NTNU – Trondheim
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Department of Physics

Examination paper for
TFY4210 Quantum theory of many-particle systems

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Examination date: 21 May 2014

Examination time (from-to): 9-13

Permitted examination support material: C

Approved calculator

Rottmann: Matematisk Formelsamling

Rottmann: Matematische Formelsammlung

Barnett & Cronin: Mathematical Formulae

Other information:

The exam has 3 problems. Some formulas can be found on the last page.

The problems were developed by John Ove Fjærestad.

Language: English

Number of pages (including front page and attachments): 8

Checked by:

Date Signature

Problem 1

Consider a gas of noninteracting electrons. For simplicity, neglect the electron spin and assume that the electrons are constrained to move in one spatial dimension. The length of the system is L, and periodic boundary conditions are imposed.

(a) In first quantization, the Hamiltonian of the system is given by

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial z_j^2} \tag{1}$$

where N is the number of electrons and z_j is the coordinate of the j'th electron ($j = 1, 2, \ldots, N$). Show that in second quantization the Hamiltonian can be written as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k \tag{2}$$

and determine ε_k. Here the operators $c_k^\dagger$ and c_k respectively create and annihilate an electron with wavevector k (due to the periodic boundary conditions the allowed (discrete) wavevectors are given by $k = 2\pi n/L$ where n is an arbitrary integer).

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In the remainder of the problem you will work in the grand canonical ensemble, so the Hamiltonian is modified to

$$H = \sum_k (\varepsilon_k - \mu) c_k^\dagger c_k \equiv \sum_k \xi_k \hat{n}_k, \tag{3}$$

where $\xi_k = \varepsilon_k - \mu$ with μ being the chemical potential and $\hat{n}_k = c_k^\dagger c_k$. Here ξ_k is an even function of k which increases monotonically with $|k|$.

(b) Consider many-particle states of the form

$$|\ell\rangle \equiv \prod_{k\in S_\ell} c_k^\dagger |0\rangle \tag{4}$$

where $|0\rangle$ is the state containing no fermions (implying $c_k|0\rangle = 0 = \hat{n}_k|0\rangle$ for all k) and S_ℓ is an arbitrary set of distinct wavevectors. Thus the set S_ℓ defines which single-particle k-states are occupied by an electron in the many-particle state $|\ell\rangle$. (To define $|\ell\rangle$ unambiguously, we take the order of the creation operators in the product to be such that if k_1 and k_2 are both in S_ℓ, and $k_2 > k_1$, then $c^\dagger_{k_2}$ is to the right of $c^\dagger_{k_1}$.)

1. Show that the states $|\ell\rangle$ defined in (4) are eigenstates of H defined in (3) and determine an expression for the associated eigenvalue E_ℓ.
2. What is the ground state, i.e. the state with the smallest value of E_ℓ? Give an expression for the ground state energy.

(c) For a general many-fermion system the single-particle spectral function $A(\nu, \omega)$ can be written

$$A(\nu, \omega) = \frac{1}{Z} \sum_{\ell, m} |\langle m | c^\dagger_\nu | \ell \rangle|^2 \left(e^{-\beta E_\ell} + e^{-\beta E_m} \right) \delta(\omega + E_\ell - E_m). \tag{5}$$

Here the sums are over the complete and orthonormal set of eigenstates $|\ell\rangle$ of the Hamiltonian H with E_ℓ being the corresponding eigenvalues, $Z = \sum_\ell e^{-\beta E_\ell}$ is the partition function, and $c^\dagger_\nu$ creates a fermion in a single-particle state characterized by the quantum number ν.

1. For a general many-fermion system, prove the sum rule

$$\int_{-\infty}^{\infty} d\omega \, A(\nu, \omega) = 1. \tag{6}$$

2. For the specific case of the fermionic system with Hamiltonian (3), calculate the right-hand side of (5) to show that

$$A(k, \omega) = \delta(\omega - \xi_k). \tag{7}$$

Problem 2

A model of a ferromagnet on a square lattice has the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - J' \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{8}$$

with $J, J' > 0$. The two terms in H only differ in the possible values of the relative position vectors $\boldsymbol{r}_j - \boldsymbol{r}_i$ (here $\boldsymbol{r}_i$ is the position vector of site i): The sum in the first term is over pairs of nearest-neighbour sites and the sum in the second term is over pairs of next-nearest-neighbour sites (in both sums, each pair is counted once). The nearest-neighbour and next-nearest-neighbour sites of a given site on the square lattice are shown in Fig. 1.

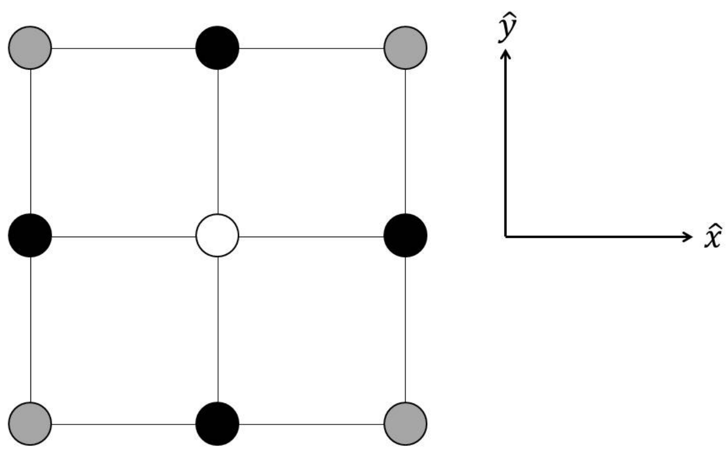

Figure 1: A given site (shown in white) has 4 nearest-neighbour sites (shown in black) and 4 next-nearest-neighbour sites (shown in grey). The unit vectors $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ are also shown (the lattice spacing is set to 1).

(a) Use spin-wave theory to calculate the ground state energy E_0 and the magnon dispersion $\omega_{\boldsymbol{k}}$ (in this analysis, neglect terms describing interactions between magnons).

(b)

1. Based on your results in (a), determine whether the magnons are gapless or gapped.
2. Briefly explain whether your answer to (b)1 is consistent with arguments/results based on symmetry.

3. Propose a term that, if added to the Hamiltonian (8), would change your answer to (b)1.

Problem 3

Consider fermions in a disordered potential (e.g. electrons interacting with impurities in a metal). In the lectures we developed a perturbation expansion for the single-particle Matsubara Green function $\mathcal{G}(\boldsymbol{k}, \boldsymbol{k}'; ip_m)$ where p_m is a fermionic Matsubara frequency. Upon averaging over the positions of the impurities, the resulting Green function became $\boldsymbol{k}$-diagonal: $\bar{\mathcal{G}}(\boldsymbol{k}, \boldsymbol{k}'; ip_m) = \bar{\mathcal{G}}(\boldsymbol{k}, ip_m)\delta_{\boldsymbol{k},\boldsymbol{k}'}$. We represented each term in the perturbation expansion for $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$ by a Feynman diagram and established the Feynman rules for translating between the diagrams and their associated mathematical expressions.

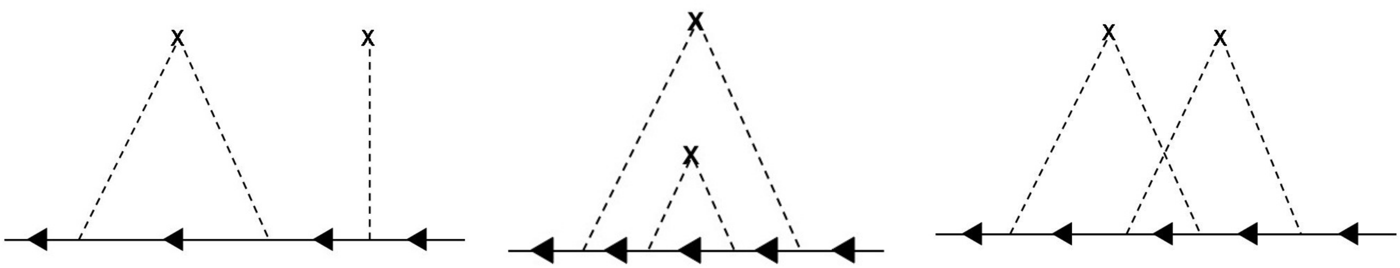

Figure 2: Three Feynman diagrams.

(a) Consider the Feynman diagrams in Fig. 2 that appear in the perturbation expansion for $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$.

1. **For the first two diagrams**, give the mathematical expression (do not attempt to evaluate any wavevector sums).
2. **For all three diagrams**, determine whether the diagram is reducible or irreducible (justify your conclusion). If the diagram is irreducible, draw the corresponding self-energy diagram.

(b) Taking as your starting point the way in which self-energy diagrams enter into the Feynman diagrams for $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$, prove the Dyson equation

$$\bar{\mathcal{G}}(\boldsymbol{k}, ip_m) = \frac{1}{[\mathcal{G}^{(0)}(\boldsymbol{k}, ip_m)]^{-1} - \Sigma(\boldsymbol{k}, ip_m)} \tag{9}$$

where $\mathcal{G}^{(0)}(\boldsymbol{k}, ip_m) = 1/(ip_m - \xi_{\boldsymbol{k}})$ is the unperturbed Green function and $\Sigma(\boldsymbol{k}, ip_m)$ is the self-energy.

The rest of the problem concerns some approximations to the self-energy.

(c) First consider "the full Born approximation" (FBA) $\Sigma_{\mathrm{FB}}(\boldsymbol{k}, ip_m)$, defined as the sum of all self-energy diagrams with a *single* impurity cross (see Fig. 3).

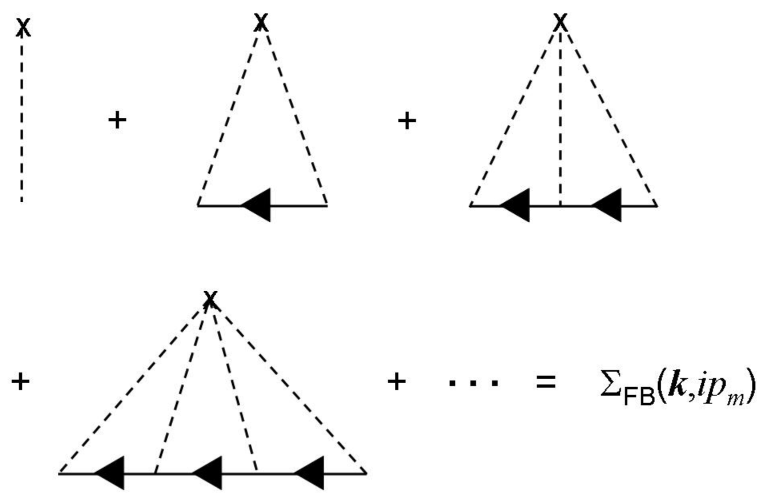

Figure 3: The full Born approximation (FBA) for the self-energy.

Let $\bar{\mathcal{G}}_{\mathrm{FB}}(\boldsymbol{k}, ip_m)$ be the approximate Green function that corresponds to the FBA for the self-energy. According to the Dyson equation,

$$\bar{\mathcal{G}}_{\mathrm{FB}}(\boldsymbol{k}, ip_m) = \frac{1}{ip_m - \xi_{\boldsymbol{k}} - \Sigma_{\mathrm{FB}}(\boldsymbol{k}, ip_m)}. \tag{10}$$

1. Which (if any) of the three Feynman diagrams in Fig. 2 are included in the diagrammatic expansion of $\bar{\mathcal{G}}_{\mathrm{FB}}$? Justify your answer.

2. Give an example of a Feynman diagram in the expansion of $\bar{\mathcal{G}}_{\mathrm{FB}}$ that is proportional to the square of the impurity density and is of sixth order in the scattering potential.

(d) Next consider a different approximation to the self-energy, "the self-consistent Born approximation" (SCBA) $\Sigma_{\rm SCB}(\boldsymbol{k}, ip_m)$. The Dyson equation for the associated Green function $\mathcal{G}_{\rm SCB}(\boldsymbol{k}, ip_m)$ is

$$\bar{\mathcal{G}}_{\rm SCB}(\boldsymbol{k}, ip_m) = \frac{1}{ip_m - \xi_{\boldsymbol{k}} - \Sigma_{\rm SCB}(\boldsymbol{k}, ip_m)}. \tag{11}$$

$\Sigma_{\rm SCB}$ is obtained from $\Sigma_{\rm FB}$ as follows (see Fig. 4): In each self-energy diagram in $\Sigma_{\rm FB}$, replace each unperturbed Green function $\mathcal{G}^{(0)}(\boldsymbol{k}', ip_m)$ (shown as full thin lines in Fig. 3) by the Green function $\bar{\mathcal{G}}_{\rm SCB}(\boldsymbol{k}', ip_m)$ (shown as full thick lines in Fig. 4). This approximation is called "self-consistent" because the rhs of (11) depends on $\bar{\mathcal{G}}_{\rm SCB}$ through $\Sigma_{\rm SCB}$. Using this approximation for the self-energy, many more Feynman diagrams are included in the approximation for the Green function.

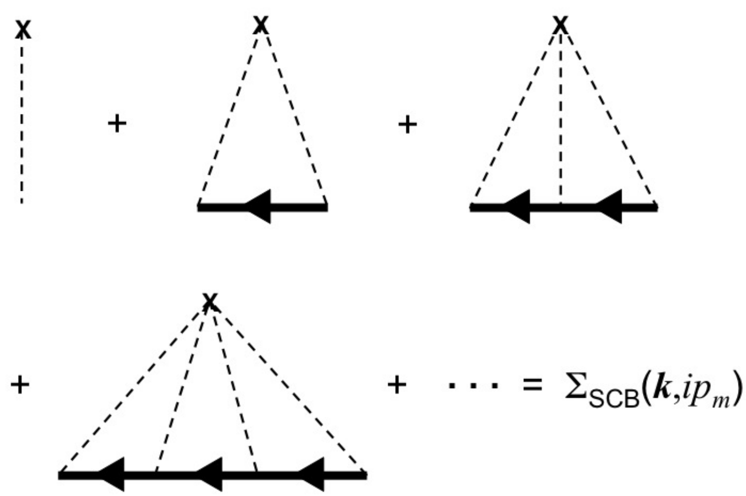

Figure 4: The self-consistent Born approximation (SCBA) for the self-energy. The full thick lines represent the Green function $\bar{\mathcal{G}}_{\rm SCB}$.

1. Which of the diagrams in Fig. 2 are included in the diagrammatic expansion of $\bar{\mathcal{G}}_{\rm SCB}$? Explain your reasoning.

2. Give an(other) example of a Feynman diagram that is included in the expansion of $\bar{\mathcal{G}}_{\rm SCB}$ but not in $\bar{\mathcal{G}}_{\rm FB}$.

Formulas

From first to second quantisation:

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

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

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

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

A commutator:

$$[\hat{n}_\nu, c_{\nu'}^\dagger] = \delta_{\nu,\nu'} c_\nu^\dagger$$

Spin interactions:

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z.$$

Holstein-Primakoff representation:

$$\begin{aligned} S_j^+ &= \sqrt{2S - \hat{n}_j}\ a_j, \\ S_j^- &= a_j^\dagger \sqrt{2S - \hat{n}_j}, \\ S_j^z &= S - \hat{n}_j, \end{aligned}$$

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

Fourier transform:

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

Lattice sum:

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