NTNU
Norwegian University of
Science and Technology

Department of Physics

Examination paper for
# TFY4210/FY8302 Quantum theory of solids

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**Examination time (from–to):** 15:00–19:00

**Permitted examination support material:** B: K. Rottman Mathematical Formulas or equivalent. Approved calculator.

**Other information:**

Maximum number of points is 100.
If you wish to submit a blank test/withdraw from the exam, go to the menu and click “Submit blank”. This cannot be undone, even if the test is still open.

Technical support during examination: Orakel support service. Phone: 73591600

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| **Informasjon om trykking av eksamensoppgave** | |
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| **Originalen er:** | |
| **1-sidig** ☐ | **2-sidig** ☒ |
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| **skal ha flervalgskjema** ☒ | |

Date Signature

**Problem 1** (Points: 5+10+10+10+10+5=50)

The fermionic Hubbard model with repulsive interactions on a lattice with $N$ sites, is given by the following Hamiltonian

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

with $U > 0$. Here, $\langle i, j\rangle$ means that the lattice sites $i$ and and $j$ are nearest neighbors, and the $(c^\dagger_{i\sigma}, c_{i\sigma})$-operators are fermion creation- and destruction operators creating/destroying a fermion at lattice site $i$ with spin $\sigma$. They satisfy anticommutation relations $c^\dagger_{i\alpha} c_{j\beta} + c_{j\beta} c^\dagger_{i\alpha} = \delta_{ij}\delta_{\alpha\beta}$, with $\delta$ being Kronecker deltas. Furthermore, $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. $\mu$ is a chemical potential regulating the average number of particles in the system.

**a)** Explain what the various terms in the Hamiltonian represent, paying special attention to the spin-structure of the third term.

**b)** An antiferromagnetic insulator on a $2D$ square lattice may be modelled by a Hamiltonian with nearest neighbor exchange interactions

$$H_{\text{AFMI}} = - \sum_{\langle i,j \rangle,\alpha} J_\alpha \, \mathbf{S}_{i\alpha} \mathbf{S}_{j\alpha}$$

with $J_\alpha < 0$ . The operators $\mathbf{S}_i$ are spin-operators, and $\alpha \in (x, y, z)$ denotes the cartesian component of the spins. We will consider the case $J_z = J$ and $J_x = J_y = \Delta J$, with $\Delta \leq 1$. Consider first $\Delta = 1$ and explain briefly how and under what conditions such a spin-model could be derived from the Hubbard model (no detailed calculations are necessary).

**c)** Using a Holstein-Primakoff transformation for this case and calculating to quadratic order in bosonic magnon-operators $a_i$ and $b_i$ (and their adjoints), the Hamiltonian may be written on the form (need not be shown!)

$$H = E_0^c - 2JS \sum_{\langle i,j \rangle} \left[ a_i^\dagger a_i + b_i^\dagger b_i + \Delta(a_i b_j + b_i^\dagger a_j^\dagger) \right]$$

Introduce Fourier-transformed operators and show that the Hamiltonian may be brought onto the following form

$$H = E_0^c - 2JS \sum_q \left[ z(a_q^\dagger a_q + b_q^\dagger b_q) + \Delta\gamma(q)(a_q b_q + b_q^\dagger a_q^\dagger) \right]$$

where $z$ is the number of nearest neighbors, and give an explicit expression for $\gamma(q)$.

**d)** For $\Delta = 1$, this Hamiltonian may be diagonalized by the Bogoliubov-transformation

$$\begin{aligned} a_q &= u_q A_q - v_q B_q^\dagger \\ b_q^\dagger &= u_q B_q^\dagger - v_q A_q \end{aligned}$$

with $u_q^2 - v_q^2 = 1$. Explicit expressions for $u_q, v_q$ will not be needed here. Then the Hamiltonian takes the form (need not be shown!)

$$\begin{aligned} H &= E_0^{\rm qm} + \sum_q \omega_q \left[ A_q^\dagger A_q + B_q^\dagger B_q \right] \\ \omega_q &= 2|J|S\sqrt{z^2 - \gamma^2(q)} \end{aligned}$$

Use this to compute $\omega_q$ for $\Delta < 1$, and sketch $\omega_q$ as a function of $q$ for small $q$.

**e)** Next, we add a uniform magnetic field to the problem $\mathbf{h} = h\hat{z}$ along the $z$-axis. This adds a Zeeman-term $-h\sum_i S_{iz}$ to the Hamiltonian. To quadratic order in the magnon-operators $a$ and $b$, this term takes the form $h\sum_q \left[ a_q^\dagger a_q - b_q^\dagger b_q \right]$. Show that the Hamiltonian now becomes

$$H = E_0^{\rm qm} + \sum_q \left[ \omega_q^A A_q^\dagger A_q + \omega_q^B B_q^\dagger B_q \right]$$

and give expressions for $\omega_q^A$ and $\omega_q^B$.

**f)** For large enough magnetic field $h$, $\omega_q^A$ or $\omega_q^B$ will become negative. Find the lowest value of $h$ where this happens, and give a physical interpretation of the sign-change in $\omega_q^A$ or $\omega_q^B$.

Fourier-transformed magnon-operators

$$\begin{aligned} a_q &= \frac{1}{\sqrt{N}} \sum_i a_i \, e^{i\mathbf{q}\cdot\mathbf{r}} \\ b_q &= \frac{1}{\sqrt{N}} \sum_i b_i \, e^{-i\mathbf{q}\cdot\mathbf{r}} \end{aligned}$$

Boson commutation relation

$$a_\lambda a_{\lambda'}^\dagger - a_{\lambda'}^\dagger a_\lambda = \delta_{\lambda\lambda'}$$

**Problem 2** (Points: 5+5+10+10+10+10=50)

The fermionic Hubbard model with attractive interactions on a lattice with $N$ sites, is defined by the Hamiltonian (in the same notation as in **Problem 1**)

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} - |U| \sum_i n_{i\uparrow} n_{i\downarrow}$$

**a)** Give the definition of a Fermi liquid.

**b)** Show that the Hamiltonian above may be written on the form

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} - |U| \sum_i P^\dagger_i P_i$$

and thus determine an expression for $P_i$.

**c)** We apply a mean-field approximation to this Hamiltonian by setting $P_i = b_i + \delta b_i$ with $b_i \equiv \langle P_i \rangle$, inserting this into H and neglecting terms quadratic in $\delta b_i$. Show that the Hamiltonian then takes the form

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} + |U| \sum_i b^\dagger_i b_i - |U| \sum_i \left[ P^\dagger_i b_i + P_i b^\dagger_i \right]$$

**d)** We now use the Ansatz $b_i = b^\dagger_i = b$ independent of $i$. Introduce Fourier-transformed operators

$$\begin{aligned} c_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_k c_{k\sigma} e^{i\mathbf{k}\cdot\mathbf{r}_i} \\ c^\dagger_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_k c^\dagger_{k\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}_i} \end{aligned}$$

and show that the Hamiltonian may be written on the form

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{N\Delta^2}{|U|} - \Delta \sum_k \left[ c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right]$$

and give expressions for $\varepsilon_k$ and $\Delta$.

**e)** We next introduce a Bogoliubov transformation to a new set of fermions $(\gamma^\dagger_k, \gamma_k)$ and $(\eta^\dagger_k, \eta_k)$.

$$\begin{aligned} c_{k\uparrow} &= u_k \eta_k - v_k \gamma_k \\ c^\dagger_{-k\downarrow} &= u_k \gamma_k + v_k \eta_k \end{aligned}$$

with $u_k^2 + v_k^2 = 1$. The Hamiltonian may then be written on the form

$$H = \sum_k \varepsilon_k + \frac{N\Delta^2}{|U|} + \sum_k E_k \left[\gamma_k^\dagger \gamma_k - \eta_k^\dagger \eta_k\right]$$

with $E_k = \sqrt{\varepsilon_k^2 + \Delta^2}$. Compute the momentum distribution $n_k = \sum_\sigma \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle$ for this system and decide, based on this computation, whether or not the system is a Fermi liquid when $\Delta \neq 0$. Here, you may use that $u_k^2 - v_k^2 = -\varepsilon_k / E_k$.

**f)** What sort of system does this Hamiltonian describe?

Some formulas and relations that may be helpful. It is assumed that the candidate understands the symbols that are being used.

For a non-interacting fermion system with Hamiltonian $H = \sum_\lambda (\varepsilon_\lambda - \mu) c_\lambda^\dagger c_\lambda$, the free energy $F$ is given by

$$F = -\frac{1}{\beta} \sum_\lambda \ln\left(1 + e^{-\beta(\varepsilon_\lambda - \mu)}\right)$$

For a non-interacting boson system with Hamiltonian $H = \sum_\lambda (\varepsilon_\lambda - \mu) c_\lambda^\dagger c_\lambda$, the free energy $F$ is given by

$$F = \frac{1}{\beta} \sum_\lambda \ln\left(1 - e^{-\beta(\varepsilon_\lambda - \mu)}\right)$$

Fermi-Dirac distribution

$$n_\lambda = \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} + 1}$$

Bose distribution

$$n_\lambda = \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} - 1}$$

Riemann $\zeta$-function

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$$

$\Gamma$-function

$$\Gamma(z) = \int_0^\infty dt \ \ t^{z-1} \ e^{-t}$$

$$\sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} = N \delta_{\mathbf{q},0}$$

Kronecker-$\delta$

$$\begin{aligned} \delta_{\alpha\beta} &= 1; \alpha = \beta \\ \delta_{\alpha\beta} &= 0; \alpha \neq \beta \end{aligned}$$

If $ad - bc = 1$, then

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$