11. Thermodynamic quantities of paramagnets

We consider a system of N non-interacting spin-$1/2$ particles which are in a static magnetic field $\vec{B} = B_0\vec{e}_z$. The Hamiltonian operator is then given by

$$\hat{H} = -B_0\hat{M}^z = \mu_B B_0 \sum_{j=1}^{N} \hat{\sigma}^z \tag{1}$$

where $\hat{M}^z$ is the magnetisation operator in z-direction and μ_B is the Bohr magneton. Furthermore, let $\hat{\rho}_N$ be the density matrix of the entire system of N spins.

(a) Show that at equilibrium and in a homogeneous system the following statement is true

$$U = \langle \hat{H} \rangle = N\mathrm{Tr}\{\hat{\rho}_1\hat{H}_1\} \tag{2}$$

with $\hat{H}_1 = \mu_B B_0 \hat{\sigma}_1^z$ and $\hat{\rho}_1 = \mathrm{Tr}_{N-1}\{\hat{\rho}_N\}$, and Tr being the trace over the $N-1$ other spins.

(1 point)

(b) Assume a Boltzmann-Gibbs distribution of spins. The density matrix of a single spin is then given by

$$\hat{\rho}_1 = \frac{e^{\beta\epsilon_0}|+\rangle\langle+| + e^{-\beta\epsilon_0}|-\rangle\langle-|}{\mathcal{Z}_1}, \tag{3}$$

with the normalisation constant $\mathcal{Z}_1 = e^{\beta\epsilon_0} + e^{-\beta\epsilon}$ and $\epsilon_0 = \mu_B B_0$. Show that the total energy U is given by

$$U = -n\mu_B B_0 \frac{e^{2\beta\mu_B B} - 1}{e^{2\beta\mu_B B} + 1} \tag{4}$$

with $\beta = 1/k_B T$ by explicitly determining the expected value of the Hamiltonian $\langle \hat{H} \rangle$. Determine its limits at $T \to 0$ and $T \ll \mu/BB_0/k_B$. Show further that the expectation value of the magnetisation in z-direction is given by

$$\langle \hat{M}^z \rangle = N\mu_B \tanh\left(\frac{\mu_B B_0}{k_B T}\right) \tag{5}$$

(1 point)

(c) Use the explicit form of the probabilities $p_\pm = e^{\mp\beta\epsilon_0}/\mathcal{Z}_1$ to derive the following formula for the entropy S of the system.

$$S = -Nk_B[p_+ \ln p_+ + p_- \ln p_-]. \tag{6}$$

(1 point)

(d) Use the formulas of entropy S or total energy U to derive a formula for the specific heat C and show that

$$C = \left.\frac{\partial U}{\partial T}\right|_{B_0} = T\left.\frac{\partial S}{\partial T}\right|_{B_0} = k_B N(\beta\mu_B B_0)^2 \mathrm{sech}^2(\beta\mu_B B_0). \tag{7}$$

How does the specific heat behave for temperatures in the limit cases $T \ll \mu_B B_0/k_B$ and $T \gg \mu_B B_0/k_B$. Show that the specific heat $C(T)$ reaches its maximum approximately at the Curie temperature $\theta = \mu_B B_0/k_B$.
Hint: You may use that the equation $x \tanh x = 1$ für $x > 0$ has only one solution at $x \approx 1.2$.

(1 point)

12. Classical approximation of the quantum gas

A gas of quantum particles of mass m at a density n and temperature T can be approximated by a classical gas if the mean distance d between the particles, defined as

$$d = \frac{1}{n^{1/3}}, \tag{8}$$

is much larger than the thermal de Broglie wavelength, namely $d \gg \lambda_{\mathrm{th}}$. For a gas of $N = 10^{19}$ particles confined in a volume $V = 1\ \mathrm{cm}^3$, determine the corresponding interparticle distance d and compare it with the de Broglie wavelength of a hydrogen molecules at $T \approx 290$ K: $\lambda_{\mathrm{th}} \approx 0.72 \times 10^{-8}$ cm. Check whether the condition to treat the gas as a classical system is fulfilled or not.

(1 point)

13. Density operator

Consider the Hilbert space $\mathfrak{H}$ onto which the density operator $\hat{\rho} : \mathfrak{H} \to \mathfrak{H}$ is defined such that it can be written as

$$\hat{\rho} = \sum_\lambda p_\lambda |\psi_\lambda\rangle\langle\psi_\lambda|, \tag{9}$$

where for all value of λ the vector $|\psi_\lambda\rangle$ are normalized states of the Hilbert space $\mathfrak{H}$. Furthermore, the coefficients $p_\lambda \geq 0$ are such that $\sum_\lambda p_\lambda = 1$.

(a) Show that the expectation value of some hermitian operator $\hat{A}$ is given by

$$\langle \hat{A} \rangle = \mathrm{Tr}\{\hat{\rho}\hat{A}\}, \tag{10}$$

where the trace is performed over a basis $\{|n\rangle\}$ of the Hilbert space $\mathfrak{H}$.

(1 point)

(b) Show that the density operator is Hermitian, namely that $\rho^\dagger = \rho$.

(1 point)

(c) Show that the density operator is definite positive, or in other words that

$$\langle \psi|\hat{\rho}|\psi\rangle \geq 0, \tag{11}$$

for any arbitrary state $|\psi\rangle$ of the Hilbert space.

(1 point)

(d) Show that the density operator is normalized: $\mathrm{Tr}\{\hat{\rho}\} = 1$.

(1 point)