Mathematical methods in chemistry. Exam for Part II.

Total = 90 points

June 2, 2023

You can freely use and do not need to derive any formulas in the provided **formula sheet** or **hints** on page 2. If you use anything else from the lecture or book, you should provide details.

Problem 1 (30 points)

Use the **Laplace transform** to solve the partial differential equation (PDE)

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial^2 u(x,t)}{\partial x^2}, \quad x \geq 0,\, t \geq 0,$$

describing wave propagation in the first quadrant, with initial conditions

$$u(x,0) = 0 \quad \text{and} \quad \left.\frac{\partial u(x,t)}{\partial t}\right|_{t=0} = 0 \quad \text{for } x \geq 0,$$

and boundary conditions

$$u(0,t) = f(t) = \sin(2t) \quad \text{and} \quad \lim_{x\to\infty} u(x,t) = 0 \quad \text{for } t \geq 0.$$

Problem 2 (30 points)

Use the **method of separation of variables** and **Fourier series** to solve the wave equation

$$\frac{\partial^2 y(x,t)}{\partial t^2} = \frac{\partial^2 y(x,t)}{\partial x^2}, \quad 0 < x < \pi,\, t > 0,$$

describing the displacement y of a string attached at $x = 0$ and $x = \pi$, with initial conditions

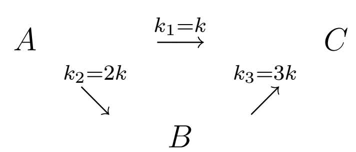
$$y(x,0) = \sin(2x) \quad \text{and} \quad \left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = 0 \quad \text{for } 0 \leq x \leq \pi,$$

and boundary conditions

$$y(0,t) = 0 \quad \text{and} \quad y(\pi,t) = 0 \quad \text{for } t \geq 0.$$

Problem 3 (30 points)

Consider the composite reaction



where the rate constants for the three elementary steps are $k_1 = k$, $k_2 = 2k$, $k_3 = 3k$, and the initial concentrations are $[A]_0 = a_0$ and $[B]_0 = [C]_0 = 0$. Let us denote the concentrations at time t by $a(t) := [A]_t$, $b(t) := [B]_t$, and $c(t) := [C]_t$. These concentrations satisfy the following system of ordinary differential equations:

$$\begin{aligned}
\dot{a}(t) &= -(k_1 + k_2)a(t), \\
\dot{b}(t) &= k_2 a(t) - k_3 b(t), \\
\dot{c}(t) &= k_1 a(t) + k_3 b(t).
\end{aligned}$$

Use the **Laplace transform** to solve this system and find explicit expressions for the concentrations $a(t)$, $b(t)$, and $c(t)$ at time t in terms of a_0, k, and t alone. (Do *not* solve the system for general k_1, k_2, k_3!) Sketch (i.e., draw qualitative graphs of) the dependence of the concentrations $a(t)$, $b(t)$, and $c(t)$ on time t.

Hints for Problems 1 to 3

You can use these formulas without deriving them:
Inverse Laplace transforms:

$$\begin{aligned}
\mathcal{L}^{-1}\left[\frac{1}{s}\right] &= 1, \\
\mathcal{L}^{-1}\left[\frac{n!}{s^{n+1}}\right] &= t^n, \quad n \in \mathbb{N}_0, \\
\mathcal{L}^{-1}\left[\frac{s}{1+s^2}\right] &= \cos(t), \\
\mathcal{L}^{-1}\left[\frac{1}{1+s^2}\right] &= \sin(t), \\
\mathcal{L}^{-1}\left[\frac{1}{s}e^{-a\sqrt{s}}\right] &= \operatorname{erfc}\left(\frac{a}{2\sqrt{t}}\right), \\
\mathcal{L}^{-1}\left[e^{-a\sqrt{s}}\right] &= \frac{a}{2\sqrt{\pi t^3}}e^{-a^2/(4t)}.
\end{aligned}$$

General solutions of homogeneous ODEs ($k \in \mathbb{R}$; $n \in \mathbb{N}$; a and b are arbitrary constants):

$$\begin{aligned}
\frac{d}{dx}y(x) + k\,x^n\,y(x) = 0 &\quad \text{has a general solution} \quad y(x) = ae^{-kx^{n+1}/(n+1)}, \\
\frac{d^2}{dx^2}y(x) + k^2 y(x) = 0 &\quad \text{has a general solution} \quad y(x) = a\cos(kx) + b\sin(kx), \\
\frac{d^2}{dx^2}y(x) - k^2 y(x) = 0 &\quad \text{has a general solution} \quad y(x) = ae^{kx} + be^{-kx}.
\end{aligned}$$

Particular solutions of inhomogeneous ODEs ($k, A, B, C \in \mathbb{R}$; a and b are suitable constants):

$$\frac{d^2}{dx^2}y(x) \pm k^2 y(x) = A\cos(Cx) + B\sin(Cx) \quad \text{has a particular solution} \quad y(x) = a\cos(Cx) + b\sin(Cx),$$

$$\frac{d^2}{dx^2}y(x) \pm k^2 y(x) = Ae^{Cx} \quad \text{has a particular solution } y(x) = ae^{Cx}.$$