Numerical methods in chemistry. Exercises 6

Problem 1

Using **separation of variables** and the **Fourier method**, solve the boundary value problem describing **heat conduction**:

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2}, \quad x \in \left[0, \frac{\pi}{4}\right]$$
$$\phi(x, 0) = x\left(\frac{\pi}{4} - x\right) \text{ at time } t = 0$$
$$\phi(0, t) = \phi\left(\frac{\pi}{4}, t\right) = 0 \text{ for all time.}$$

Hint: Use the methods you have learned to determine the **Fourier sine series** representation of the function $f(x) := x\left(\frac{\pi}{4} - x\right)$ on the (nonstandard) interval $\left[0, \frac{\pi}{4}\right]$.

Problem 2

Use the **Laplace transform** to solve the PDE describing **heat conduction**

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial \phi}{\partial t}$$

with boundary conditions $\phi(x, 0) = 0$, $\phi(0, t) = 1$, $t > 0$ and

$$\lim_{x \to \infty} \phi(x, t) = 0.$$

Hint: You will need the inverse Laplace transform $\mathcal{L}^{-1}\left[\frac{1}{s} e^{-x\sqrt{s}}\right] = \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right)$, where the **complementary error function** is defined by

$$\operatorname{erfc}(x) := \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt.$$

Express the solution in terms of $\operatorname{erfc}(x)$; do not try to simplify it further.