NTNU

Department of Physics

Examination paper for
TFY4210 Quantum Theory of Many-Particle Systems

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The problems were developed by Even Thingstad and discussed with John Ove Fjærestad.

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This exam consists of 4 problems. Each problem has several subproblems. Problems typically have an introduction. Some times, context and some explanation is needed also between subproblems. This is indicated by starting the paragraph with a box (□). The last page of this exam contains some formulae that may be of use.

Good luck!

1: Quick questions

The questions in this problem should be answered very briefly. One sentence may be enough, but your answer should not be longer than roughly three sentences. Strive to make your answers concise, and focus on the most important points. Use equations if appropriate.

a) What is a single particle operator, and how do you obtain the single particle operator in second quantization, assuming you know what this operator looks like in first quantization?

b) Consider a system consisting of 2 identical bosons described by coordinates x_1, x_2 and interacting with 2 identical fermions described by coordinates y_1, y_2. What are the symmetry properties of the many-particle wave function describing this system?

c) What is the difference between a Mott insulator and a band insulator?

d) How is the generator of a continuous unitary symmetry related to Noethers theorem?

e) How do you obtain the Lehmann representation for a Greens function?

f) What is analytic continuation in the context of Greens functions?

g) What is the Bogoliubov approximation in the context of Bose-Einstein condensates?

h) What is the main idea behind the derviation of the Landau criterion of superfluidity?

2: Su-Schrieffer-Heeger model

The Su-Schrieffer-Heeger (SSH) model is a one-dimensional hopping model that was developed to describe conduction of electrons in polymer chains. It is known as one of the simplest models to exhibit so-called topological features. In this problem, we **consider the electrons to be spinless.**

Consider a one-dimensional lattice with L unit cells, and let each unit cell consist of two lattice sites. We consider hopping only between nearest neighbour lattice sites. The SSH model is characterized by different hopping amplitudes for hopping between lattice sites within the same (amplitude α) and in different (amplitude β) unit cells. The Hamiltonian can therefore be modelled as

$$H = -\alpha \sum_i \left(a_i^\dagger b_i + \text{h.c.} \right) - \beta \sum_i \left(b_i^\dagger a_{i+1} + \text{h.c.} \right), \tag{1}$$

where $\alpha, \beta > 0$ are two different real hopping amplitudes, and where a_i and b_i are annihilation operators for an electron at the two different lattice sites inside unit cell i. Let d be the distance between lattice sites, and let $a = 2d$ be the distance between unit cells.

We first consider periodic boundary conditions, i.e. $i + L = i$ and the sums running from $i = 1$ to $i = L$. Then, in subproblem (d), we switch to a chain with an edge. Then, the first sum in the Hamiltonian of Eq. (1) (amplitude α) still runs from $i = 1$ to $i = L$, while the second sum (amplitude β) runs from $i = 1$ to $i = L - 1$.

(a) Diagonalize the Hamiltonian and show that it can be brought to the form

$$H = \sum_k \epsilon_k (c_k^\dagger c_k - d_k^\dagger d_k), \tag{2}$$

where c_k and d_k are some new Fermion operators, and where

$$\epsilon_k = \sqrt{\alpha^2 + \beta^2 + 2\alpha\beta \cos ka}. \tag{3}$$

You do not have to give explicit expressions for the new operators c_k and d_k. The sum over k is over the reduced Brillouin zone $(-\pi/a, \pi/a)$.

(b) Sketch the single particle dispersion relation as function of the quasimomentum.

(c) Assume the system has $N = L$ (spinless) electrons, i.e. half filling with one electron per unit cell. For what values of α and β is the system a conductor at low temperature? When is it an insulator?

(d) The system is invariant under $\alpha \leftrightarrow \beta$. This is not the case when **we let the system have edges instead of using periodic boundary conditions** (see introduction to problem). Explain why and determine the energy eigenvalues in the two special cases $\alpha \neq 0,\ \beta = 0$ (case 1) and $\alpha = 0,\ \beta \neq 0$ (case 2). Compare with the bulk dispersion relation from subproblem (a). (Hint: It may be useful to make a figure.)

☐ An edge state is an energy eigenstate where an electron in this state is localized at the edge of the sample. The probability amplitude typically decays exponentially with the distance from the edge. For the Su-Schrieffer-Heeger model, edge states are only possible in one out of the two cases $\alpha > \beta$ and $\beta < \alpha$. These two cases are said to topologically inequivalent.

(e) Explain how one may demonstrate the presence of edge states choosing some appropriate finite system size and using numerical tools. You should include relevant equations and matrices in your answer. What properties do you expect the edge states to have based on subproblem (d).

3: Spin currents in the Heisenberg model

Consider the ferromagnetic Heisenberg model in a magnetic field on a qubic, d-dimensional lattice,

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i h_i^z(t) S_i^z. \tag{4}$$

Applying a static magnetic field gradient ∇h, one may induce a spin current j. To linear order,

$$\langle j \rangle = \sigma \nabla h, \tag{5}$$

where σ is the spin conductivity. The determination of this conductivity is very similar to what we did in the impurity scattering problem.

(a) Consider first a static, homogeneous magnetic field $h_i^z(t) = h$. Derive the excitation spectrum in linear spin wave theory and discuss the result in light of Goldstones theorem. You may use that the excitation spectrum of the ferromagnetic Heisenberg model is

$$\omega_k^{h=0} = 2JS \sum_{\delta} \left(1 - \cos \mathbf{k} \cdot \boldsymbol{\delta}\right), \tag{6}$$

where $\boldsymbol{\delta}$ are the nearest neighbour vectors in one direction, e.g. $\boldsymbol{\delta} \in \{\hat{x}, \hat{y}\}$ in $d = 2$.

□ We now return to the general case of a magnetic field that can be both time- and spatially dependent. The total magnetization $M = \sum_i S_i^z$ is a conserved quantity, and we must therefore have a continuity equation

$$\dot{S}_l^z + \sum_{\delta} \left(j_\delta(l) - j_\delta(l - \delta)\right) = 0, \tag{7}$$

where $j_\delta(l)$ is the spin current flowing from lattice site l to lattice site $l + \delta$.

(b) Use the Heisenberg equation of motion $i\partial_t A = [A, H]$ to identify the spin current. Express it in terms of the spin raising and lowering operators S_i^+ and S_i^-. Briefly discuss whether the obtained expression is reasonable.

(c) Express the total spin current $j_\delta = \sum_l j_\delta(l)$ in terms of the magnon creation and annihilation operators $a_k^\dagger$ and a_k. You may disregard terms that correspond to interaction between magnons. Check that $\langle j_\delta \rangle = 0$ when we set $h_i = 0$ for all i.

□ Using linear response theory, one may show that

$$\langle j_\delta(\mathbf{q}, \omega) \rangle = \chi(\mathbf{q}, \omega) h^z(\mathbf{q}, \omega), \tag{8}$$

with response function

$$\chi_\delta(\mathbf{q},\omega) = \frac{i}{N}\int_0^\infty dt\ e^{i\omega t}\langle[j_\delta(\mathbf{q},t), S^z(-\mathbf{q},0)]\rangle, \tag{9}$$

where the second argument of S^z is a time argument. The expectation value is with respect to the unperturbed Hamiltonian, i.e. without the magnetic field. The spatial and temporal Fourier transformations are given by

$$A(\mathbf{q}) = \frac{1}{\sqrt{N}}\sum_l e^{-i\mathbf{q}\cdot\mathbf{r}_l}A(l) \tag{10}$$

$$A(\omega) = \int_{-\infty}^{\infty} dt\ e^{i\omega t}A(t). \tag{11}$$

(d) How do you obtain the spin conductivity σ, assuming we have calculated $\chi(\mathbf{q},\omega)$? (Hint: Fourier transform equation (5).)

(e) The Kubo formula relates the electrical conductivity for the electrical current to the current-current response function. Explain how one may use the continuity equation to show that the current-spin response function χ of equation (9) can be written as a current-current response function, and with this how one may obtain the spin current analog of the Kubo formula. Do not try to perform the calculation, simply identify and describe the main steps. (Hint: $e^{i\omega t} = (1/i\omega)(d/dt)e^{i\omega t}$.)

4: Greens functions and impurity scattering

(a) The Matsubara Greens function of a time translational invariant system is defined as $\mathcal{G}(\nu,\nu',\tau) = -\langle T_\tau c_\nu(\tau)c^\dagger_{\nu'}(0)\rangle$, where we restrict the argument τ to the interval $-\beta < \tau \leq \beta$. Show that

$$\mathcal{G}(\nu,\nu',\tau+\beta) = \zeta\mathcal{G}(\nu,\nu',\tau) \tag{12}$$

with $\zeta = 1$ for bosons and $\zeta = -1$ for fermions.

□ The Matsubara Greens functions in the imaginary time and frequency domains are related through

$$\begin{aligned} \mathcal{G}(\nu,\nu';\tau) &= \frac{1}{\beta}\sum_{\omega_n} e^{-i\omega_n\tau}\mathcal{G}(\nu,\nu';i\omega_n) & (13)\\ \mathcal{G}(\nu,\nu';i\omega_n) &= \int_0^\beta e^{i\omega_n\tau}\mathcal{G}(\nu,\nu';\tau) & (14)\end{aligned}$$

(b) Determine the possible values of ω_n for fermions (case 1) and bosons (case 2).

□ We now consider the impurity scattering problem, as discussed in the lectures and lecture notes. We have developed Feynman diagrams and Feynman rules for the impurity averaged single particle Greens function in this problem. For a given diagram, we let n be the order of the diagram in the impurity potential, while m is the order in the impurity density n_{imp}.

(c) Draw all Feynman diagrams for the impurity averaged single particle Greens function up to order $n = 3$ in the impurity potential. Identify the irreducible diagrams. Write down the expressions for the irreducible diagrams at order $n = 3$. Do not try to evaluate the momentum sums.

(d) Assume we calculate the self energy Σ up to order $n = 3$ and use the Dyson equation to obtain the impurity averaged Greens function. This corresponds to summing up a given subset of all possible diagrams for the impurity averaged Greens function. Draw all inequivalent[1] diagrams that belong to this subset, are of order $n = 5$, and have $m = 3$ impurity crosses. Explain your reasoning.

[1]With inequivalent diagrams, we mean diagrams that do not correspond to the same expression.

Formulae

The meaning and domain of applicability for the formulae and symbols below is assumed to be known.

Spins:

$$S^{\pm} = S^x \pm iS^y \tag{15}$$

Spin commutation relations:

$$[S^\alpha, S^\beta] = i\sum_\gamma \epsilon_{\alpha\beta\gamma} S^\gamma, \quad [S^z, S^{\pm}] = \pm S^{\pm} \tag{16}$$

Holstein-Primakoff representation:

$$S_i^+ = \sqrt{2S - a_i^\dagger a_i}\; a_i\;, \quad S_i^- = a_i^\dagger \sqrt{2S - a_i^\dagger a_i}\;, \quad S_i^z = S - a_i^\dagger a_i \tag{17}$$

Lattice fourier transform:

$$d_i = \frac{1}{\sqrt{N}} \sum_q e^{i\mathbf{q}\cdot\mathbf{r}_i} d_q \tag{18}$$

Lattice sum:

$$\frac{1}{N}\sum_i e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}_i} = \delta_{kq} \tag{19}$$

Time ordering:

$$T_\tau \left\{A(\tau)B(\tau')\right\} = \left\{ \begin{array}{rl} A(\tau)B(\tau'), & \tau' < \tau \\ \zeta B(\tau')A(\tau), & \tau < \tau' \end{array} \right\} \tag{20}$$

Kubo formula:

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) = \frac{i}{\omega}\left[\Pi^R_{\alpha\beta}(\mathbf{q},\omega) + \frac{ne^2}{m}\delta_{\alpha\beta}\right] \tag{21}$$

with current-current response function defined as the Fourier transform of

$$\Pi^R_{\alpha\beta}(\mathbf{r}-\mathbf{r}', t-t') = -i\theta(t-t')\langle[j^P_\alpha(\mathbf{r},t), j^P_\beta(\mathbf{r}',t')]\rangle \tag{22}$$