Homework 3

Due: Monday, 2/9/26, 23:59:59

Problem 1 — Unitary matrices

Show that $\mathbb{U} = e^{\mathbb{A}}$ is unitary if and only if $\mathbb{A}$ is anti-Hermitian, $\mathbb{A}^\dagger = -\mathbb{A}$.

Problem 2 — Rotating a Spin-1/2 Particle

The operator that rotates the state of a spin-1/2 particle around the x axis through angle ϕ is

$$\hat{R}_x(\phi) = e^{-i\hat{S}_x\phi/\hbar}$$

where $\hat{S}_x$ is the angular momentum operator along the x direction. We say that angular momentum is the *generator of rotation*.

The basis of the eigenstates of spin along the z axis has two orthonormal states: $|\uparrow\rangle$ and $|\downarrow\rangle$. In this basis, the matrix representing $\hat{S}_x$ has the form

$$\hat{S}_x \xrightarrow{\hat{S}_z \text{ basis}} \frac{\hbar}{2}\mathbb{X} \qquad \text{where} \qquad \mathbb{X} \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

a. Describe in words what the matrix $\mathbb{X}$ does. What happens when you apply it twice?

b. Using the Taylor series for the exponential function, write out enough terms of the matrix representation of $\hat{R}_x(\phi)$ that you see the pattern and can sum it to yield a simple 2×2 matrix.

c. Show that multiplying the matrix representation of $\hat{R}_x(\phi)$ by its adjoint (conjugate transpose) yields the identity. This shows that $\hat{R}_x(\phi)$ is a unitary operator.

Problem 3 — Orthonormal basis

Find the coefficients $a_0, b_0, b_1, c_0, c_1, c_2$ such that

$$\{a_0, b_0 + b_1 t, c_0 + c_1 t + c_2 t^2\}$$

form orthonormal polynomials on $(0, 1)$ using the inner product

$$\langle f, g \rangle = \int_0^1 f(t) g(t)\, \mathrm{d}t$$

Problem 4 — Invertibility

For which values of α are the following matrices invertible? Find the inverses whenever possible. (You may do this analytically or by using code, or both!)

$$\mathbb{A} = \begin{pmatrix} 1 & \alpha & 0 \\ \alpha & 1 & \alpha \\ 0 & \alpha & 1 \end{pmatrix} \qquad \mathbb{B} = \begin{pmatrix} 0 & 1 & \alpha \\ 1 & \alpha & 0 \\ \alpha & 0 & 1 \end{pmatrix}$$

Problem 5 — Thermal average energy of a simple harmonic oscillator

By midsemester in Physics 52, you will show that the energy levels of a simple harmonic oscillator of angular frequency ω are

$$\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \text{where} \qquad n = 0, 1, 2, \ldots$$

That is, the energy of the oscillator is quantized in units of $\hbar\omega$, with a minimum energy (zero-point offset) of $\hbar\omega/2$.

When such an oscillator is in contact with a reservoir held at absolute temperature T, its energy is not fixed. Rather, the probability of observing it to have any particular energy depends on the ratio of that energy to thermal energy, defined as $k_\mathrm{B}T$, where k_B is Boltzmann's constant $(1.38 \times 10^{-23}\ \mathrm{J/K})$. Specifically, the probability that the oscillator will have energy ϵ_n is given by

$$P(n) = \frac{e^{-\beta\epsilon_n}}{Z}$$

where $\beta \equiv \frac{1}{k_\mathrm{B}T}$ and

$$Z = \sum_{n=0}^{\infty} e^{-\beta\epsilon_n}$$

is called the **partition function**. (It's just the sum of all the Boltzmann factors; dividing by Z produces a normalized probability.) Therefore, the average energy in the oscillator is

$$\bar{E} = \sum_{n=0}^{\infty} P(n)\epsilon_n = \sum_{n=0}^{\infty} \frac{\epsilon_n e^{-\beta\epsilon_n}}{Z}$$

Write a function to compute the (approximate) thermal average energy in an oscillator of angular frequency ω at temperature T by summing N terms in the series. Make a plot of $\bar{E}(x)$, where $x = k_\mathbf{B}T/\hbar\omega$ for $0.025 \leq x \leq 2$. (Note that the “right” way to handle dimensions such as temperature and energy is to define a variable x that is formed by a dimensionless ratio, as we do here.]

NB: Should you wish to compare your result to the exact expression, the following results are derived early in Physics 117 (Statistical Mechanics and Thermodynamics),

$$\bar{E} = -\frac{\partial(\ln Z)}{\partial\beta} \qquad \text{and} \qquad Z = \frac{1}{2\sinh(\beta\hbar\omega/2)}$$

Here's the template:

In [1]:
```
def energy(N:int, x:float)->float:
    """
    Using the first N terms of the sum that gives the
    energy of an oscillator in contact with a heat reservoir
    at absolute temperature T, estimate its average energy.

    Inputs:
        N: the number of terms to include in the sum
        b: the dimensionless ratio of thermal energy to the energy,
        quantum, k_B T / hbar ω.

    Output:
        average energy / hbar omega
    """
```

In [ ]: