Mathematical methods in chemistry. Exam for Part I.

Total = 90 points

April 8, 2025

You do not need to derive any formulas in the provided **formula sheet** or **hints** *on page 2.*

Problem 1 (30 points)

Let $f(x) = \sin(x/2)$ for $-\pi < x \leq \pi$ and $f(x + 2\pi) = f(x)$ for all $x \in \mathbb{R}$.
(a) Find the Fourier series of $f(x)$.
(b) To what values does this Fourier series converge at $x = 0$ and $x = \pi$?
Now let $g(t) = \sin(t/2)$ for all $t \in \mathbb{R}$.
(c) Find the Laplace transform of $g(t)$.

Problem 2 (30 points)

Consider the motion in a harmonic potential with friction, where a particle of mass m feels both the harmonic force $F_1 = -kx(t)$ and friction force $F_2 = -\gamma v(t)$, proportional to the velocity $v(t) = \dot{x}(t)$. Displacement $x(t)$ of the particle satisfies the ordinary differential equation (ODE)

$$m\ddot{x}(t) = F_1 + F_2.$$

Assume that $m = k = 1$, $\gamma = 2$, and that the initial displacement and velocity are $x(0) = 0$ and $\dot{x}(0) = 1$. (Do not solve the problem for general values of parameters.)
(a) **Use the Laplace transform** to solve this ODE, i.e., find the function $x(t)$ explicitly.
(b) What is the velocity of the particle at time t?
(c) What are the limiting values of the displacement and velocity at infinitely long times?
(d) What is the maximum displacement $x(t)$ of the particle?
(e) Plot (by hand) the displacement $x(t)$ as a function of time t.
All answers should be expressed in terms of t only.

Problem 3 (30 points)

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

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

with boundary conditions

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

and initial conditions

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

Hints for Problems 1 to 3

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

$$\frac{d}{dx}y(x) + k\,x^n\,y(x) = 0 \quad \text{has a general solution} \quad y(x) = ae^{-kx^{n+1}/(n+1)},$$

$$\frac{d^2}{dx^2}y(x) + k^2 y(x) = 0 \quad \text{has a general solution} \quad y(x) = a\cos(kx) + b\sin(kx),$$

$$\frac{d^2}{dx^2}y(x) - k^2 y(x) = 0 \quad \text{has a general solution} \quad y(x) = ae^{kx} + be^{-kx}.$$