Freie Universität Berlin
Fachbereich Physik
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Prof. Dr. Roland Netz
Douwe Bonthuis
Jan Daldrop
Philip Loche

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

$$\int_{-\infty}^{\infty} dx \, \exp\left(g(x)\right) \tag{1}$$

can be approximated by the so-called saddle point approximation

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

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

b) Estimate the integral

$$\int_{-\infty}^{\infty} dx \, \frac{1}{1+x^2} \tag{3}$$

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

$$\int_{-\infty}^{\infty} dx \, \frac{1}{1+x^2} = \pi. \tag{4}$$

(3 points)

c) Now approximate the integral

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

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

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

(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 $\rho(\boldsymbol{p}, \boldsymbol{q}, t)$ is only a function of the energy $\mathcal{H}(\boldsymbol{p}, \boldsymbol{q})$ and the time t, i.e.

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

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

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

(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:

$$K_1 = S^2/V + S^5/(VN^3) + S^7/(VN^5) \tag{9}$$
$$K_2 = S^5/V^3 \tag{10}$$
$$K_3 = S^4/N^4 \tag{11}$$

(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

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

has a constrained, extremal value with the conditions

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

at (and only at)

$$\rho_n = \exp(-\beta E_n)/Z \tag{14}$$

with the canonical partition function

$$Z = \sum exp(-\beta E_n). \tag{15}$$

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 $\sum_{n=1}^{N} \rho_n$.