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Blatt 4 zur Theoretischen Physik IV, WS 2023/2024

(Abgabe bis 01.12.2023, 8:30 Uhr)

Exercise 1: A d-dimensional sphere

A d-dimensional sphere with radius R is defined by

$$x_1^2 + x_2^2 + \ldots + x_d^2 \leq R^2,$$

where x_i represents the Cartesian coordinates.

a) Calculate the volume and surface area of such a sphere.
   Hint: Consider the integral $I = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-(x_1^2+\ldots+x_d^2)} \, \mathrm{d}x_1 \cdots \mathrm{d}x_d$.

b) Determine the thickness Δr at which the volume of the surface layer with this thickness is exactly equal to the volume of the inner sphere.

c) Consider the limit $d \to \infty$ for the answer of part (b).

[6.5+4.5+2=13 Points]

Exercise 2: Functional form of entropy

Assume that S is an additive quantity, and the relationship with the number of microstates Ω is given by an arbitrary function $S = f(\Omega)$.

Show that the additive nature of S, in conjunction with the multiplicative nature of Ω, necessarily implies that the function $f(\Omega)$ is of the form $S = k \ln \Omega$ (with $k = \text{const}$). Thus, the quantity S indeed represents the entropy of the system.

[6 Points]

Exercise 3: Extremal entropy and probability distributions

Consider a system with N different stationary states with probabilities ω_i. The entropy is then given by $S = -k_B \sum_{i=1}^{N} \omega_i \ln \omega_i$.

a) Use the method of Lagrange multipliers to determine the values of ω_i such that $S(\omega_1, \ldots, \omega_N)$ becomes extremal. The normalization condition $\sum_{i=1}^{N} \omega_i = 1$ serves as a constraint.
   Hint: You should maximize $S' = S + \lambda \times \text{constraint}$. This results in the distribution of the microcanonical ensemble.

b) Repeat the procedure of part (a) for the additional constraint $\sum_{i=1}^{N} E_i \omega_i = E$, where E and E_i are constants.

Hint: Determine the first Lagrange multiplier λ from normalization and then use $\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{\partial S}{\partial \eta}\frac{\partial \eta}{\partial E}$ to express the second Lagrange multiplier η in terms of temperature. You will see next week that the result of this exercise is indeed the distribution of the canonical ensemble.

Now consider a composite system with states (i, j) consisting of two such systems with probability distributions p_i and q_i.

c) Show that for uncorrelated sub-systems, i.e. $w_{i,j} = p_i q_j$, the total entropy is equal to the sum of the entropies of the subsystems.

Finally, consider a continuous system with distribution $\omega(x)$. The entropy is then

$$S[\omega(x)] = -k_B \int_{-\infty}^{\infty} \omega(x) \ln \omega(x)\, dx.$$

The mean and variance of $\omega(x)$ are given as

$$\langle x \rangle = \int_{-\infty}^{\infty} x\omega(x)\, dx = 0 \quad \text{and} \quad \langle (x - \langle x \rangle)^2 \rangle = \int_{-\infty}^{\infty} (x - \langle x \rangle)^2 \omega(x)\, dx = \sigma^2.$$

d) Demonstrate that the entropy becomes extremal when $\omega(x)$ is given by a Gaussian distribution with width σ. Also, provide all three Lagrange multipliers.

Hint: Use the Euler-Lagrange equation: $\frac{\partial L}{\partial \omega} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial L}{\partial \omega'} = 0$.

[2+7+2+6=17 Points]

Exercise 4: Computational task (Shannon entropy)

Suppose that the frequency f_n of the n-th most frequent word in English decreases proportional to $\frac{1}{n}$ for $n \leq 12000$ and it is zero otherwise. If we assume that English is generated by picking words at random according to this distribution, what is the Shannon entropy of English (per word)? Compare the result with the case of a $\frac{1}{n^2}$ distribution. As a guide, there is a Python code in the exercise folder (Blatt4-ShannonEntropy-PythonCode1.py), where the contribution of the n-th most frequent word in the Shannon entropy is calculated. You can complete it.

[4 Points]