Exercise 6.1: Differential entropy (3P)

Let $p(x)$ be a probability density normalized by $\int_{-\infty}^{+\infty} p(x)\,\mathrm{d}x = 1$. Then the corresponding *differential entropy* is defined by

$$H_c = -\int_{-\infty}^{+\infty} p(x) \ln p(x)\ \mathrm{d}x.$$

Consider a discretization of the x-axis into equidistant intervals with size Δx and let $p_j = \frac{p(j\,\Delta x)}{\mathcal{N}}\Delta x$ be a discrete probability distribution which approximates $p(x)$, where $\mathcal{N} = \sum_{j=-\infty}^{+\infty} p(j\,\Delta x)\Delta x$ is the normalization. Show that in the limit $\Delta x \to 0$ the entropy H_c differs from the usual discrete Shannon entropy $H = -\sum_{j=-\infty}^{\infty} p_j \ln p_j$ only by an offset $\Delta H := H - H_c$ and compute this offset to leading order in Δx. Explain your findings qualitatively.

Exercise 6.2: Saddle point method (3P)

In Statistical Physics one is often confronted with integrals of the type

$$I = \int_a^b \exp\bigl(Nf(x)\bigr)$$

in the limit $N \to \infty$. Such integrals can be evaluated by using the so-called *saddle point method*. Starting point is the observation that for very large N the integral is dominated by contributions around the maximum of $f(x)$. The solution reads

$$I \;\approx\; \exp\bigl(Nf(x_0)\bigr)\sqrt{\frac{2\pi}{N|f''(x_0)|}} \qquad \text{for large } N \to \infty\,,$$

where x_0 is the value where the function $f(x)$ reaches its global maximum. This implies that

$$\frac{1}{N}\ln I \;\approx\; f(x_0) + \frac{1}{2N}\ln\frac{2\pi}{N|f''(x_0)|}$$

(a) Prove the saddle point method, assuming that $f(x)$ is can be differentiated continuously infinitely many times. (2P)

(b) Employ the saddle point method to prove Stirlings formula (1P)

$$N! \approx \sqrt{2\pi N}\, N^N e^{-N} \qquad \text{for } N \to \infty\,.$$

Here it is convenient to use the following integral representation of the Γ-function:

$$N! = \Gamma(N+1) = \int_0^\infty x^N e^{-x}\,\mathrm{d}x$$

Please turn over ⇒

Exercise 6.3: Density of states of N harmonic oscillators (6P)

Let $\mathbf{H}$ be the Hamiltonian of a quantum-mechanical system acting on the Hilbert space $\mathcal{H}$. Furthermore let us denote by $\mathbb{1}$ the identical map on $\mathcal{H}$. The so-called *density of states* corresponding to the energy $E \in \mathbb{R}$ is defined by

$$\boxed{\Omega(E) = \mathrm{Tr}\big[\delta(E\mathbb{1} - \mathbf{H})\big].}$$

(a) Use the well-known representation of the Dirac delta function $\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, e^{ikx}$ to prove the following relation: (1P)

$$\Omega(E) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}k\, e^{ikE}\, \mathrm{Tr}\left[e^{-ik\mathbf{H}}\right]$$

(b) Let us now consider an N-dimensional harmonic oscillator defined by the Hamiltonian

$$\mathbf{H} = \sum_{j=1}^{N} \hbar\omega(\mathbf{a}_j^\dagger \mathbf{a}_j + \frac{1}{2}) .$$

Show that the density of states of this system is given by (2P)

$$\Omega(E) = \frac{1}{2\pi}\int \mathrm{d}k\, e^{ikE} \left(\sum_{n=0}^{\infty} e^{-i\hbar k\omega(n+\frac{1}{2})}\right)^N .$$

(c) The expression derived in (b) can be understood as a geometric series. Convert this expression by evaluating the geometric series, showing that (1P)

$$\Omega(\epsilon) = \frac{1}{2\pi}\int \mathrm{d}k\, \exp\left(N\left[ik\epsilon - \ln\Big(2i\sin\frac{k\hbar\omega}{2}\Big)\right]\right) ,$$

where $\epsilon = E/N$.

(d) Evaluate the resulting integral with the help of the saddle point approximation in the limit $N \to \infty$ and show that the average entropy per oscillator $\bar{s}$ for $\epsilon > \hbar\omega/2$ takes on the following value: (1P)

$$\bar{s}(\epsilon) = \lim_{N\to\infty}\frac{\ln\Omega(\epsilon)}{N} = \left(\frac{\epsilon}{\hbar\omega}+\frac{1}{2}\right)\ln\left(\frac{\epsilon}{\hbar\omega}+\frac{1}{2}\right) - \left(\frac{\epsilon}{\hbar\omega}-\frac{1}{2}\right)\ln\left(\frac{\epsilon}{\hbar\omega}-\frac{1}{2}\right)$$

Hint: The saddle point approximation works also with complex phases. This means that you can simply ignore the emerging imaginary unit i, computing the integral as if it was real-valued. Attention: There are several maxima, use only one of them.

Moreover, show that $\bar{s}(\epsilon) \approx \ln(\epsilon/\hbar\omega)$ for large $\epsilon \to \infty$. (1P)

(Σ = 12P)

To be handed in electronically until Wednesday, June 03, 2020, 12:00, on WueCampus according to our Corona guidelines on the web page `cs.hayehinrichsen.de`.