Übungen zur Theorie der Kondensierten Materie II SS 16

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Blatt 4
Besprechung 20.05.2016

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1. Thermodynamics from the single-particle Green's function (6 Points)

In this exercise we will show that all thermodynamic properties of an in general interacting system are determined by the imaginary part of its single-particle Green's function. To this end, consider the interacting Hamiltonian

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \frac{1}{2} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}\sigma\sigma'} v_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{q}) c^\dagger_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'} c_{\boldsymbol{k}-\boldsymbol{q}\sigma}, \tag{1}$$

where $c^\dagger_{\boldsymbol{k}\sigma}$ and $c_{\boldsymbol{k}\sigma}$ denote fermionic creation and annihilation operators (σ is the spin index).

(a) Express the energy $E := \langle H \rangle$ at arbitrary temperature $T = \beta^{-1}$ in terms of retarded and advanced 2-fermion and 4-fermion Green's functions of the schematic form $\langle [c, c^\dagger]_+ \rangle$ and $\langle [c^\dagger c c, c^\dagger]_+ \rangle$ where $[\cdot, \cdot]_+$ denotes the anticommutator. (1 Pt.)

(b) The explicit dependence on 4-fermion Green's functions can be eliminated by taking advantage of the equations of motion of the Green's functions. Show that one can write

$$E(T) = \frac{1}{4\pi} \sum_{\boldsymbol{k}\sigma} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{\omega + \epsilon_{\boldsymbol{k}}}{e^{\beta\omega} + 1} \mathcal{A}(\boldsymbol{k}, \omega), \qquad \mathcal{A}(\boldsymbol{k}, \omega) = -2\mathrm{Im}\left(G^R_{c_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}\sigma}}(\omega) \right) \tag{2}$$

with $G^R_{c_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}\sigma}}(\omega)$ representing the retarded single-particle Green's function as defined in the lecture. (3 Pts.)

(c) Convince yourself that Eq. (2) reproduces the correct result in the noninteracting limit $v_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{q}) = 0$. (1 Pt.)

(d) Why does Eq. (2) determine all thermodynamic properties of the system? (1 Pt.)

2. Jordan-Wigner transformation (12 Points)

In the following we will explore how spin-models can be expressed in terms of fermionic creation and annihilation operators. We will be investigating the anisotropic 1D Heisenberg magnet in an external magnetic field h which is defined by the Hamiltonian

$$H = -\sum_{j=1}^{N-1} \left(J_x S^x_j S^x_{j+1} + J_y S^y_j S^y_{j+1} + J_z S^z_j S^z_{j+1} \right) + h \sum_{j=1}^{N} S^z_j, \tag{3}$$

where S^a_j, $a = x, y, z$, are spin-1/2 operators satisfying the usual commutation relations

$$[S^a_j, S^b_{j'}]_- = i\delta_{j,j'} \epsilon_{abc} S^c_j. \tag{4}$$

(a) For simplicity, let us first investigate a single site and, hence, drop the index j for the moment. Show that $S^+ := S^x + iS^y$, $S^- := S^x - iS^y$ and S^z satisfy the same commutation relations as $c^\dagger$, c and $c^\dagger c - 1/2$ where c and $c^\dagger$ are fermionic annihilation and creation operators. (1 Pt.)

(b) With this observation in mind, it is natural to introduce fermionic operators c_j for every site $j = 1, 2, \dots N$ of the Heisenberg chain in Eq. (3) and assign $S_j^+ = c_j^\dagger$, $S_j^- = c_j$ and $S_z = n_j - 1/2$ with $n_j = c_j^\dagger c_j$. However, the problem is that the fermionic operators at different sites anticommute while spatially distinct spin operators commute. This can be reconciled by adding "string operators", $\exp(\pm i\pi \sum_{j'<j} n_{j'})$, as suggested by Jordan and Wigner:

$$S_j^+ = c_j^\dagger\, e^{-i\pi \sum_{j'<j} n_{j'}}, \qquad S_j^- = c_j\, e^{i\pi \sum_{j'<j} n_{j'}}, \qquad S_z = n_j - 1/2. \tag{5}$$

Show that Eq. (5) yields indeed the correct behavior. (3 Pts.)

(c) Insert this transformation into the Heisenberg chain model (3) and show that it can be brought into the form

$$\begin{aligned} H = &- \sum_{j=1}^{N-1} \left[t\, c_j^\dagger c_{j+1} + \Delta\, c_j c_{j+1} + \text{H.c.} \right] - \mu \sum_{j=1}^{N} \left(n_j - \frac{1}{2} \right) \\ &+ U \sum_{j=1}^{N-1} \left(n_j - \frac{1}{2} \right) \left(n_{j+1} - \frac{1}{2} \right). \end{aligned} \tag{6}$$

Express the parameters t, Δ, μ and U in terms of the parameters of the original magnetic model. Eq. (6) represents a system of spinless fermions hopping (with amplitude t) on a 1D lattice with chemical potential μ and superconducting nearest-neighbor pairing Δ and additional nearest-neighbor interaction U. (4 Pts.)

(d) In the following we will focus on $U = 0$. What is the corresponding limit in Eq. (3)? In this case, Eq. (6) assumes the form of a noninteracting model[1] and can, hence, be readily diagonalized which also reveals the spectrum of the associated magnetic model in Eq. (3).

To diagonalize Eq. (6), first rewrite it in terms of the Fourier-transformed operators, $c_j \to c_k$, $-\pi/a < k \le \pi/a$, assuming periodic boundary conditions (a denotes the lattice constant and k is the 1D crystal momentum). As a second step, perform a Bogoliubov transformation, i.e., introduce new operators a_k and $a_k^\dagger$ as superpositions of electrons and holes,

$$\begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix} = U_k \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}. \tag{7}$$

The 2×2 matrix U_k is chosen such that the Hamiltonian becomes diagonal in the new operators. Calculate the eigenvalues that determine the spectrum of the system. (3 Pts.)

(e) Plot the spectrum for the special case of $\mu = 0$. Under which conditions does the gap close? Do you understand this behavior in terms of the original magnetic model in Eq. (3)? (1 Pt.)

[1] This model is known as the *Kitaev chain model*.