Vv286 Honors Mathematics IV
Ordinary Differential Equations

Assignment 3

Date Due: 10:00 AM, Thursday, the 15th of October 2015

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Exercise 1. Consider the initial value problem

$$y' = y^2 + x^2, \qquad y(0) = 0. \tag{$**$}$$

i) Use Picard iteration to find a succession of approximate solutions y_1, y_2, y_3, y_4, starting from $y_0(x) = 0$. You may use Mathematica to help perform the integrations.

ii) Use Mathematica to obtain a numerical solution to $(**)$. Plot the numerical solution as well as y_1, y_2, y_3, y_4 in a single graph.

(2 + 3 Marks)

Exercise 2. In classical analytical mechanics, the total energy of a system is represented by the *Hamilton function* $H = T + V$, where T represents the kinetic energy and V is the potential energy. For a harmonic oscillator,

$$H(x,p) = \frac{p^2}{2m} + \frac{k}{2}x^2,$$

where m is the mass, p the momentum, x the position and k the spring constant of the oscillator. By non-dimensionalizing, we can obtain $H = p^2 + x^2$. In quantum mechanics, the classical Hamilton function is translated to a *Schrödinger operator* (also denoted H) on a certain Hilbert space. This operator is obtained by replacing p by $i\frac{d}{dx}$ and the potential V by a multiplication operator with $V(x)$. For the harmonic oscillator this yields

$$H = -\frac{d^2}{dx^2} + x^2.$$

The eigenvalue problem

$$H\psi = \lambda\psi$$

is called the *Schrödinger equation* and the eigenvalues λ determine the possible energy levels of the quantum-mechanical harmonic oscillator.

The goal of this exercise is to investigate the eigenvalues λ_n and eigenfunctions ψ_n of H in a simplified setting. We assume that the domain of H is

$$V := \{\psi \in C^\infty(\mathbb{R})\colon \psi(x) = e^{-x^2/2}p(x),\ p \in \mathcal{P}(\mathbb{R})\},$$

where $\mathcal{P}(\mathbb{R})$ is the (infinite-dimensional) vector space of real polynomials over $\mathbb{R}$. On V we define a scalar product by

$$\langle \psi, \varphi \rangle = \int_{-\infty}^{\infty} \psi(x)\varphi(x)\,dx.$$

The results below essentially agree with calculations in quantum mechanics textbooks. In physics, the quantum mechanical harmonic oscillator can be used to model, for example, two-atom molecules such as HCl (hydrogen chloride) as two masses joined by a spring. The eigenvalues below correspond to the possible quantized oscillation/vibration energy levels (after norming with physical constants) and can be observed through spectroscopy (e.g., Raman spectroscopy).

i) Prove that H is well-defined, i.e., prove that $H\psi \in V$ if $\psi \in V$.

ii) Prove that H is symmetric, i.e., $\langle H\psi, \varphi\rangle = \langle \psi, H\varphi\rangle$ for all $f, g \in V$. We will show later that this guarantes that the eigenvalues are real and that the eigenfunctions are orthogonal, i.e., $\langle \psi_n, \psi_m\rangle = 0$ if $n \neq m$. You may use these two facts for now without proof.

iii) We define the *creation operator* $A\colon V \to V$, $A = -\frac{d}{dx} + x$. Show the *commutation relation*

$$[H, A] := HA - AH = 2A.$$

iv) Let $\psi \in V$ be an eigenfunction of H for the eigenvalue $\lambda \in \mathbb{R}$. Assume that $A\psi \neq 0$. Prove that then $A\psi$ is an eigenfunction of H for the eigenvalue $\lambda + 2$.

v) For $n \in \mathbb{N}$ the *Hermite polynomials* are defined by $H_n(x) := (-1)^n e^{x^2} \dfrac{d^n}{dx^n}(e^{-x^2})$. Calculate H_0, H_1 and H_2 and use Mathematica to plot their graphs.

vi) Verify that

$$H(e^{-x^2/2}) = e^{-x^2/2} \qquad \text{and} \qquad Af(x) = e^{x^2/2}\left(-\frac{d}{dx}\right)(e^{-x^2/2}f(x)). \qquad (***)$$

Use $(***)$ to show that the eigenfunctions of H to eigenvalues $\lambda_n = 2n+1$, $n \in \mathbb{N}$, may be written in the form $\psi_n(x) = e^{-x^2/2}H_n(x)$.

vii) Prove by induction that $H_n' = 2nH_{n-1}$ for $n \in \mathbb{N} \setminus \{0\}$. (*Hint*: prove first that $H_{n+1}(x) = 2xH_n(x) + H_n'(x)$.)

viii) Show that $\|\psi_n\|^2 = \langle \psi_n, \psi_n \rangle = \sqrt{\pi}2^n n!$. Recall that $\int_{\mathbb{R}} e^{-x^2/2}\, dx = \sqrt{2\pi}$.

(1 + 1 + 1 + 2 + 2 + 2 + 2 + 2 Marks)