Numerical methods in chemistry. Exercises 5

Problem 1

Consider the function $f(x)$ where

$$f(x) = \begin{cases} 0 & -\pi \leq x \leq 0 \\ \sin x & 0 \leq x \leq \pi \end{cases},$$

and $f(x) = f(x + 2\pi)$ for all $x \in \mathbb{R}$. Determine:
(a) The Fourier series of the function on interval $-\pi \leq x \leq \pi$.
(b) The sine Fourier series of $f(x)$ on interval $0 \leq x \leq \pi$.
(c) The cosine Fourier series of $f(x)$ on interval $0 \leq x \leq \pi$.
(d) The complex Fourier series of $f(x)$ on interval $-\pi \leq x \leq \pi$.
Sketch the graph of $f(x)$ as well as of each of the four Fourier series on the interval $-\pi \leq x \leq \pi$.

Problem 2

In quantum chemistry, you will learn how to solve the *time-independent* **Schrödinger equation** for a particle in a box as well as for an electron in the hydrogen atom. In the next lecture, we shall solve the *time-dependent* **Schrödinger equation** for an electron in a 1-dimensional box of length l, and for the example I will present, I will need the following Fourier series. Find the Fourier sine series of the function $f(x)$ on the interval $0 \leq x \leq l$, where

$$f(x) = \begin{cases} 0 & 0 \leq x \leq l/2 \\ -\sin(2\pi x/l) & l/2 \leq x \leq l. \end{cases},$$