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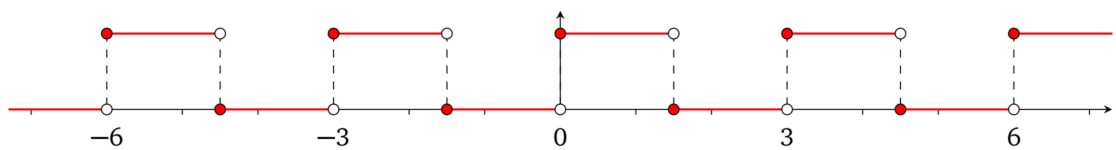
11. exercise sheet for Mathematics for Advanced Materials Science

11.1. *(3-periodic functions)*
Let $g\colon \mathbb{R} \to \mathbb{R}$ be the 3-periodic function defined by $g(x) = 1$ for $0 \leq x < 3/2$ and $g(x) = 0$ for $3/2 \leq x < 3$:



(a) What are the values of r for which one might be interested in computing $\hat{g}(r)$? (Hint: "$r \in \mathbb{Z}$" is a *wrong* answer. You should consult Example 4.9 from the lecture notes.)

(b) Compute the Fourier coefficients $\hat{g}(r)$ of g for r as in (a). (Hint: because g is 3-periodic, but not 1-periodic, the Fourier coefficients are *not* given by $\int_0^1 g(x)e^{-2\pi i k x}\,\mathrm{d}x$ which, incidentally, would be zero for all $k \neq 0$. Once you are done, you may compare your answer with the Fourier coefficients $\hat{\chi}(k)$ from Example 4.7. Moreover, you may check your result using $\hat{g}(3) \approx -0.1061\mathrm{i}$.)

11.2. *(Differentiation)*
Consider the two maps $f\colon \mathbb{R}^2 \to \mathbb{R}^2$, $(x, y) \mapsto (xy^2, \exp(x))$, and $g\colon \mathbb{R}^2 \to \mathbb{R}$, $(v, w) \mapsto v - w$. Compute the following:

(a) $(g \circ f)(x, y)$;

(b) the Jacobian matrices $J_f(x, y)$, $J_g(v, w)$, and $J_{g\circ f}(x, y)$,

(c) the matrix–matrix product $J_g(f(x, y))J_f(x, y)$.

(Hint: examples for computing the Jacobian matrices can be found in § 5.1.3.)

11.3. *(Polar coordinates, differentiation)*
Consider the function

$$f\colon \mathbb{R}^2 \setminus \{\vec{0}\} \to \mathbb{R}, \quad (x, y) \mapsto \frac{2xy}{(x^2 + y^2)^2},$$

as well as the well-known polar coordinate map $\vec{P}\colon \mathbb{R}^2 \to \mathbb{R}^2$, $(r, \varphi) \mapsto (r\cos\varphi, r\sin\varphi)$. Let $\vec{v} = (1/\sqrt{2}, 1/\sqrt{2})$. Compute the following quantities.

(a) $\partial_1 f(x, y)$ and $\partial_2 f(x, y)$.

(b) $\dfrac{\partial f}{\partial \vec{v}}(x, y)$. (Hint: Lemma 5.1.)

(c) $(f \circ \vec{P})(r, \varphi)$.

(d) $\dfrac{\partial f}{\partial r}(r, \varphi)$ and $\dfrac{\partial f}{\partial \varphi}(r, \varphi)$.
(Hint: this notation means $\partial_1(f \circ \vec{P})$ and $\partial_2(f \circ \vec{P})$.)

11.4. *(Heat equation)*
Imagine some thin, heated wire spanned between two points which are kept at equal temperature by means of an external heat source/sink. We model the wire by the interval $[0, 1]$ and let $u(t, x)$ denote the temperature of the wire at the point $x \in [0, 1]$ and time $t \geq 0$. Abstracting away all units and constants of proportionality, the evolution of the resulting function $u\colon \mathbb{R}_{\geq 0} \times [0, 1] \to \mathbb{R}$ in this model problem can be seen to be governed by the ***heat equation***

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

at all points $(t, x) \in \mathbb{R}_{>0} \times (0, 1)$, where $\frac{\partial^2}{\partial x^2}$ means differentiating with respect to x *twice*. (A glimpse of how one may derive this equation from physical principles and Gauß's integral theorem can be found in § 8.2 of the lecture notes, but here we take this equation for granted.)

In this exercise, we shall first find a number of particular solutions to the head equation. Subsequently, we shall apply Fourier analysis to show that the few solutions we have already found suffice, by means of (infinite) linear combination, to construct solutions to the heat equation that match (basically any) initial temperature distribution that we may choose. The underlying principles here can be used to treat a number of other partial differential equations appearing in physics, also modelling higher-dimensional problems, although the computations quickly become more involved.

(a) For $k \in \mathbb{N}$, verify that $x \mapsto \sin(\pi k x)$ is an eigenfunction of the operator mapping infinitely often differentiable functions $\mathbb{R} \to \mathbb{R}$ to their second derivative.
(Hint: the exercise just asks you to take the second derivative of that function and observe that you get a multiple of the original function. What is this multiple?)

(b) (***Particular solutions***:) Verify that, for every $k \in \mathbb{N}$, the function

$$b_k\colon \mathbb{R}^2 \to \mathbb{R}, \quad (t, x) \mapsto e^{-\pi^2 k^2 t} \sin(\pi k x),$$

satisfies the heat equation, as well as the "boundary condition" $b_k(t, 0) = 0 = b_k(t, 1)$ for all t and $b_k(0, x) = \sin(\pi k x)$ for all x.
(Hint: here you are just supposed to compute $\frac{\partial}{\partial t}$ and $\frac{\partial^2}{\partial x^2}$ of b_k and observe that both expressions coincide.)

(c) (***Superposition principle***:) Verify that any linear combination $\lambda f + \mu g$ (with numbers λ and μ) of any two functions f, g satisfying the heat equation again satisfies the heat equation.

(d) Let $f\colon [0,1] \to \mathbb{R}$ be a continuous, piecewise continuously differentiable function with $f(0) = 0 = f(1)$. Show that f can be written as

$$f(x) = \sum_{k=1}^{\infty} \tilde{f}(k) \sin(\pi k x) \quad \text{with} \quad \tilde{f}(k) := 2\int_0^1 f(x)\sin(\pi k x)\,\mathrm{d}x.$$

(Guide: define a 2-periodic function $F\colon \mathbb{R} \to \mathbb{R}$ by $F(x) = f(x)$ for $0 \le x \le 1$ and $F(x) = -f(-x)$ for $-1 \le x < 0$. Use Theorem 4.1 to see that F is represented everywhere by its Fourier series. Recall that the Fourier coefficients of the 2-periodic function F need to be computed as in Example 4.9 and show that $\hat{F}(-r) = -\hat{F}(r)$ for $r = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \ldots$; now proceed as in exercise 10.3 to rewrite the Fourier series for F as a series with sines and cosines. You should see that the coefficients in front of the cosine terms vanish. By the definition of F using f, you should arrive at the desired formula for $f(x)$.)

(e) (***Grand finale***:) Use your insights from all of the above exercises to find an infinite series representing a (the) continuous function $u\colon \mathbb{R}_{\ge 0} \times [0,1] \to \mathbb{R}$ that

- solves the heat equation,
- satisfies the *boundary condition* $u(t,0) = 0 = u(t,1)$ for all $t \ge 0$, and
- satisfies the *initial condition* (initial temperature distribution)

$$u(0,x) = (\chi * \chi)(x) \quad \text{for } 0 \le x \le 1,$$

where $\chi * \chi$ should be taken from Example 4.8 with parameter $c = 1/2$.

(Hint: you may assume that a convergent infinite series $f(x) = \sum_{k=1}^{\infty} f_k(x)$ of differentiable functions f_k produces a differentiable function whose derivative can be computed by differentiating term-wise: $f'(x) = \sum_{k=1}^{\infty} f_k'(x)$; use this also when multiple variables are involved and one is speaking of partial derivatives. This is actually not always true, but it holds in many important cases and the details of this shall not concern us here.)