Universität des Saarlandes
Fakultät 7 – Physik und Mechatronik

Fachrichtung 7.1 – Theoretische Physik
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Blatt 9 zur Theoretischen Physik IV, WS2023/2024

(Abgabe bis 12.01.2024, 8.30 Uhr)

Exercise 1 *Harmonic oscillators in the grand canonical ensemble* [13 Points]

We consider a system of N quantum mechanical harmonic oscillators, which are to be distinguishable and independent. The energy eigenvalues of the individual oscillators are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{1}$$

a) Calculate the canonical sum of states $Z_N(T)$ and the free energy $F(T, N)$.

b) Determine the entropy $S(T, N)$ and energy $E(T, N)$.

c) Show that for the grand canonical state sum $Z_g(T, \mu)$,

$$Z_g(T,\mu) = \frac{1}{1 - e^{\beta\mu} Z_1(T)} \quad \text{mit } \beta = \frac{1}{k_B T} \text{ und } Z_1(T) = \frac{1}{2\sinh\left(\frac{\hbar\omega}{2k_B T}\right)}$$

applies. What condition must be satisfied for the convergence of Z_g?

d) Set up the grand canonical potential $\Phi(T, V, \mu)$ and use it to determine $N(T, \mu)$, $S(T, \mu)$ and $E(T, \mu)$.

e) Approximate the expressions for S and E for large N and compare with the result from b).

Exercise 2 *Photon density matrices*[1] [9 Points]

a) Write the density matrix for a vertically polarized photon $|V\rangle$ in the basis where $|V\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and a horizontal photon $|H\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Calculate $\mathrm{Tr}(\boldsymbol{\rho})$, $\mathrm{Tr}(\boldsymbol{\rho}^2)$, and $S = -k_B \mathrm{Tr}(\boldsymbol{\rho}\log\boldsymbol{\rho})$.
Hint: A bra $\langle V|$ can be written $(1\ 0)$.

b) Write the density matrix for a diagonally polarized photon, $|H\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$, and the density matrix for unpolarized light. Calculate $\mathrm{Tr}(\boldsymbol{\rho})$, $\mathrm{Tr}(\boldsymbol{\rho}^2)$, and $S = -k_B \mathrm{Tr}(\boldsymbol{\rho}\log\boldsymbol{\rho})$. **Hint:** For the unpolarized photo the denisty matrix is given by $\boldsymbol{\rho}_u = \frac{1}{2}|V\rangle\langle V| + \frac{1}{2}|H\rangle\langle H|$.

c) Interpret the values of the three traces physically. (One is a check for pure states, one is a measure of information, and one is a normalization.)

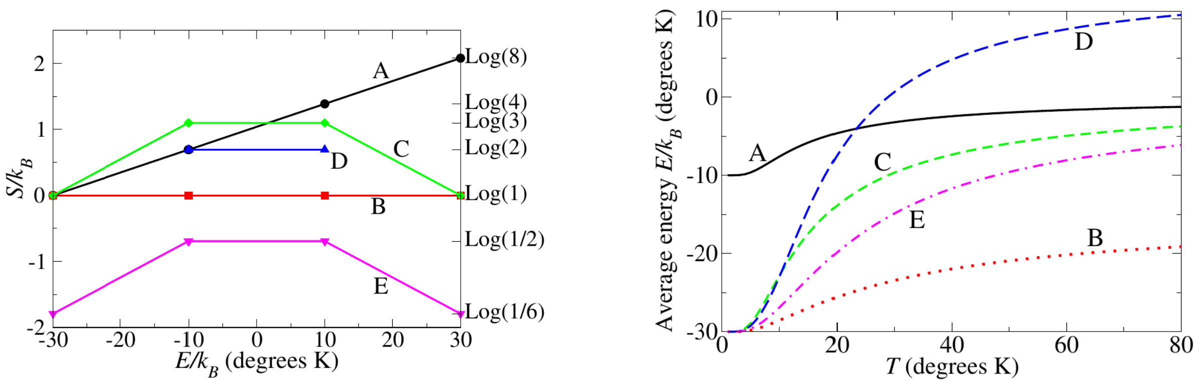
[1] From the book of Sethna, James P., Statistical Mechanics: Entropy, Order Parameters, and Complexity, 2nd edn (Oxford, 2021; online edn, Oxford Academic, 22 Apr. 2021), https://doi.org/10.1093/oso/9780198865247.001.0001.

Exercise 3 *Ensembles and quantum statistics*[2] [14 Points]

A system has two single-particle eigenfunctions, with energies (measured in degrees Kelvin) $E_0/k_B = -10$ and $E_2/k_B = 10$. Experiments are performed by adding three noninteracting particles to these two states, either identical spin-1/2 fermions, identical spinless bosons, distinguishable particles, or spinless identical particles obeying Maxwell–Boltzmann statistics.
Hints: As a consequence of the Pauli exclusion principle, only one fermion can occupy a particular quantum state at a given time. Bosons don't obey Pauli exclusion principle. Maxwell–Boltzmann statistics is often described as the statistics of distinguishable classical particles, but this assumption leads to the Gibbs paradox which is resolved by the Gibbs factor $1/\sqrt{N}$ with N the number of particles.

a) The system is first held at constant energy. In Fig. 1a which curve represents the entropy of the fermions as a function of the energy? Bosons? Distinguishable particles? Maxwell–Boltzmann particles? Substantive calculations are needed.

b) The system is now held at constant temperature. In Fig. 1b which curve represents the mean energy of the fermions as a function of temperature? Bosons? Distinguishable particles? Maxwell–Boltzmann particles? Substantive calculations are needed.



(a) Microcanonical three particles

(b) Canonical three particles

Figure 1: Three particles mixed states

Exercise 4 *Computational task: quantum harmonic oscillator* [4 Points]

The quantum harmonic oscillator is a fundamental system in quantum mechanics that describes a particle in a potential well created by a harmonic oscillator. In classical mechanics, a harmonic oscillator follows Hooke's Law, where the force exerted on the particle is proportional to its displacement from the equilibrium position. In quantum mechanics, the energy levels of a quantum harmonic oscillator are quantized, meaning they can only take on discrete values.
The wave functions of a quantum harmonic oscillator are given by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n \cdot n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{2}$$

Here:

- $\psi_n(x)$ is the wave function for the n-th energy level.
- n is the quantum number, taking values $0, 1, 2, \ldots$.
- m is the mass of the particle.
- ω is the angular frequency of the oscillator.

[2] *Ibid.*

- $\hbar$ is the reduced Planck constant.
- $H_n(x)$ is the n-th Hermite polynomial.

Make a simple simulation of a quantum harmonic oscillator by calculating the wave function of an electron in 1 dimension. Visualize the wave function for $n = 0, 1, 2$. As a guide, there is a Python code in the exercise folder (blatt09_QHarmOscill.py), you can complete it.