Mathematical Methods

Problem Sheet 3: "Ordinary differential equations and special functions"

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1) (Green function)
Consider the differential operator $T = \frac{d^2}{dx^2} + 2c\frac{d}{dx} + 1$, where $0 < c < 1$.

a) Determine the value of ω for which $y_1(x) = e^{-cx}\cos(\omega x)$ and $y_2(x) = e^{-cx}\sin(\omega x)$ solve the homogeneous equation $Ty = 0$.

(b) Show that the solutions y_1 and y_2 are linearly independent by computing the Wronski determinant $W = y_1 y_2' - y_1' y_2$.

(c) Find the Green function $G(x,t) = \frac{y_1(t)y_2(x) - y_1(x)y_2(t)}{W(t)}$ for the operator T.

(d) Write down the general solution for the inhomogeneous equation $Ty = f$, where f is a given function, in terms of the Green function.

2) (Hermite polynomials again)
Consider the space $L^2_w(\mathbb{R})$ with weight function $w(x) = e^{-x^2}$. The Hermite polynomials $H_n \in L^2_w(\mathbb{R})$ can be defined by the Rodriguez formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \ . \tag{1}$$

(a) Show that the H_n form an orthogonal system on $L^2_w(\mathbb{R})$ with $\langle H_n, H_m \rangle = \sqrt{\pi} 2^n n!\, \delta_{nm}$.

(b) Show that the Hermite polynomials satisfy the recursion relation $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$ and $H_n' = 2nH_{n-1}$.

(c) Show that H_n satisfies the differential equation $y'' - 2xy' + 2ny = 0$.

(d) Solve the differential equation from part (c) with a power series Ansatz.

(e) Using reduction of order, show that the second solution to the Hermite differential equation for $n = 1$ (in addition to $H_1(x) = 2x$) is given by

$$\tilde{y}(x) = \sum_{k=0}^{\infty} \frac{x^{2k}}{2(2k-1)k!} \ . \tag{2}$$

Verify that the above solution $\tilde{y}$ is consistent with the recursion relation for the coefficients obtained in part (d).

3) (Hermitian and unitary operators)
Let V be the vector space of infinitely many times differentiable functions $f : \mathbb{R} \to \mathbb{C}$ with $x^n f(x) \to 0$ for $x \to \pm\infty$ and any $n \geq 0$. On V we have the usual scalar product

$$\langle f, g \rangle = \int_{\mathbb{R}} dx\, f(x)^* g(x) \ . \tag{3}$$

(a) Let $T : V \to V$ and $S : V \to V$ be two hermitian operators. Show that $T \circ S$ is hermitian iff $[T, S] = 0$.

(b) For $T : V \to V$ anti-hermitian, show that iT is hermitian. Show that every linear operator $T : V \to V$ can be written as a sum of a hermitian and an anti-hermitian operator.

(c) Which of the following operators are hermitian? (i) $i\frac{d}{dx}$, (ii) x^k, (iii) $\frac{d}{dx} + x^2$, (iv) $i\frac{d^3}{dx^3}$, (v) $ix\frac{d}{dx}$. Write the ones which are not hermitian as a sum of a hermitian and an anti-hermitian operator.

(d) Show that eigenvalues λ of a unitary operator $U : V \to V$ must satisfy $|\lambda| = 1$.

(e) Show that the translation operator $T_a : V \to V$ defined by $T_a(f)(x) := f(x-a)$ is unitary.

4) (Quantum harmonic oscillator)
Consider the operator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{d\xi^2} + \frac{1}{2}m\omega^2\xi^2 \ , \tag{4}$$

associated to the quantum harmonic oscillator, where $\xi \in \mathbb{R}$. We would like to solve the eigenvalue problem $H\Psi = E\Psi$.

(a) Introduce the new coordinate $x = \sqrt{\frac{m\omega}{\hbar}}\xi$ and $\epsilon = \frac{E}{\hbar\omega}$ and show that the equation $H\Psi = E\Psi$ can be re-written as

$$\mathcal{H}\psi = \epsilon\psi \ , \qquad \mathcal{H} = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right) \ . \tag{5}$$

Comment on the practical and physical significance of this re-writing.

(b) Write $\psi(x) = y(x)e^{-x^2/2}$. Show that ψ satisfies the differential equation (5) iff y satisfies the Hermite differential equation $y'' - 2xy' + (2\epsilon - 1)y = 0$.

(c) Show that the solutions to equation (5) in $L^2(\mathbb{R})$ are given by the hermite functions $h_n(x) = H_n(x)e^{-x^2/2}/A_n$ with $\epsilon = n + \frac{1}{2}$. (Here, $A_n = \pi^{1/4}2^{n/2}\sqrt{n!}$ is a normalisation factor such that $\| h_n \| = 1$.)

(d) Define the operators $a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right)$, $a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$ and $N = a^\dagger a$ and show that $\mathcal{H} = N + \frac{1}{2}$.

(e) Define $|n\rangle := |h_n\rangle$ and show that $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, $a|n\rangle = \sqrt{n}|n-1\rangle$ and $N|n\rangle = n|n\rangle$. (Hint: Use the relations for Hermite polynomials from question 2(b).) Hence, verify that $\mathcal{H}|n\rangle = \left(n + \frac{1}{2}\right)|n\rangle$.

5) (Sturm-Liouville operators)

(a) Show that every second order differential operator

$$T = \alpha_2(x)\frac{d^2}{dx^2} + \alpha_1(x)\frac{d}{dx} + \alpha_0(x) \quad (6)$$

where $\alpha_2(x) \neq 0$ can be written in Sturm-Liouville form.

(b) Write the Legendre, Laguerre and Hermite differential equations as a Sturm-Liouville eigenvalue problem, $T_{\rm SL}y = \lambda y$, and find the explicit form of $T_{\rm SL}$ in each case.

(c) For the cases in part (b), explain what the relevant inner product vector spaces are and show that the Sturm-Liouville operators $T_{\rm SL}$ are hermitian.

6) (Bessel functions)
The Bessel differential equation is given by

$$x^2y'' + xy' + (x^2 - \nu^2)y = 0\ . \quad (7)$$

(a) Solve this equation with a power series Ansatz of the form $y(x) = \sum_{k=0}^{\infty} a_k x^{k+\alpha}$, where $\alpha = \pm\nu$. Show that all a_k with k odd must vanish and find a recursion relation for the a_k with k even.

(b) Solve the recursion relation to find a formula for a_{2k} in terms of a_0 and write down the complete series solutions $J_{\pm\nu}$ for $\alpha = \pm\nu$, choosing $a_0 = (2^\alpha\Gamma(\alpha+1))^{-1}$.

(c) Show that $J_{1/2}(x) = \sqrt{\frac{2}{\pi x}}\sin x$ and $J_{-1/2}(x) = \sqrt{\frac{2}{\pi x}}\cos x$.

Additional computational problems

Computational methods, both numerical and symbolic, are of increasing importance in physics and symbolic computational tools have become significantly more powerful over the past decade or so. This is changing the way physicists work. Much as the introduction of the pocket calculator some 50 years ago has made by-hand numerical calculations unnecessary, modern systems such as Mathematica, can now take over standard symbolic calculations, such as algebraic manipulations or integration. This facilitates powerful checks of by-hand calculations but also allows for calculations which are virtually intractable with a pen-and-paper approach. The following problems present an opportunity to practice some of these methods in the context of topics from the Mathematical Methods course. They are supplementary and voluntary but strongly recommended and hopefully a fun way to engage with symbolic computations early on. The problems are meant for realisation in Mathematica which can be downloaded from the university server. Mathematica is easy to use, has good built-in documentation and many high-level mathematical functions - you can start to experiment immediately.

C1) (Hermite polynomials)

(a) For the first few Hermite polynomials, check the Rodriguez formula, the differential equation and orthogonality. Expand the function $f : \mathbb{R} \to \mathbb{R}$ given by $f(x) = x^2/(1+x^2)$ (truncate at finite order) and compare the truncated series and the function f by plotting.

(b) Compute the (first few) Hermite polynomials from their generating function.

(c) Find the matrix which describes the Hamilton operator H of the harmonic oscillator, relative to an ortho-normal basis of eigenfunctions of H (focusing on the first few smallest eigenvalues). Introduce a new Hamilton operator $H_1 = H + \epsilon x^4$ for an anharmonic oscillator and find the matrix which describes H_1 relative to the eigenbasis of H. Analyse how the lowest eigenvalues change as ϵ increases.

C2) (Potentials and gradients)

(a) Define an electrostatic potential V for a set of point charges at specified locations in the x-y plane and compute the associated electric field $\mathbf{E}$. In the x-y plane, visualise V by a contour plot and $\mathbf{E}$ by a vector plot.

(b) Introduce a probe charge q i(also located in the x-y plane) into the system and show how the vector plot for $\mathbf{E}$ for varying locations (x_0, y_0) of the probe charge. (You can use the Manipulate module.)

C3) (Simple spin systems)

(a) Consider a two-dimensional Hilbert space (over the complex numbers) with ortho-normal basis $(|\uparrow\rangle, |\downarrow\rangle)$ which describes a simple two-state spin system. The matrix elements $\mathcal{H}_{ss'} = \langle s|H|s'\rangle$, where $s, s' = \uparrow, \downarrow$, for the Hamilton operator H of the system form a hermitian 2×2 matrix. Write the most general such matrix as $\mathcal{H} = b_0 \mathbb{1}_2 + \sum_{i=1}^{3} b_i \sigma_i$, where b_0 and b_i are real number and σ_i are the Pauli matrices. Find the eigenvalues and eigenvectors of $\mathcal{H}$ and write down the energy eigenstates of H as a linear combination of the basis $(|\uparrow\rangle, |\downarrow\rangle)$.

(b) Write down the general solution $\psi(t)$ to the time-dependent Schrödinger equation, using the results from part (a) and specialise to $b_0 = b_1 = 1$ and $b_2 = b_3 = 0$.

(c) Find the specific solution $\psi(t)$ to the time-dependent Schrödinger equation for which $\psi(0) = |\uparrow\rangle$. For this solution, compute the probabilities $p_\uparrow(t)$ and $p_\downarrow(t)$ of finding the system in the spin up and down states, as a function of time.