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Methods of Statistical Physics
NFPL088, Tue 11:30, F052 (KFKL)

Problem Sheet 7

1 Quantum correction to the specific heat of an ideal atomic gas

Start with the expression for the internal energy of ideal fermions (bosons), $U = \sum_k \varepsilon_k / (e^{\beta(\varepsilon_k - \mu)} \pm 1)$.

(a) Perform the continuum limit and prove the exact relation $U = -\frac{3}{2}\Phi$ (see the expression for Φ from the lecture).

(b) Calculate the specific heat ($c_V = (\partial U/\partial T)_{V,N}$) in the limit of high temperatures using the fugacity expansion; give the quantum correction, which has the lowest nonzero order of $\hbar$.

(c) Discuss your result: what do you learn from it?

Remark: Alternative calculation proceeds via the entropy $S = -(\partial\Phi/\partial T)_{\mu,V}$ and $c_V = T\,(\partial S/\partial T)$. Note, however, that the chemical potential must be fixed when these derivatives are calculated.

2 Variance of particles in the BEC

The number of particles in the condensate is $\langle n_{\mathbf{p}=0}\rangle$. Calculate the variance of the number of particles in the condensate, $(\Delta n_{\mathbf{p}=0})^2 = \left\langle (n_{\mathbf{p}=0} - \langle n_{\mathbf{p}=0}\rangle)^2 \right\rangle = \langle n^2_{\mathbf{p}=0}\rangle - \langle n_{\mathbf{p}=0}\rangle^2$ for a BEC under the critical temperature!

(a) Look into the Problem 1, Sheet 3 (Fermi-Dirac). Use the same technique to calculate the variance of the number of particles in a state $\mathbf{p}$, $n_{\mathbf{p}}$. Prove the thermodynamic relation

$$(\Delta n_{\mathbf{p}=0})^2 = \beta^{-1} \left(\frac{\partial \langle n_{\mathbf{p}=0}\rangle}{\partial \mu} \right)_{T,V}. \tag{1}$$

(b) Express the ground-state occupation through the fugacity z,

$$\langle n_{\mathbf{p}=0}\rangle = \frac{z}{1-z}. \tag{2}$$

Use this expression and Eq. (1) to show, that $(\Delta n_{\mathbf{p}=0})^2 = \langle N\rangle + \langle N\rangle^2$. Discuss the result.

3 Bosons that do not condense

Show, that bosons with a quadratic dispersion, moving in two dimensions, do not undergo BEC. Use the continuum expression for the particle number, $N = \int \mathrm{d}\epsilon\, N(\epsilon)/(e^{\beta\epsilon}/z - 1)$. Unlike in the 3D case, the density of states in 2D is constant; for a square of length L it is easy to get $N(\epsilon) = L^2/\delta E$ for $\epsilon > 0$ and zero otherwise (The physical meaning of the constant δE is the average spacing between eigenenergies per unit area.). Now the integral for N can be calculated exactly. For fixed N and L^2, you obtain a relationship between the fugacity and the temperature, allowing you to express the temperature dependence of the chemical potential. Inspect the low- and high-T limits and sketch a graph of $\mu(T)$ at a fixed density N/L^2 (no computer!). Discuss the result.

4 **Statistical mechanics of neutron beams**

Suppose that a neutron beam is prepared in the following way: half of the neutrons have their spin aligned with the (positive) x-axis and the other half along the z-axis.

(a) Define the appropriate density operator $\hat{\rho}$ for the beam. Verify that $\hat{\rho}$ satisfies the three basic properties: hermiticity, positivity and unitarity. Does the beam represent a pure state?

(b) Calculate the average spin vector $\langle \mathbf{s} \rangle = \frac{1}{2}\hbar\langle \hat{\boldsymbol{\sigma}} \rangle$ and the corresponding variances $\langle \hat{s}_i^2 \rangle - \langle s_i \rangle^2$, $i = x, y, z$. Discuss your results.

(c) Calculate the eigenvalues P_+, P_- of the density operator and the so called degree of polarization defined through

$$\Pi := \frac{P_+ - P_-}{P_+ + P_-}. \tag{3}$$

How do you interpret your result?

5 **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.

6 **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.

7 **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 Sheet 6, Problem **2** (atom in a field).

(a) Calculate the mean energy, and the heat capacity $c_V = \mathrm{d}E/\mathrm{d}T$. Hint: you can use the results of the Sheet 3, Problem **2** **(a)**

(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.

8 Specific heat of a glass material

Consider a solid from the Problem **7** 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 **3** 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.