

Statistical Physics and Thermodynamics (SS 2018)

Problem sheet 4

Hand in: Friday, May 25 during the lecture

<http://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-netz/lehre>

1 Saddle point approximation (6 points)

If a function $g(x)$ has a sharp maximum at x_0 , integrals of the form

$$\int_{-\infty}^{\infty} dx \exp(g(x)) \quad (1)$$

can be approximated by the so-called saddle point approximation

$$\int_{-\infty}^{\infty} dx \exp(g(x)) \approx \int_{-\infty}^{\infty} dx \exp\left(g(x_0) + \frac{1}{2}g''(x_0)x^2 + \frac{1}{6}g'''(x_0)x^3 + \dots\right). \quad (2)$$

a) Derive eq. (2). **(1 point)**

b) Estimate the integral

$$\int_{-\infty}^{\infty} dx \frac{1}{1+x^2} \quad (3)$$

by using the leading order saddle point approximation. Compare your result to the exact value

$$\int_{-\infty}^{\infty} dx \frac{1}{1+x^2} = \pi. \quad (4)$$

(3 points)

c) Now approximate the integral

$$\int_{-\infty}^{\infty} dx \frac{1}{(1+x^2)^k} \quad (5)$$

and compare your results to the exact values for $k = 10$ and $k = 100$:

$$\int_{-\infty}^{\infty} dx \frac{1}{(1+x^2)^k} = \frac{\Gamma(k-1/2)\sqrt{\pi}}{(k-1)!} = \frac{(1/2)(3/2)\cdots(k-3/2)\pi}{(k-1)!} \approx \begin{cases} 0.582673 & \text{for } k = 10 \\ 0.177914 & \text{for } k = 100 \end{cases}. \quad (6)$$

(2 points)

2 Stationary phase space distributions (5 points)

Consider an ensemble of states so that different energies are populated with different probabilities in such a way that the phase space probability density $\rho(\mathbf{p}, \mathbf{q}, t)$ is only a function of the energy $\mathcal{H}(\mathbf{p}, \mathbf{q})$ and the time t , i.e.

$$\rho(\mathbf{p}, \mathbf{q}, t) = \rho(\mathcal{H}(\mathbf{p}, \mathbf{q}), t). \quad (7)$$

a) Show that in this case $\rho(\mathbf{p}, \mathbf{q}, t)$ must be independent of time, and thus

$$\rho(\mathcal{H}(\mathbf{p}, \mathbf{q}), t) = \rho(\mathcal{H}(\mathbf{p}, \mathbf{q})). \quad (8)$$

(4 points)

b) Does this also imply that ρ must be the canonical Boltzmann distribution? (1 point)

3 Extensive and intensive functions (4 points)

a) Determine which of the following functions $K_i(S, V, N)$ of the entropy S , the volume V , and the number of particles N , are extensive or intensive:

$$K_1 = S^2/V + S^5/(VN^3) + S^7/(VN^5) \quad (9)$$

$$K_2 = S^5/V^3 \quad (10)$$

$$K_3 = S^4/N^4 \quad (11)$$

(1 point)

b) Explain whether the derivatives $\frac{\partial K_i}{\partial S}$ and $\frac{\partial^2 K_i}{\partial S^2}$ with respect to the entropy S are extensive or intensive for $i = 1, 2, 3$. (3 points)

4 Canonical ensemble (5 points)

Prove the following theorem for the canonical ensemble by using Lagrange multipliers:

The entropy function

$$S(\rho_1, \dots, \rho_N) = -k \sum_{n=1}^N \rho_n \ln \rho_n \quad (12)$$

has a constrained, extremal value with the conditions

$$\sum_{n=1}^N \rho_n = 1 \quad \text{and} \quad \sum_{n=1}^N \rho_n E_n = E, \quad (13)$$

at (and only at)

$$\rho_n = \exp(-\beta E_n)/Z \quad (14)$$

with the canonical partition function

$$Z = \sum \exp(-\beta E_n). \quad (15)$$

Express β as a function of k and of the Lagrange multiplier λ_E for the energy and interpret your result.

Hint: Get rid of the logarithms before eliminating the Lagrange multiplier λ_ρ that couples to the sum $\sum_{n=1}^N \rho_n$.