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Methods of Statistical Physics
NFPL088, Tue 17:20, F155 (KFM)

Problem Sheet 6

1 Two-spin correlations in the mean-field approximation (MFA)
In the MFA to the Ising model, calculate $\langle s_n s_m \rangle_0$ (directly perform the phase space average).

2 Model of an atom in a radiation field
We consider an atom which can be excited, either thermally or by the external field. For simplicity, we focus on the ground state and the first excited state only, separated by the excitation energy 2Δ. Naturally, it is convenient to use Pauli matrices $\hat{\sigma}_i$, acting on the two atomic states. The Hamiltonian of the atom reads $\hat{H}_\mathrm{A} = \Delta\hat{\sigma}_z$. The Hamiltonian of the field, capable at inducing transitions, is $\hat{H}_\mathrm{F} = \varepsilon\hat{\sigma}_x$, where ε is proportional to the field intensity.
Study the linear response to $\hat{H}_\mathrm{F}$ in the following steps:

(a) To familiarize yourself with the model, give the spectrum of $\hat{H}_\mathrm{A}$, the energetic gap and the probability of finding the atom in an excited state at a given temperature.

(b) Compute the susceptibility $\kappa_{AB}(T)$ with $\hat{A} = -\hat{B} = \hat{\sigma}_x$ following the definition given in the lecture [Eq. (41) therein]. You can think that the operator σ_x measures the dipole moment.

(c) For $\Delta \neq 0$, evaluate the limits $T = 0$ and ∞ of the susceptibility. Then, evaluate the limit $\Delta = 0$ for any T. If the ground state is degenerate, the zero-temperature susceptibility should diverge.

(d) Compute the susceptibility $\kappa_{AB}(T)$ with $\hat{A} = \hat{\sigma}_x, \hat{B} = \hat{\sigma}_z$. Discuss the result: what does it imply?

Further reading: Quantum optics often employs the so called Jaynes–Cummings model, where $\hat{H}_\mathrm{A}$ is used to model an atom. The field is quantized, unlike in this problem, where it is classical and static.

3 Curie-like temperature behavior
Using the definition of the susceptibility [Eq. (41) from the lecture] show, that the susceptibility of a non-degenerate system is finite at low temperatures, and diverges if the system has a ground-state degeneracy. Discuss the examples: magnetic susceptibility of a Fermi gas and of a free magnetic moment.

4 **Two-spin molecule**

Consider Ising Hamiltonian for a two-atomic molecule (with spins 1/2 - valued $\{+1, -1\}$ on each atom) in an external field B (no interaction outside the molecule).

- **(a)** Find the partition sum of this system.
- **(b)** Find the free energy and the heat capacity c_V of this system assuming $B = 0$.
- **(c)** Decide whether a phase transition is possible, find the temperature of the maximum of c_V.

5 **One-dimensional Ising chain**

Consider Ising Hamiltonian for a 1D chain of N equivalent spins with only nearest neighbor interaction, no external field, exact (no MFA).

- **(a)** Calculate the partition sum (Hint: prove the recurrence relation $Z_{N+1} = 2Z_N \cosh(J/kT)$). Give the free energy, heat capacity c_V, mean spin value at site n; correlation between different sites m, n.
- **(b)** Decide whether a phase transition is possible, find the temperature of the maximum of c_V, compare to phase transition temperature in MFA.

6 **Specific heat of a two-level system**

Consider a solid, which has N atoms, and each of them has two energy levels, with eigenenergies Δ and $-\Delta$ as in the Problem **2** (atom in a field, but with $\varepsilon = 0$).

- **(a)** Calculate the mean energy, and the heat capacity $c_V = \mathrm{d}E/\mathrm{d}T$. Hint: Didn't we calculate the energy in Sheet 1, Problem **2** already?
- **(b)** What is the behavior of the heat capacity for $kT \gg \Delta$ and $kT \ll \Delta$?
- **(c)** Sketch a plot of $c_V(T)$ based on these two limits (no computer plot!).
- **(d)** Discussion: Read about the Schottky anomaly and name some materials, where it is observed.

7 **Specific heat of a glass material**

Consider a solid from the Problem **6** with a modification. The solid is disordered (*e.g.* a glass), so that the values of Δ are random. We assume they are uniformly distributed in the interval $0 \leq \Delta \leq \Delta_0$. Obviously, $2\Delta_0$ is a maximal excitation gap of the atom.

- **(a)** Use the expression for the inner energy from the Problem **6** and perform an average over Δ. Focus on the limit of low temperatures, when $\beta\Delta \gg 1$. Hint: Approximate $\tanh(\beta\Delta) \approx 1 - 2e^{-\beta\Delta}$.
- **(b)** Calculate the heat capacity of the glass and show, that it is linear in T at low temperatures, apart from terms which are exponentially small. Compare this behavior to other paradigmatic models of solids.