PH434 Autumn 2025 – Programming Lab.

Practical Class 6 (Dated: 26.09.2025)

Question 1

The composite Simpson's rule is a numerical integration technique that builds on the trapezoidal method. Here, the integration interval $[a, b]$ is divided into n equal and even divisions ($\textbf{be careful here}$), such that the integration is given by,

$$\begin{aligned}\int_a^b f(x)dx &\approx \frac{\Delta x}{3} \sum_{\substack{j=0 \\ j\, even}}^{n-2} \left[f(x_j) + 4f(x_{j+1}) + f(x_{j+2})\right] \\ &= \frac{\Delta x}{3}[f(x_0) + 4\sum_{\substack{j=1 \\ j\, odd}}^{n-1} f(x_j) + 2\sum_{\substack{j=2 \\ j\, even}}^{n-2} f(x_j) + f(x_n)],\end{aligned}$$

where $\Delta x = x_{i+1} - x_i,\ \forall\, i \in [0, n)$. Write a function that implements the Simpson's method and integrate the function $f(x) = x^2 \log(x)$, between $x = 1$ and $x = 10$.

Question 2

Compare the above results obtained using the **integrate.quad** function and **trapezoidal** rule method.

This question requires you to define a function for the trapezoidal rule.

Now, taking $n = 100$ in both cases, show whether the **Simpson's** or **trapezoidal** rule gives you a value closer to the inbuilt function.

Question 3

Consider the quantum operator: $\mathcal{H} = \frac{1}{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) + \frac{1}{4}(\sigma_z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_z)$, where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\mathbb{I}$ is the 2×2 identity matrix.

1. Write down the Hamiltonian $\mathcal{H}$.
2. Find the eigenvalues and eigenvectors of $\mathcal{H}$.
3. Show that $\mathcal{D} = P^{-1}\mathcal{H}P$, where $\mathcal{D}$ is the diagonal matrix containing the eigenvalues of $\mathcal{H}$ and P is an invertible matrix formed by the eigenvectors.

   Note that $P^{-1} = (P^*)^T$ as P is unitary.

Question 4

Time-evolution in quantum mechanics can be written as: $|\psi(t)\rangle = e^{-i\mathcal{H}t}|\psi(0)\rangle$.

Write a function to find $|\psi(t)\rangle$, with arguments $|\psi(0)\rangle$, and time t.

Print the output for $|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right]$ and $t = 0.1$.

Challenge:

Imagine you work for a transport company. Your job is to transfer large containers using barges (something like a boat) from one state to another. These containers are always stacked (arranged vertically) such that only a smaller sized container be kept on top of another (no containers can lie beside each other, but the boats can in principle hold several such containers). See the image.

Your daily routine is to transfer these containers from one boat to another using a lift crane. This lift crane can only carry one container at a time. But there is an empty land between the boats that can be used to keep the containers during transferring, with an area to hold the largest container (you can only stack containers in this area during transferring).

How many times must you use the lift crane to transfer n containers from one boat to another, ensuring that there is never a situation where a large container lies above a smaller one.

Show, what this number is for $n = 3$.

In [11]:

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Out[11]: