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. The percentage in parentheses after each problem number indicates the presumable weighting of the problem. 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 page. The problems were developed by John Ove Fjærestad.

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In this exam, a white box (□) at the start of a line signifies the beginning of new text that is not part of the preceding question.

Problem 1 (25%)

Consider a system that can contain bosons in two different states, labeled ↑ and ↓. The basis state with $n_\uparrow$ ↑-bosons and $n_\downarrow$ ↓-bosons is written $|n_\uparrow, n_\downarrow\rangle$. Creation and annihilation operators $b_\alpha^\dagger$ and b_α ($\alpha = \uparrow, \downarrow$) are defined by their action on the basis states as follows:

$$\begin{aligned} b_\uparrow^\dagger|n_\uparrow, n_\downarrow\rangle &= \sqrt{n_\uparrow + 1}|n_\uparrow + 1, n_\downarrow\rangle, & b_\downarrow^\dagger|n_\uparrow, n_\downarrow\rangle &= \sqrt{n_\downarrow + 1}|n_\uparrow, n_\downarrow + 1\rangle, \\ b_\uparrow|n_\uparrow, n_\downarrow\rangle &= \sqrt{n_\uparrow}|n_\uparrow - 1, n_\downarrow\rangle, & b_\downarrow|n_\uparrow, n_\downarrow\rangle &= \sqrt{n_\downarrow}|n_\uparrow, n_\downarrow - 1\rangle. \end{aligned} \tag{1}$$

(a) Show that $[b_\uparrow, b_\uparrow^\dagger] = 1$. Also write down (without proof) the other bosonic commutation relations that follow from (1).

□ A spin operator $\hat{\boldsymbol{S}} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$ can be represented in terms of the ↑- and ↓-boson operators by defining (here $\hat{S}^\pm = S^x \pm iS^y$)

$$\hat{S}^+ = b_\uparrow^\dagger b_\downarrow, \tag{2}$$

$$\hat{S}^- = b_\downarrow^\dagger b_\uparrow, \tag{3}$$

$$\hat{S}^z = \frac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow), \tag{4}$$

where $\hat{n}_\alpha \equiv b_\alpha^\dagger b_\alpha$. This is known as the **Schwinger boson representation**.

(b) Use the bosonic commutation relations to show that the Schwinger boson representation satisfies the spin commutation relations

$$[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z \quad \text{and} \quad [\hat{S}^z, \hat{S}^\pm] = \pm\hat{S}^\pm. \tag{5}$$

□ Since both $n_\uparrow$ and $n_\downarrow$ range over all the nonnegative integers, the bosonic Hilbert (or, more precisely, Fock) space spanned by the basis states $|n_\uparrow, n_\downarrow\rangle$ is infinite-dimensional. In contrast, the Hilbert space corresponding to a value S for the total spin quantum number is $(2S+1)$-dimensional, and is spanned by the basis states $|S, m\rangle$ which satisfy $\hat{\boldsymbol{S}}^2|S, m\rangle = S(S+1)|S, m\rangle$ and $\hat{S}^z|S, m\rangle = m|S, m\rangle$, where m, the eigenvalue of $\hat{S}^z$, can take the values $m = -S, -S+1, \ldots, S$.

(c) Show from the Schwinger boson representation that

$$\hat{\boldsymbol{S}}^2 = \frac{\hat{n}_\uparrow + \hat{n}_\downarrow}{2}\left(\frac{\hat{n}_\uparrow + \hat{n}_\downarrow}{2} + 1\right), \tag{6}$$

and show that if

$$n_\uparrow + n_\downarrow = 2S, \tag{7}$$

it follows that

$$\hat{\boldsymbol{S}}^2|n_\uparrow, n_\downarrow\rangle = S(S+1)|n_\uparrow, n_\downarrow\rangle. \tag{8}$$

□ As a consequence of these various results, the spin Hilbert space corresponds to a $(2S+1)$-dimensional **sub**space, defined by the constraint (7), of the infinite-dimensional bosonic Fock space. More precisely, one can take

$$|S, m\rangle = |n_\uparrow, n_\downarrow\rangle \quad \text{where } n_\uparrow = S + m \text{ and } n_\downarrow = S - m. \tag{9}$$

For some applications it is useful to know how the boson operators are affected by various transformations. Here we will consider spin rotations around the z axis.

(d) Give an expression for the operator $U(\theta)$ that produces a rotation about the z axis by the angle θ, and use this to calculate

$$U(\theta)b_\alpha^\dagger U^\dagger(\theta). \tag{10}$$

As a check of your result for (10), use it to show that

$$U(2\pi)|S, m\rangle = (-1)^{2S}|S, m\rangle. \tag{11}$$

(Hint for proving (11): Up to a normalization factor, the basis state $|n_\uparrow, n_\downarrow\rangle$ can be written

$$(b_\uparrow^\dagger)^{n_\uparrow}(b_\downarrow^\dagger)^{n_\downarrow}|0, 0\rangle \tag{12}$$

where $|0, 0\rangle$ is the bosonic vacuum state satisfying $b_\uparrow|0, 0\rangle = b_\downarrow|0, 0\rangle = 0$.)

Problem 2 (45%)

Consider a system of electrons on a 1-dimensional lattice with periodic boundary conditions. For simplicity we will neglect the spin degree of freedom, thus treating the electrons as spinless fermions. The Hamiltonian is given by

$$H = -t \sum_j (c_j^\dagger c_{j+1} + \text{h.c.}) + \Delta \sum_j (-1)^j c_j^\dagger c_j. \tag{13}$$

Here, the operators $c_j^\dagger$ and c_j respectively create and annihilate a spinless fermion at site j ($j = 1, 2, \ldots, N$). The number of lattice sites N is assumed to be an even number. The first term in H represents hopping between nearest-neighbour sites with hopping matrix element t. The second term in H implies that the energy cost for a fermion to occupy a site j equals Δ for even j and $-\Delta$ for odd j. The constant parameters t and Δ are both real, with $t > 0$, while Δ can be either positive, negative, or 0. We set the lattice spacing to 1.

(a) Introduce new fermionic operators c_k defined as

$$c_k = \frac{1}{\sqrt{N}} \sum_j e^{-ikj} c_j. \tag{14}$$

Show that $c_{k+2\pi m} = c_k$, where m is an arbitrary integer, and show that the Hamiltonian can be written in the form

$$H = \sum_{k \in 1\text{BZ}} \left[\varepsilon_k c_k^\dagger c_k + \Delta c_{k+\pi}^\dagger c_k \right], \tag{15}$$

where the k-sum is over the 1st Brillouin zone (1BZ). Give the form of the function ε_k and show that it satisfies $\varepsilon_{k\pm\pi} = -\varepsilon_k$.

(b) Show that H can be rewritten as

$$H = \sum_{k \in \text{MBZ}} \left[\varepsilon_k (c_k^\dagger c_k - c_{k+\pi}^\dagger c_{k+\pi}) + \Delta (c_k^\dagger c_{k+\pi} + c_{k+\pi}^\dagger c_k) \right], \tag{16}$$

where the k-sum is now restricted to the "magnetic Brillouin zone" (MBZ) (i.e. $|k|$ is not greater than $\pi/2$).

(c) Introduce new fermionic operators α_k and β_k by defining

$$c_k = u_k \alpha_k - v_k \beta_k, \tag{17}$$

$$c_{k+\pi} = v_k \alpha_k + u_k \beta_k. \tag{18}$$

Here u_k and v_k are real parameters satisfying $u_k^2 + v_k^2 = 1$, which can be used to write $u_k = \cos\theta_k$, $v_k = \sin\theta_k$. Show that by a proper choice of θ_k, the Hamiltonian can be written in the diagonal form

$$H = \sum_{k \in \mathrm{MBZ}} \left[E_k^{(\alpha)} \alpha_k^\dagger \alpha_k + E_k^{(\beta)} \beta_k^\dagger \beta_k \right] \tag{19}$$

and give the form of the two functions $E_k^{(\alpha)}$ and $E_k^{(\beta)}$.

In the remainder of the problem we assume that there are $N/2$ fermions in the system.

(d) Characterize the ground state in terms of occupation numbers of the appropriate fermionic modes. Based on this, give an expression for the ground state energy in the form $\sum_{k \in \mathrm{MBZ}} f_k$, where f_k is a specific function of k.

(e) Consider the operator

$$\hat{N}_{\mathrm{even}} - \hat{N}_{\mathrm{odd}} = \sum_j (-1)^j c_j^\dagger c_j \tag{20}$$

which measures the difference between the number of fermions on even and odd sites. Find an expression for the ground state expectation value $\langle(\hat{N}_{\mathrm{even}} - \hat{N}_{\mathrm{odd}})\rangle$ in the form $\sum_{k \in \mathrm{MBZ}} g_k$, where g_k is a specific function of k. Discuss whether the expression is physically reasonable by commenting on (i) its magnitude in the two limits $|\Delta| \ll t$ and $|\Delta| \gg t$ and (ii) its sign for the two cases $\Delta > 0$ and $\Delta < 0$.

Problem 3 **(30%)**

Consider electrons scattering with impurities in a metal (we neglect the electron spin). In the lectures we developed a perturbation expansion (in the electron-impurity scattering potential) for the impurity-averaged Matsubara 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.

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

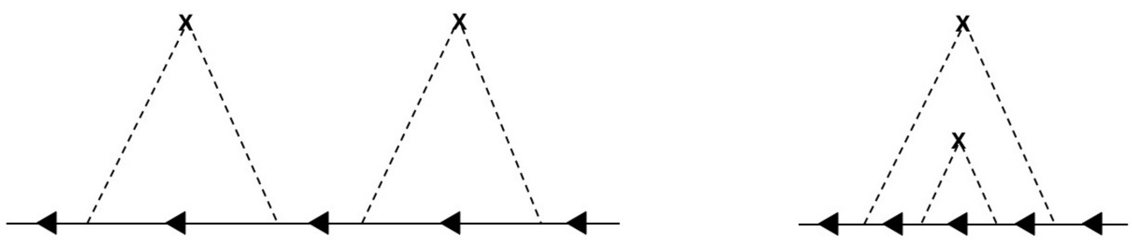

Figure 1: Two Feynman diagrams.

1. For each diagram, give its mathematical expression (do not attempt to evaluate any wavevector sums).
2. For each diagram, determine whether it is reducible or irreducible (justify your conclusion). If the diagram is irreducible, draw the corresponding self-energy diagram.

☐ In the lectures we showed that $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$ can be expressed as

$$\bar{\mathcal{G}}(\boldsymbol{k}, ip_m) = \frac{1}{(\mathcal{G}^{(0)}(\boldsymbol{k}, ip_m))^{-1} - \Sigma(\boldsymbol{k}, ip_m)} = \frac{1}{ip_m - \xi_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, ip_m)} \tag{21}$$

where $\Sigma(\boldsymbol{k}, ip_m)$ is the self-energy.

(b)

1. Explain (e.g. by drawing diagrams or otherwise) in what way self-energy diagrams are "building blocks" in the perturbation (Feynman diagram) expansion for the Green function $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$. Include an explanation of how, by using an approximate self-energy that may only

include a **finite** number of self-energy diagrams, one still obtains an approximation to the Green function that includes an **infinite** subset of all Feynman diagrams in the full perturbation expansion for the Green function.

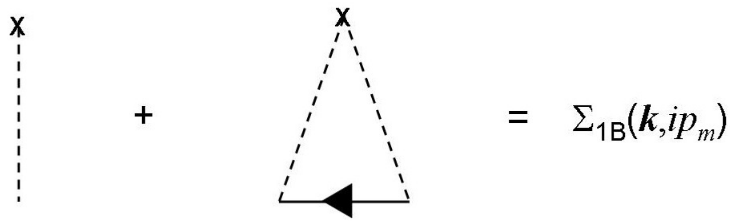

Figure 2: The approximation to the self-energy known as the first Born approximation.

2. In the lectures we found an approximate result for $\bar{\mathcal{G}}(\boldsymbol{k}, ip_m)$ by approximating the self-energy $\Sigma(\boldsymbol{k}, ip_m)$ as shown in Fig. 2. This is called the "first Born approximation" for the self-energy and denoted by $\Sigma_{1\mathrm{B}}(\boldsymbol{k}, ip_m)$. Determine which (if any) of the Feynman diagrams in Fig. 1 are included when one approximates the self-energy by $\Sigma_{1B}(\boldsymbol{k}, ip_m)$.

(c) In the lectures we showed that for a very short-ranged potential, $\Sigma_{1B}(\boldsymbol{k}, ip_m)$ is approximately given by

$$\Sigma_{1B}(\boldsymbol{k}, ip_m) = \Delta - \frac{i}{2\tau}\mathrm{sgn}(p_m), \tag{22}$$

where Δ and τ are real constants. Use this to find expressions for the retarded Green function $\overline{G^R}(\boldsymbol{k}, \omega)$ and for the spectral function $A(\boldsymbol{k}, \omega) = -(1/\pi)\mathrm{Im}\, \overline{G^R}(\boldsymbol{k}, \omega)$ (for real ω).

(d) Sketch the spectral function as a function of ω for fixed $\boldsymbol{k}$. Also sketch the spectral function in the absence of any impurity scattering, i.e. for just noninteracting electrons. Describe how the parameters Δ and τ are responsible for the differences between these two functions.

Formulas

Commutator relations:

$$\begin{aligned} [\hat{n}_\mu, a_\nu] &= -a_\nu \delta_{\mu\nu}, && (23) \\ [\hat{n}_\mu, a_\nu^\dagger] &= a_\nu^\dagger \delta_{\mu\nu}. && (24) \end{aligned}$$

Baker-Hausdorff theorem:

$$e^{-B} A e^{B} = \sum_{n=0}^{\infty} \frac{1}{n!} [A, B]_n, \tag{25}$$

where $[A, B]_n$ is defined recursively as

$$\begin{aligned} [A, B]_n &\equiv [[A, B]_{n-1}, B], \qquad (n = 1, 2, \ldots) && (26) \\ [A, B]_0 &\equiv A. && (27) \end{aligned}$$

Lattice sum:

$$\frac{1}{N} \sum_j e^{ijF(k-k')} = \begin{cases} 1 & \text{if } F(k-k') = 2\pi \times \text{ integer,} \\ 0 & \text{otherwise} \end{cases} \tag{28}$$

where $F(k)$ is a function of k that satisfies $NF(k) = 2\pi \times$ integer.

Trigonometric identities:

$$\begin{aligned} \cos 2x &= \cos^2 x - \sin^2 x, && (29) \\ \sin 2x &= 2 \sin x \cos x, && (30) \\ \cos^2 x &= \frac{1}{1 + \tan^2 x}. && (31) \end{aligned}$$

Dirac delta function identity:

$$\operatorname{Im} \frac{1}{x + i\eta} = -\pi \delta(x) \tag{32}$$

where $\eta = 0^+$.