Universität des Saarlandes
Fakultät 7 – Physik und Mechatronik

Fachrichtung 7.1 – Theoretische Physik
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Blatt 5 zur Theoretischen Physik IV, WS2023/2024

(Abgabe bis 08.11.2023, 8.30 Uhr)

Exercise 1 *Heat capacities of solid state models.* [14 Points]

a) Assume that a particle assumes discrete energy levels ϵ_n $(n = 0, 1, 2, \dots)$, where the probability of assuming the energy level ϵ_n follows the canonical ensemble $P(n) \propto e^{-\beta\epsilon_n}$ $(\beta = 1/(k_B T))$. Here T denotes the temperature. The sum of states is given by $Z = \sum_{n=0}^{\infty} e^{-\beta\epsilon_n}$. Derive a formula for the average energy level $\langle\epsilon_n\rangle$.

b) The atoms or molecules oscillate in the crystal lattice of a solid. We now want to describe this in the context of statistical mechanics. To do this, we denote the number of atoms (or molecules) by N. Calculate $\langle\epsilon_n\rangle$ if $\epsilon_n = (\frac{1}{2} + n)h\nu$ (h: Planck's quantum of action).

c) **Einstein model.** We now consider a solid consisting of N atoms. Each atom has three degrees of freedom (x, y and z direction) and therefore has the energy levels $\epsilon_{(n_x,n_y,n_z)} = (\frac{3}{2} + n_x + n_y + n_z)h\nu$ $(n_x, n_y, n_z = 0, 1, 2, \dots)$ with the frequency ν.

   i) Calculate the total energy U if the temperature is T.

   ii) Also calculate the heat capacity at constant volume $C_V = \frac{\partial U}{\partial T}$.

d) **Debye model.** The number of modes between the frequencies ν and $\nu + \Delta\nu$ is proportional to ν^2 , corresponding to

$$\rho(\nu)\Delta\nu = \frac{4\pi V}{c^3}\nu^2\Delta\nu$$

where V denotes the volume and c a velocity. Debye introduced a *cut-off* frequency ν_m so that

$$\int_0^{\nu_m} \rho(\nu)d\nu = 3N$$

   i) Calculate the total energy U if the temperature is T.

Hint: You can use the Debye function $D_3(x) = \int_0^x \frac{x'^3}{e^{x'}-1}dx'$ in the final expression of U. Here, $\lim_{x\to\infty} D_3(x) = \frac{\pi^4}{15}$

   ii) Calculate an expression of ν_m depending on N.

   iii) Show that when $T \to \infty$, $D_3(\nu_m\beta h) \approx \frac{1}{3}(\nu_m\beta h)^3$.

   iv) Find the exponent α so that $\frac{C_V}{T^\alpha}$ converges to a constant that is greater than 0 but is smaller than ∞ and determine the constant in the two limiting cases: $T \to \infty$ and $T \to 0$.

Exercise 2 *Negative temperature.* [1] [22 Points]

Consider a system of N atoms, each with two electronic states at energies $\pm\epsilon/2$. The atoms are isolated from the outside world. There are only weak couplings between the atoms, sufficient to bring them into internal equilibrium but without significantly affecting the energy of the system.

a) Show that the number m of excited atoms can be express as:

$$m = \frac{E}{\epsilon} + \frac{N}{2} \tag{1}$$

if the total energy is E.

b) What is the microcanonical entropy $S_m(E)$ of our system? Simplify your expression using Stirling's formula, $\ln n! \approx n \ln n - n$.

c) Find the temperature, using your simplified expression from part (b). What happens to the temperature when $E > 0$?

d) Take one of our atoms and couple it to a heat bath of temperature $k_B T = 1/\beta$. Write explicit formulae for Z_c , E_c , and S_c in the canonical ensemble, as a sum over the two states of the atom. (E_c should be the energy of each state multiplied by the probability ρ_n of that state, and S_c should be the sum of $-k_B \rho_n \ln \rho_n$ of each state.)

e) Compare the results with what you get by using the thermodynamic relations:

i) Using Z_c, calculate the Helmholtz free energy A,

ii) S_c as a derivative of A,

iii) and E_c from $A = E_c - TS_c$. Do the thermodynamically derived formulæ you get agree with the statistical sums?

f) What happens to E in the canonical ensemble as $T \to \infty$? Can you get into the negative-temperature regime discussed in part (c)?

g) **Canonical–microcanonical correspondence.**

i) Find the entropy in the canonical distribution for N of our atoms coupled to the outside world, from your answer to part (d).

ii) Explain the value of $S(T = \infty)$ and $S(T = 0)$.

iii) Using the approximate form of the entropy from part (b) and the temperature from part (c), show that the canonical and microcanonical entropies agree, $S_m(E) = S_c(T(E))$ for large N .
Hint: $\operatorname{arctanh}(x) = \frac{1}{2} \ln \left(\frac{1+x}{1-x} \right)$.

iv) Explain in words why the microcanonical entropy is smaller than the canonical entropy.

[1] From the book of Sethna, James P., Statistical Mechanics: Entropy, Order Parameters, and Complexity, 2nd edn (Oxford, 2021; online edn, Oxford Academic, 22 Apr. 2021), https://doi.org/10.1093/oso/9780198865247.001.0001.

Exercise 3 *Computational task: Spin in External Field* [4 Points]

We want to simulate a magnetic dipole moment of atomic spin in an external field h (and immobile). The spin S can be in one of two states $S = +1$ or $S = -1$. For this, we use a *Metropolis algorithm* that allow stochastic flips of the spin, but tends to reduce the energy of the particle $E = -hS$.
Draw the mean spin $\langle S \rangle$ as a function of the reduced magnetic field βh ($\beta = 1/k_B T$) for βh between -3 and 3. Discuss the result. As a guide, there is a Python code in the exercise folder (blatt05_1spin.py) where the magnetic dipole moment is simulated using the *Metropolis algorithm*. You can complete it.