



Norwegian University of
Science and Technology

Department of Physics

Examination paper for **TFY4210/FY8302 Quantum theory of solids**

Academic contact during examination: Asle Sudbø

Phone: 40485727

Examination date: May 27 2024

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

Language: English

Number of pages: 5

Number of pages enclosed: 0

Checked by:

Informasjon om trykking av eksamensoppgave

Originalen er:

1-sidig ☐ 2-sidig ☒

sort/hvit ☒ farger ☐

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

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

with $U > 0$. Here, $\langle i, j \rangle$ means that the lattice sites i and j are nearest neighbors, and the $(c_{i\sigma}^\dagger, c_{i\sigma})$ -operators are fermion creation- and destruction operators creating/destroying a fermion at lattice site i with spin σ . They satisfy anticommutation relations $c_{i\alpha}^\dagger c_{j\beta} + c_{j\beta} c_{i\alpha}^\dagger = \delta_{ij} \delta_{\alpha\beta}$, with δ being Kronecker deltas. Furthermore, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. μ 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!)

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

Use this to compute ω_q for $\Delta < 1$, and sketch ω_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 $h \sum_q [a_q^\dagger a_q - b_q^\dagger b_q]$. Show that the Hamiltonian now becomes

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

and give expressions for ω_q^A and ω_q^B .

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

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

a) Give the definition of a Fermi liquid.

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

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

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 δb_i . Show that the Hamiltonian then takes the form

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i, \sigma} n_{i, \sigma} + |U| \sum_i b_i^\dagger b_i - |U| \sum_i [P_i^\dagger b_i + P_i b_i^\dagger]$$

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

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

and show that the Hamiltonian may be written on the form

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

and give expressions for ε_k and Δ .

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

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

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

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

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 ζ -function

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

Γ -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- δ

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

If $ad - bc = 1$, then

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