Coursework 3

(1) Consider the PDE

$$u_{tt} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) - \frac{4u}{r^2\sin^2\theta} \qquad 0\le r\le 1 \qquad 0\le\theta\le\pi$$

with boundary condition, $u=0$ at $r=1$. Use separation of variables to demonstrate that the solution of the initial-value problem, $u(r,\theta,0)=f(r,\theta)$ and $u_t(r,\theta,0)=0$, can be written as the superposition of normal modes

$$u = \sum_{j=1}^{\infty}\sum_{n=0}^{\infty} c_{nj}\cos(\varpi_{nj}t)F_{nj}(r)G_n(\cos\theta),$$

where you should determine the functions $F_{nj}(r)$ and $G_n(\cos\theta)$, along with the normal-mode frequencies ϖ_{nj}. Provide an expression for the coefficients c_{nj} in terms of integrals over r for the initial condition $f(r,\theta)=F(r)(\cos\theta-\cos 3\theta)$.

(2) The Schrödinger equation and Hermite polynomials: Consider the PDE,

$$i\phi_t = \phi_{xx} - V(x)\phi,$$

where $V(x)$ is a prescribed potential function and $-\infty<x<\infty$; $\phi(x,t)$ is known as the wavefunction. The separation of variables, $\phi = e^{iEt}X(x)$, reduces the PDE to the eigenvalue problem,

$$X'' + (E-V)X = 0,$$

where $X(x)\to 0$ for $x\to\pm\infty$.

(a) For the potential of the simple harmonic oscillator, $V(x)=x^2/4$, introduce the transformation, $X=e^{-x^2/4}y(x)$, to show that the solutions satisfy Hermite's ODE (see below).

(b) By posing the polynomial solution, $y(x)=\sum_{m=0}^{\infty}a_m x^m$, obtain a recurrence relation for the coefficients, a_m, and thence determine for what values of E the series terminates.

(c) Calculate $H_n(x)$ for $n=2, 3, ..., 5$, using the recurrence relation of (b). Verify your results using the recursion relation for the polynomials themselves (given below), and Rodrigues formula (also given below).

(d) By writing Hermite's ODE in standard Sturm-Liouville form, establish that the weight function is indeed $\sigma = e^{-x^2/2}$; what is $p(x)$ and how is E related to the Sturm-Liouville eigenvalue? What kind of boundary conditions are being imposed on the Sturm-Liouville problem for $y(x)$?

(e) Evaluate the integral

$$\int_{-\infty}^{\infty} H_n(x)\frac{d^n}{dx^n}(e^{-x^2/2})dx$$

by repeatedly integrating by parts. Hence verify the integral relation at the bottom of the next page, given Rodrigues formula.

(f) Collect together the previous results to write down a solution for the wavefunction $\phi(x,t)$, when the initial condition is $\phi(x,0)=f(x)$, expressing any coefficients as integrals involving the Hermite polynomials and $f(x)$.

(g) Find the wavefunction for all time for $\phi(x,0)=x^3(x-1)e^{-x^2/4}$ and $\phi(x,0)=e^{-x^2/4+x}$.

Helpful information:

Bessel's equation is

$$r^2y'' + ry' + (k^2r^2 - m^2)y = 0,$$

and has the solution, $y(r) = J_m(kr)$, which is regular at $r = 0$. The more general ODE,

$$x^2y'' + (1 - 2\alpha)xy' + (\omega^2\beta^2x^{2\beta} + \alpha^2 - \nu^2\beta^2)y = 0,$$

has solutions $y = x^\alpha \mathcal{C}_\nu(\omega x^\beta)$ where $\mathcal{C}_\nu(z)$ is a Bessel function.

Legendre's equation is

$$\frac{d}{dx}\left[(1 - x^2)\frac{dy}{dx}\right] + \lambda y = 0;$$

the solutions that are regular at $x = \pm 1$ are $\lambda = n(n+1)$ and $y = P_n(x)$ (the Legendre polynomial of degree n), with $n = 0, 1, 2, \ldots$ Also, $P_n(1) = 1$ and

$$\int_{-1}^{1} [P_n(x)]^2 dx = \frac{2}{1 + 2n}.$$

A summary of the properties of Hermite polynomials:
Hermite's ODE: $y'' - xy' + \lambda y = 0$
Weight function: $\sigma(x) = e^{-x^2/2}$
Interval: $-\infty < x < \infty$
Regular solutions: $y(x) = H_n(x)$ and $\lambda = n$
Normalization: The leading coefficient of the polynomial is unity. i.e. $H_n(x) = x^n + \ldots$, so $H_0(x) = 1$ and $H_1(x) = x$, etc.
Recurrence relation: $H_{n+1} - xH_n + nH_{n-1} = 0$
Rodrigues formula:

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

Integral relation:

$$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2/2} dx = n!\sqrt{2\pi}.$$

A warm-up problem

Consider the PDE

$$u_t = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right), \qquad 0 \le r \le 1 \qquad 0 \le \theta \le \pi$$

with boundary condition, $u_r(1,\theta,t) = 0$. Use separation of variables to demonstrate that the solution of the initial-value problem, $u(r,\theta,0) = g(r,\theta)$, can be written as the superposition,

$$u = \sum_j \sum_n c_{nj} T_{nj}(t) F_j(r) G_n(\cos\theta),$$

where you should determine the functions $T_{nj}(t)$, $F_j(r)$ and $G_n(\cos\theta)$. Be careful to include all possible choices for these functions, including the constant solution if that is acceptable.

Provide an expression for the coefficients c_{nj} in terms of integrals over the initial condition $g(r,\theta)$. Make this expression as explicit as you can by using the helpful information given below and proving that

$$\frac{1}{2}[J_1^2(k) + J_0^2(k)] = \int_0^1 rJ_0^2(kr)dr, \qquad k\int_0^1 rJ_0(kr)dr = J_1(k),$$

$$\int_{-1}^1 P_0(x)dx = 2 \qquad \text{and} \qquad \int_{-1}^1 P_n(x)dx = 0 \quad \text{if } n > 0.$$

Hence, establish that the solution will in general converge to a constant for large times, unless

$$\int_0^\pi g(r,\theta)\sin\theta \, d\theta = 0,$$

in which case the solution decays exponentially with time.

Let $u = T(t)R(r)Y(x)$ with $x = \cos\theta$. Then

$$T' + \Lambda T = 0, \qquad r^2R'' + rR' + k^2r^2R = 0, \qquad \frac{d}{dx}\left[(1-x^2)\frac{dY}{dx}\right] + \lambda Y = 0,$$

with $\Lambda = k^2 + \lambda$. Thus, demanding regularity at $r = 0$ and $x = \pm 1$, we find that $T(t)$, $R(r)$ and $Y(x)$ are given by $e^{-\Lambda t}$, $J_0(kr)$ and $P_n(x)$, respectively, along with $\lambda = n(n+1)$ and $n = 0$, 1, ... The boundary condition at $r = 1$ implies $J_0'(k) = 0$, and so $k = z_j$, the j^{th} zero of $J_0'(z)$, or $J_1(z)$. But the solution with $j = 0$, corresponding to $k = z_0 = 0$ and $R = constant$, is also possible.

We now write a general solution,

$$u = \sum_{n=0}^{\infty}\sum_{j=0}^{\infty} c_{nj} J_0(z_j r) P_n(x) e^{-\Lambda_{nj} t}, \qquad \Lambda_{nj} = n(n+1) + z_j^2.$$

Note that the double sum includes a term with $j = n = 0$ term corresponding to $c_0 = c_{00}$ (because $J_0(z_0 r)P_0(x)e^{-\Lambda_{00}t} = 1$), which we will need to deal further with later.

To simplify the formulae for the coefficients, we may show that $\int_{-1}^1 P_n dx = 0$ if $n \neq 0$, by integrating Legendre's equation in x, and that $\int_{-1}^1 P_0 dx = 2$ since $P_0 = 1$. Also, the integral of one of the relations satisfied by J_0 and J_1 implies that $J_1(k) = k\int_0^1 rJ_0(kr)dr$, which vanishes if k is a zero of J_1.

The initial condition now demands

$$c_{nj} = \frac{2n+1}{[J_0(z_j)]^2}\int_0^1\int_0^\pi g(r,\theta)J_0(z_j r)P_n(\cos\theta) r\sin\theta \, d\theta \, dr,$$

in view of the results derived or provided for $\int_0^1 r[J_0(z_j r)]^2 \, dr$ and $\int_{-1}^1 [P_n(x)]^2 \, dx$. The constant c_0 follows as:

$$c_0 = \int_0^\pi\int_0^1 g(r,\theta)\, r\sin\theta \, dr \, d\theta,$$

again given the relations proven earlier. When this latter integral of the initial condition is finite, $u \to c_0$ for $t \to \infty$. Otherwise, $c_0 = 0$, leaving a sum with purely exponentially decaying terms.

Solutions

1. (11 points) Let $u = T(t)R(r)Y(x)$ with $x = \cos\theta$. Then

$$T'' + \omega^2 T = 0, \qquad r^2 R'' + 2rR' + \omega^2 r^2 R - n(n+1)R = 0, \qquad \frac{d}{dx}\left[(1-x^2)\frac{dY}{dx}\right] + n(n+1)Y - \frac{4Y}{1-x^2} = 0,$$

Thus, given $u(r,\theta,0) = 0$ and demanding regularity at $r = 0$ and $x = \pm 1$, we find that $T(t)$, $R(r)$ and $Y(x)$ are given by $\sin\omega t$, $r^{-1/2}J_\nu(\omega r)$ and $P_n^2(x)$, respectively, along with $\nu^2 = \frac{1}{4} + n(n+1)$ and $n = 2, 3, \ldots$ *(5 points)*. The boundary condition at $r = 1$ implies $J_\nu(\omega) = 0$, and so $\omega = z_{nj}$, the j^{th} zero of $J_\nu(z)$ *(1 point)*. We now write a general solution,

$$u = r^{-1/2} \sum_{n=2}^{\infty} \sum_{j=1}^{\infty} c_{nj} J_\nu(z_{nj} r) P_n^2(x) \sin(\varpi_{nj} t), \qquad \nu = n + \frac{1}{2}, \qquad \varpi_{nj} = z_{nj}.$$

(1 point). The initial condition now demands

$$c_{nj} = \left(n + \frac{1}{2}\right) \frac{(n-2)!}{(n+2)!} \frac{\int_0^1 \int_0^\pi f(r,\theta) J_\nu(z_{nj} r) P_n^2(\cos\theta)\, r^{3/2} \sin\theta\, d\theta\, dr}{\int_0^1 [J_\nu(z_{nj} r)]^2 r dr},$$

given that the weight function of the Sturm-Liouville problem for $R(r)$ is $\sigma = r^2$. When the $\theta-$dependence is $\cos\theta - \cos 3\theta = 2\sin 2\theta \sin\theta = 4(1-x^2)x = 4P_3^2(x)/15$, the coefficients $c_{nj} = 0$ for $n \neq 3$ and

$$c_{3j} = \frac{4}{15} \frac{\int_0^1 \int_0^\pi F(r) J_\nu(z_{nj} r) r^{3/2}\, dr}{\int_0^1 [J_\nu(z_{nj} r)]^2 r dr},$$

(4 points).

2. (19 points)(a) With the given substitution, we find that y satisfies Hermite's ODE with $\lambda = E - \frac{1}{2}$. *(2 points)*

(b) By posing the power series solution, $y(x) = \sum_m a_m x^m$, and substituting into the ODE, we find the recurrence relation,

$$a_{m+2} = \frac{(m-\lambda)a_m}{(m+2)(m+1)}.$$

Thus $\lambda = n$ gives a polynomial solution provided that we take $a_1 = 0$ if n is even, or $a_0 = 0$ if n is odd. This corresponds to $E = n + \frac{1}{2}$. *(4 points)*

(c) Using the recurrence relation and normalization, we find that

$$H_0 = 1, \quad H_1 = x, \quad H_2 = x^2 - 1, \quad H_3 = x^3 - 3x, \quad H_4 = x^4 - 6x^2 + 3, \quad H_5 = x^5 - 10x^3 + 15x.$$

We find the same results by evaluating the derivatives in Rodrigues formula, or by taking $H_0 = 1$ and $H_1 = x$, and then using the recursion relation, $H_{n+1} = xH_n - nH_{n-1}$. *(5 points)*

(d) The ODE can be rearranged into the standard form of a Sturm-Liouville problem using the integrating factor, $\exp\int(-x)dx = e^{-x^2/2}$. This gives

$$\frac{d}{dx}\left(e^{-x^2/2}\frac{dy}{dx}\right) + \lambda e^{-x^2/2} y = 0.$$

Hence, $p(x) = \sigma(x) = e^{-x^2/2}$ and the Sturm-Liouville eigenvalue is $\lambda = E - \frac{1}{2}$. For $x \to \pm\infty$, $p(x) \to 0$; the boundary conditions are regularity conditions. *(4 points)*

(e) We write

$$\int_{-\infty}^{\infty} H_n \frac{d^n e^{-x^2/2}}{dx^n} dx = (-1)^n \int_{-\infty}^{\infty} e^{-x^2/2} \frac{d^n H_m}{dx^n} dx,$$

after integrating by parts n times. But $d^n H_n/dx^n = n!$, and the remaining integral is evaluated as $\sqrt{2\pi}$. Finally, exploiting Rodrigues formula give the desired integral relation. *(3 points)*

(f) The solution to the PDE can be written as

$$\phi(x,t) = \sum_{n=0}^{\infty} c_n e^{i(n+\frac{1}{2})t - x^2/4} H_n(x)$$

where

$$c_n = \frac{1}{n!\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2/4} dx.$$

(2 points)

(g) Now, $x^3(x-1) \equiv H_4 - H_3 + 6H_2 - 3H_1 + 3H_0$. Hence, the solution for the first case is

$$\phi = \left[H_4(x)e^{9it/2} - H_3(x)e^{7it/2} + 6H_2(x)e^{5it/2} - 3xe^{3it/2} + 3e^{it/2}\right] e^{-x^2/4}$$

(2 points). In the second case, we must use the full expansion formula, in which the coefficients can be evaluated as

$$c_n = \frac{1}{n!\sqrt{2\pi}} \int_{-\infty}^{\infty} H_n(x) e^{-x^2/2} e^x \, dx$$

The integrals can be determined using the Rodrigues formula and integration by parts:

$$c_n = \frac{(-1)^n}{n!\sqrt{2\pi}} \int_{-\infty}^{\infty} e^x \frac{d^n}{dx^n}(e^{-x^2/2}) dx = \frac{1}{n!\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2+x} dx = \frac{1}{n!} e^{1/2}.$$

Hence

$$\phi = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(x) e^{i(n+\frac{1}{2})t - x^2/4 + 1/2}$$

(3 points).