SAMPLE SOLUTIONS EXERCISE 6

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.

SAMPLE SOLUTION

We can split the full Shannon entropy $H = -\sum_{j=-\infty}^{\infty} p_j \ln p_j$ into two parts: (1P)

$$\begin{aligned} H &= -\sum_{j=-\infty}^{+\infty} \Big(\frac{p(j\Delta x)}{\mathcal{N}}\Delta x\Big) \ln\Big(\frac{p(j\Delta x)}{\mathcal{N}}\Delta x\Big) \\ &= \underbrace{-\sum_{j=-\infty}^{+\infty} \Delta x\Big(\frac{p(j\Delta x)}{\mathcal{N}}\Big)\ln\Big(\frac{p(j\Delta x)}{\mathcal{N}}\Big)}_{\text{tends to } H_c} - \ln(\Delta x)\underbrace{\sum_{j=-\infty}^{+\infty}\Delta x\Big(\frac{p(j\Delta x)}{\mathcal{N}}\Big)}_{=1} \end{aligned}$$

The first term tends to H_c for $\Delta x \to 0$ since $\mathcal{N} = 1 + \mathcal{O}(\Delta x)$. (1P)

This means that $H - H_c \approx -\ln \Delta x$. The interpretation is clear: The finer the discretization is, the more information has to be provided to specify one of the bins. This gives an information offset which can be interpreted as the information to select one of the bins on an interval of unit size. Thus to leading order it scales as $-\ln \Delta x$ (or $-\log_2 \Delta x$ when measured in bits). (1P)

Remark: Note that the formulas are only correct if x does not carry a physical unit such as centimeter. If it does all arguments have to be divided by a reference length.

EXERCISE 6.2: SADDLE POINT METHOD (3P)

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

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

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

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

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:

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

Sample Solution

(a) This proof can be found in any textbook. Let $x_0 \in [a,b]$ be the point where the function $f(x)$ is maximal, i.e., $f'(x_0) = 0$ and $f''(x_0) < 0$. We Taylor-expand around x_0:

$$I = \int_a^b e^{Nf(x)} = \int_a^b \exp\Big(N\sum_{k=0}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,(x-x_0)^k\Big)\,\mathrm{d}x$$

We pull out the zeroeth order and take into account that $f'(x_0) = 0$:

$$I = e^{Nf(x_0)}\int_a^b \exp\Big(N\sum_{k=2}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,(x-x_0)^k\Big)\,\mathrm{d}x$$

Next we change variables by setting $y = \sqrt{N}(x-x_0)$:

$$I = e^{Nf(x_0)}\int_{-\sqrt{N}(a-x_0)}^{\sqrt{N}(b-x_0)} \exp\Big(\sum_{k=2}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,N^{1-k/2}y^k\Big)\,\frac{\mathrm{d}y}{\sqrt{N}}$$

Now we bring the leading exponential and $\sqrt{N}$ to the other side and take the limit:

$$\lim_{N\to\infty} I\sqrt{N}e^{-Nf(x_0)} = \lim_{N\to\infty}\int_{-\sqrt{N}(a-x_0)}^{\sqrt{N}(b-x_0)} \exp\Big(\sum_{k=2}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,N^{1-k/2}y^k\Big)\,\mathrm{d}y$$

On the r.h.s. the boundaries go to $\pm\infty$ and only the second-order term survives:

$$\lim_{N\to\infty} I\sqrt{N}e^{-Nf(x_0)} = \int_{-\infty}^{+\infty}\exp\Big(\frac{1}{2}f''(x_0)y^2\Big)\,\mathrm{d}y = \sqrt{-\frac{2\pi}{f''(x_0)}}$$

Hence

$$I \approx e^{-Nf(x_0)}\sqrt{-\frac{2\pi}{Nf''(x_0)}}$$

Correction advice: The solution should contain: (i) pull out zeroth order (ii) isolate second order as a Gauss integral, and (iii) somehow argue that the higher order go away as $N\to\infty$.

(b) We rewrite the integral as

$$N! = \int_0^{\infty} e^{n\ln x - x}$$

and identify the function $f(x)$ and its derivatives as

$$f(x) = \ln x - \frac{x}{N}\,,\quad f'(x) = \frac{1}{x} - \frac{1}{N}\,,\quad f''(x) = -\frac{1}{x^2}.$$

This function is extremal at $x_0 = N$, hence

$$f(x_0) = \ln N - 1\,,\quad f'(x_0) = 0\,,\quad f''(x_0) = -\frac{1}{N^2}.$$

Inserting this into (a) yields (1P)

$$I \approx e^{N(lnN-1)}\sqrt{\frac{2\pi}{N(1/N^2)}} = \Big(\frac{N}{e}\Big)^N\sqrt{2\pi N}.$$

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)

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

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)

Sample Solution

(a) If a function is applied to an operator (for example exp/sin/sinh), one possible way to compute the result is to switch to the diagonal representation of the operator and then to apply the function separately to each of the elements along the diagonal. In our case we go to the energy eigenbasis of the Hamiltonian: (1P)

$$\Omega(E) = \sum_m \delta(E-E_m) = \sum_m \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}k e^{ik(E-E_m)} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}k e^{ikE}\underbrace{\sum_m e^{-ikE_m}}_{=\mathrm{Tr}[e^{-ik\mathbf{H}}]} .$$

Here E_m are the eigenvalues of $\mathbf{H}$.

(b) First we perform the sum over all states in terms of the occupation numbers n_j which are the eigenvalues of the number generator $\mathbf{a}_j^\dagger \mathbf{a}_j$: (1P)

$$\mathrm{Tr}\left[e^{-ik\mathbf{H}}\right] = \mathrm{Tr}\left[e^{-ik\sum_{j=1}^{N}\hbar\omega(\mathbf{a}_j^\dagger \mathbf{a}_j+\frac{1}{2})}\right] = \sum_{n_1=0}^{\infty}\cdots\sum_{n_N=0}^{\infty} e^{-ik\sum_{j=1}^{N}\hbar\omega(n_j+\frac{1}{2})}$$

Then we reorganize the sum, observing that the contributions decouple and thus can be written as a simple power: (1P)

$$\begin{aligned}\mathrm{Tr}\left[e^{-ik\mathbf{H}}\right] &= \sum_{n_1=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\prod_{j=1}^{N} e^{-ik\hbar\omega(n_j+\frac{1}{2})} = \prod_{j=1}^{N}\sum_{n=0}^{\infty} e^{-ik\hbar\omega(n+\frac{1}{2})} \\ &= \left(\sum_{n=0}^{\infty} e^{-ik\hbar\omega(n+\frac{1}{2})}\right)^N .\end{aligned}$$

(c) This is straight-forward: (1P)

$$\left(\sum_{n=0}^{\infty} e^{-ik\hbar\omega(n+\frac{1}{2})}\right)^N = \left(\frac{e^{-\frac{1}{2}ik\hbar\omega}}{1-e^{-ik\hbar\omega}}\right)^N$$

$$= \left(\frac{1}{2i\sin\left(\frac{k\hbar\omega}{2}\right)}\right)^N = \exp\left(N\ln\left(-2i\sin\left(\frac{k\hbar\omega}{2}\right)\right)\right)$$

Inserting this into (a) completes the proof.

(d) According to the saddle point approximation, we identify the function f with:

$$f(k) = ik\epsilon - \ln\left[2i\sin\left(\frac{1}{2}k\hbar w\right)\right]$$

The derivatives read

$$f'(k) = i\epsilon - \frac{1}{2}\hbar\omega\cot\left[\frac{1}{2}\hbar\omega\right], \quad f''(k) = \frac{1}{4}\hbar^2\omega^2\sin^{-2}\left[\frac{1}{2}\hbar\omega\right].$$

Searching the extrema by solving $f'(k_0) = 0$, we find many solutions, namely

$$k_0 = \frac{\left(2\pi j - 2i\,\mathrm{arccoth}\left(\frac{2\epsilon}{\hbar\omega}\right)\right)}{\hbar\omega} \qquad (j \in \mathbb{Z})$$

At these extrema, the second derivative is negative and independent of j:

$$f''(k_0) = \frac{1}{4}\hbar^2\omega^2 - \epsilon^2 < 0$$

According to the guidelines in the exercise, we take only one of them, setting $j = 0$. Now the saddle point approximation tells us that $\Omega(E) \propto e^{Nf(k_0)}$, hence

$$\bar{s}(\epsilon) = \lim_{N\to\infty}\frac{\ln\Omega(E)}{N} = \lim_{N\to\infty}\frac{Nf(k_0) + const}{N} = f(k_0)$$

We compute

$$f(k_0) = \frac{2\epsilon\,\mathrm{arccoth}\left(\frac{2\epsilon}{\hbar\omega}\right)}{\hbar\omega} - \ln\frac{\hbar\omega}{\epsilon\sqrt{1-\frac{\hbar^2\omega^2}{4\epsilon^2}}}$$

and after some elementary algebra we arrive at (1P)

$$\bar{s}(\epsilon) = f(k_0) = \left(\frac{\epsilon}{\hbar\omega} + \frac{1}{2}\right) \ln\left(\frac{\epsilon}{\hbar\omega} + \frac{1}{2}\right) - \left(\frac{\epsilon}{\hbar\omega} - \frac{1}{2}\right) \ln\left(\frac{\epsilon}{\hbar\omega} - \frac{1}{2}\right)$$

Now we consider the limit of large ϵ, where

$$\ln\Big(\frac{\epsilon}{\hbar\omega} \pm \frac{1}{2}\Big) = \ln\Big(\frac{\epsilon}{\hbar\omega}\Big) \ln\Big(1 \pm \frac{\hbar\omega}{2\epsilon}\Big) \approx \pm\frac{\hbar\omega}{2\epsilon} \ln\Big(\frac{\epsilon}{\hbar\omega}\Big)$$

Inserting this approximation into the equation before yields

$$s(\epsilon) = f(k_0) \approx \ln\frac{\epsilon}{\hbar\omega}\,.$$

(Σ = 12P)