Quantum matter (Block 4, 2015/16)

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Exam (70 points)
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- Use a separate sheet for every exercise.
- Write your name on each sheet, on the first sheet also your student ID.
- Write clearly, unreadable work cannot be corrected.
- Except in exercise 1, give the motivation, explanation and calculations.
- Do not spend a large amount of time on finding (small) calculation errors. If you suspect you have made such an error, point it out in words.

1. Conceptual questions (3 points each = 15 points)

Answer the questions below by a few sentences, a sketch, a formula or the like.

(a) Sketch a one-dimensional lattice with lattice constant a and two-site basis with basis vectors 0 and $a/4$.

(b) State the Bloch theorem.

(c) Briefly describe the Hartree and Hartree–Fock equations, ie, what are they used for and what is the difference between them (you do not have to write them down).

(d) What is the difference between ferromagnetic and antiferromagnetic ordering? Describe in words or use a sketch.

(e) What is a Cooper pair? What is its electrical charge and quantum statistics?

2. Phonons (3+9+7+5+4 points = 28 points)

Consider the lattice vibrations of a one-dimensional lattice described by the quantum Hamiltonian

$$H = \sum_k \hbar\omega_k \left(\underline{a_k^\dagger a_k} + \frac{1}{2} \right), \tag{1}$$

where k labels the one-dimensional momentum, $a_k^\dagger$ and a_k are operators that create and annihilate phonon modes with momentum k and ω_k denotes the dispersion relation of the phonons, which is assumed to bounded from above and below by $0 < \omega_1 \le \omega_k \le \omega_2$.

(a) First consider an individual momentum k. What are the energy eigenvalues for this mode? What is the ground-state energy?

(b) Now consider the whole lattice, ie, the full Hamiltonian (1). Determine the energy eigenvalues, the canonical partition function, the free energy F and the entropy $S = -\partial F/\partial T$. Show that the internal energy U is given by

$$U = F + TS = \sum_k \frac{\hbar\omega_k}{2} + \sum_k \frac{\hbar\omega_k}{e^{\beta\hbar\omega_k} - 1}, \tag{2}$$

where $\beta = 1/(k_B T)$. Give a physical interpretation of the two terms in (2).

(c) Determine the high-temperature expansion for $C = \partial U/\partial T$ including up to $\mathcal{O}(T^{-2})$. For which temperatures is the high-temperature expansion applicable? $\hbar\omega << k_B T$

(d) Similarly obtain an expansion of C for low temperatures up to leading order. For which temperatures is this expansion valid?

(e) Consider the additional perturbation $V = g\sum_{p\neq q}(a_p^\dagger a_q + a_q^\dagger a_p)$. Determine the change in the ground-state energy to linear order in g. Justify your answer.

3. Two-dimensional electron gas (3+4+3 points = 10 points)

Consider a two-dimensional electron gas which possesses the band structure

$$E(\vec{k}) = E(k_x, k_y) = t_x + t_y - t_x\cos(k_x a) - t_y\cos(k_y a), \tag{3}$$

with $t_x, t_y > 0$ and a denoting the lattice constant.

(a) Expand the energy band (3) around $\vec{k} = \vec{0}$ up to leading non-trivial order.

(b) Now consider the special case $t_x = t_y = 2/a^2$. Calculate the density of states $D(\epsilon)$.

(c) Finally consider the effect of a perpendicular magnetic field $\vec{B} = B\vec{e}_z$. Describe qualitatively how the energy spectrum changes.

4. Ferromagnetism (3+4+4+3+3 points = 17 points)

Consider a ferromagnetic Ising model on a two-dimensional triangular lattice, ie, the Hamiltonian

$$H = -J\sum_{\langle ij\rangle} \sigma_i\sigma_j, \tag{4}$$

where $J > 0$, $\sigma_i = \pm 1$ denotes the Ising spin at site i and the sum is over all pairs of nearest-neighbours on the lattice. Note that there is no external magnetic field.

(a) Sketch the two-dimensional triangular lattice. Determine the coordination number z, ie, the number of nearest neighbours for each site.

(b) Introduce the average magnetisation per lattice site $\bar{\sigma} = \langle\sigma_i\rangle$. Write the Ising spins as $\sigma_i = \bar{\sigma} + \delta\sigma_i$ and expand the Hamiltonian (4) to leading order in the deviation $\delta\sigma_i$. Rewrite the resulting Hamiltonian in terms of the original Ising spins.

(c) Argue that the result you obtained in (b) can be interpreted as a collection of Ising spins in a magnetic field $B_{MF} = 2Jz\bar{\sigma}$. Derive a self-consistency condition for the average magnetisation $\bar{\sigma}$ from this.

Hint: The average magnetisation of an Ising spin in a magnetic field B is given by $\langle\sigma\rangle = \tanh\frac{B}{k_B T}$, which can be used without derivation.

(d) Argue that at temperatures below a critical temperature T_c the system will possess ferromagnetic order. Determine the value of the critical temperature from the self-consistency equation derived in (d).

(e) Imagine that the lattice is restricted to the positive half plane $x > 0$, ie, there is a boundary at $x = 0$. Will the average magnetisation at the boundary be larger or smaller than the bulk value $\bar{\sigma} = \lim_{x\to\infty}\bar{\sigma}(x)$? Justify your answer.