the fermionic anticommutation relations to show that $\hat{n}^2_j = \hat{n}_j$. Use the Jordan-Wigner transformation to show that the spin commutation relation $[\hat{S}^+_j, \hat{S}^-_j] = 2\hat{S}^z_j$ is satisfied.

(b) Show that $\hat{S}^+_j \hat{S}^-_{j+1} = c^\dagger_j c_{j+1}$. Express the Hamiltonian (6) in terms of fermion operators (you may assume without justification that also the fermions satisfy periodic boundary conditions, i.e. $c_{N+1} = c_1$).

□ **In the remainder of this problem we set $J_z = 0$.**

(c) By introducing new fermion operators c_k and $c_k^\dagger$ via a Fourier transformation

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ikj} c_k, \tag{12}$$

show that the Hamiltonian can be written in the form $H = \sum_k \varepsilon_k c_k^\dagger c_k$, and give an expression for the function ε_k. What are the allowed wavevectors k?

(d) Describe the ground state (in terms of the fermions).[1] Calculate the ground-state energy per site (you may take the limit $N \to \infty$).

(e) Calculate the ground-state expectation value of $\hat{S}_j^z$ for an arbitrary site j (again you may take the limit $N \to \infty$).

[1] Do not concern yourself with potential degeneracy issues (to avoid such complications, it is possible to choose N such that the ground state is nondegenerate).

Problem 3

Consider a noninteracting gas of electrons in three dimensions. In first quantization, the Hamiltonian is

$$H_0 = \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m}. \tag{13}$$

(a) Neglecting the electron spin and working in the grand canonical ensemble with chemical potential μ, show that in second quantization the Hamiltonian can be written as

$$H_0 = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} \quad \text{where} \quad \xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu. \tag{14}$$

(You may assume that the electrons are confined within a cube of side length L and with periodic boundary conditions.) Give an expression for $\varepsilon_{\boldsymbol{k}}$. Describe the electron state created by $c_{\boldsymbol{k}}^\dagger$. What are the allowed values of $\boldsymbol{k}$?

□ Consider the Matsubara single-particle Green function

$$\mathcal{G}(\boldsymbol{k}, \tau) = -\langle T_\tau (c_{\boldsymbol{k}}(\tau) c_{\boldsymbol{k}}^\dagger(0))\rangle, \tag{15}$$

where τ takes values between $-\beta$ and β (where $\beta = 1/(k_B T)$ is the inverse temperature), and T_τ orders the operators by increasing time from right to left, introducing a minus sign when a reordering is needed. The time dependence of the operators is given by $A(\tau) = e^{H\tau} A(0) e^{-H\tau}$ (where $A(0) \equiv A$). The Fourier transform of $\mathcal{G}(\boldsymbol{k}, \tau)$ is given by

$$\mathcal{G}(\boldsymbol{k}, ip_m) = \int_0^\beta d\tau \; e^{ip_m \tau} \mathcal{G}(\boldsymbol{k}, \tau) \tag{16}$$

where $p_m = (2m+1)\pi/\beta$ is a fermionic Matsubara frequency (m is an integer).

(b) Calculate $\mathcal{G}(\boldsymbol{k}, ip_m)$ for the Hamiltonian (14). Use the result to find the retarded single-particle Green function $G^R(\boldsymbol{k}, \omega)$.

□ Next, consider electrons scattering with impurities in a metal (again we neglect the electron spin). In the lectures we developed a perturbation expansion (in the electron-impurity scattering potential) for the impurity-averaged Matsubara single-particle Green function $\overline{\mathcal{G}}(\boldsymbol{k}, ip_m)$. We represented each term in the perturbation expansion for $\overline{\mathcal{G}}(\boldsymbol{k}, ip_m)$ by a Feynman diagram and established the Feynman rules for translating between the diagrams and their associated mathematical expressions.

(c) Consider the two Feynman diagrams in Fig. 1 that appear in the perturbation expansion for $\overline{\mathcal{G}}(\boldsymbol{k}, ip_m)$.

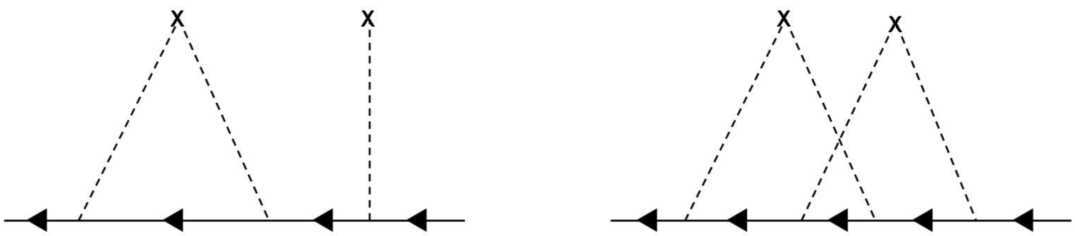

Figure 1: Two Feynman diagrams.

For each diagram:

1. Give its mathematical expression (do not attempt to evaluate any wavevector sums).
2. Determine whether it is reducible or irreducible (justify your conclusion).

(d) Explain how the self-energy $\Sigma(\boldsymbol{k}, ip_m)$ is defined (feel free to draw diagrams as part of your explanation).

□ Consider the impurity-averaged retarded single-particle Green function $\overline{G}^R(\boldsymbol{k}, \omega)$ for this problem (ω real). It obeys a Dyson equation which can be written as

$$\overline{G}^R(\boldsymbol{k}, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} + i\eta - \Sigma^R(\boldsymbol{k}, \omega)}. \tag{17}$$

This equation is obtained from the Dyson equation for the Matsubara Green function $\overline{\mathcal{G}}(\boldsymbol{k}, ip_m)$ by the analytic continuation $ip_m \to \omega + i\eta$. The quantity $\Sigma^R(\boldsymbol{k}, \omega)$ obtained from $\Sigma(\boldsymbol{k}, ip_m)$ in this way is called the retarded self-energy. Write it as $\Sigma^R(\boldsymbol{k}, \omega) = \Sigma^R_r(\boldsymbol{k}, \omega) + i\Sigma^R_i(\boldsymbol{k}, \omega)$ where Σ^R_r and Σ^R_i are its real and imaginary parts, respectively. We will assume that the imaginary part Σ^R_i is nonzero, in which case $i\eta$ in the denominator in (17) can be neglected.

(e) Use Eq. (17) to find an expression for the single-particle spectral function $A(\boldsymbol{k}, \omega) \equiv -(1/\pi)\text{Im}\, \overline{G}^R(\boldsymbol{k}, \omega)$ in terms of ω, $\xi_{\boldsymbol{k}}$, $\Sigma^R_r(\boldsymbol{k}, \omega)$ and $\Sigma^R_i(\boldsymbol{k}, \omega)$. Based on your knowledge of the general properties of $A(\boldsymbol{k}, \omega)$, can you deduce the sign of $\Sigma^R_i(\boldsymbol{k}, \omega)$?

Formulas

Spin operators:

$$\hat{S}_j^x = \frac{1}{2}(\hat{S}_j^+ + \hat{S}_j^-), \tag{18}$$

$$\hat{S}_j^y = \frac{1}{2i}(\hat{S}_j^+ - \hat{S}_j^-). \tag{19}$$

Holstein-Primakoff representation:

$$\hat{S}_j^+ = \sqrt{2S - \hat{n}_j}\, a_j, \tag{20}$$

$$\hat{S}_j^- = a_j^\dagger \sqrt{2S - \hat{n}_j}, \tag{21}$$

$$\hat{S}_j^z = S - \hat{n}_j, \tag{22}$$

where $\hat{n}_j \equiv a_j^\dagger a_j$.

Fourier transform:

$$a_j = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_j} a_{\boldsymbol{k}}. \tag{23}$$

Lattice sum:

$$\frac{1}{N} \sum_j e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_j} = \delta_{\boldsymbol{k},\boldsymbol{k}'}. \tag{24}$$

General commutator identities:

$$[A, BC] = [A, B]C + B[A, C], \tag{25}$$

$$[A, BC] = \{A, B\}C - B\{A, C\}. \tag{26}$$

Commutator relations:

$$[\hat{n}_\mu, a_\nu] = -a_\nu \delta_{\mu\nu}, \tag{27}$$

$$[\hat{n}_\mu, a_\nu^\dagger] = a_\nu^\dagger \delta_{\mu\nu}. \tag{28}$$

(there are more formulas on the next page)

From first to second quantization:

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}(x_i) \quad \Longrightarrow \quad \sum_{\alpha,\beta} \langle \alpha | \hat{h} | \beta \rangle c_\alpha^\dagger c_\beta, \tag{29}$$

$$\langle \alpha | \hat{h} | \beta \rangle = \int dx \; \phi_\alpha^*(x) \hat{h}(x) \phi_\beta(x). \tag{30}$$

$$\hat{H}_I = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \hat{v}(x_i, x_j) \quad \Longrightarrow \quad \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma, \tag{31}$$

$$\langle \alpha\beta | \hat{v} | \gamma\delta \rangle = \int \int dx \; dx' \; \phi_\alpha^*(x) \phi_\beta^*(x') \hat{v}(x, x') \phi_\gamma(x) \phi_\delta(x'). \tag{32}$$

Fermi-Dirac distribution:

$$n_F(\xi) = \frac{1}{e^{\beta\xi} + 1}. \tag{33}$$