Mathematical Methods MT2011: Problems 4

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(mostly recycled from Fabian Essler's MT2009 problems)

1. *Orthogonality*

In problem set 2 you showed that N orthogonal vectors are automatically linearly independent. Let the functions $\Psi_n(x)$ be orthogonal over the interval $[a, b]$ with respect to the weight function $w(x)$. Show that the functions $\Psi_n(x)$ are linearly indepdendent.

2. *Orthogonal, normalised eigenfunctions*

The real functions $u_n(x)$ ($n = 1$ to ∞) are an orthogonal, normalised set on the interval (a, b) with weight function $w(x) = 1$. The function $f(x)$ is expressed as a linear combination of the $u_n(x)$ via

$$f(x) = \sum_{n=1}^{\infty} a_n u_n(x). \qquad \text{(Q2.1)}$$

Show that

(i)

$$a_n = \int_a^b u_n(x) f(x)\,\mathrm{d}x; \qquad \text{(Q2.2)}$$

(ii)

$$\int_a^b [f(x)]^2\,\mathrm{d}x = \sum_{n=1}^{\infty} a_n^2. \qquad \text{(Q2.3)}$$

[Hint for part (ii): writing out the left-hand side in long-hand notation gives

$$\begin{aligned}&\int_a^b (a_1u_1(x) + a_2u_2(x) + \cdots)(a_1u_1(x) + a_2u_2(x) + \cdots)\,\mathrm{d}x \\ &\qquad = \int_a^b \left[a_1^2[u_1(x)]^2 + a_2^2[u_2(x)]^2 + \cdots + 2a_1a_2u_1(x)u_2(x) + \cdots\right]\,\mathrm{d}x.\end{aligned} \qquad \text{(Q2.4)}$$

Why do the $\int [u_n(x)]^2 \mathrm{d}x$ terms each give 1? Why do the $\int u_n(x)u_m(x)\,\mathrm{d}x$ terms with $n \neq m$ each give 0?]

3. *Eigenvalues and eigenfunctions*

By substituting $x = \mathrm{e}^t$, find the normalized eigenfunctions $y_n(x)$ and the eigenvalues λ_n of the operator $\hat{\mathcal{L}}$ defined by

$$\hat{\mathcal{L}}y = x^2y'' + 2xy' + \frac{1}{4}y, \qquad 1 \le x \le \mathrm{e}, \qquad \text{(Q3.1)}$$

with boundary conditions $y(1) = y(\mathrm{e}) = 0$.

4. *Hermiticity*

Consider the set of functions $\{f(x)\}$ of the real variable x defined on the interval $-\infty < x < \infty$ that go to zero faster than $1/x$ for $x \to \pm\infty$, i.e.,

$$\lim_{x\to\pm\infty} x f(x) = 0. \tag{Q4.1}$$

For unit weight function, determine which of the following linear operators is Hermitian when acting upon $\{f(x)\}$: (a) $\frac{\mathrm{d}}{\mathrm{d}x} + x$ (b) $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} + x^2$ (c) $\mathrm{i}x\frac{\mathrm{d}}{\mathrm{d}x}$ (d) $\mathrm{i}x\frac{\mathrm{d}^3}{\mathrm{d}x^3}$.

5. *More Hermiticity*

Recall that an operator A is Hermitian if $\langle u|\, A\, |v\rangle = \langle v|\, A\, |u\rangle^\star$, or, equivalently,

$$\int_a^b u^\star(x)\,[Av(x)]\; w(x)\mathrm{d}x = \left[\int_a^b v^\star(x)\,[Au(x)]\; w(x)\mathrm{d}x\right]^\star = \int_a^b [Au(x)]^\star\, v(x)\, w(x)\mathrm{d}x. \tag{Q5.1}$$

The dual $A^\dagger$ of the operator A is defined such that $\langle u|\, A^\dagger\, |v\rangle = \langle v|\, A\, |u\rangle^\star$, or, equivalently

$$\int_a^b u^\star(x)\left[A^\dagger v(x)\right]\; w(x)\mathrm{d}x = \int_a^b [Au(x)]^\star\, v(x)\, w(x)\mathrm{d}x. \tag{Q5.2}$$

(a) Let A be a non-Hermitian operator. Show that $A + A^\dagger$ and $\mathrm{i}(A - A^\dagger)$ are Hermitian operators.
(b) Using the preceding result, show that every non-Hermitian operator may be written as a linear combination of two Hermitian operators.

6. *Sturm–Liouville Problem*

The equation

$$\hat{\mathcal{L}}y(x) = \lambda y(x) \tag{Q6.1}$$

is a Sturm–Liouville equation for the operator

$$\hat{\mathcal{L}} = \frac{1}{w(x)}\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)\right], \tag{Q6.2}$$

where $p(x)$, $q(x)$ and $w(x)$ are real functions with $w(x) > 0$. Any two real solutions $y_n(x)$, $y_m(x)$ with distinct eigenvalues λ_n, λ_m satisfy the boundary condition

$$\left[y_m p\frac{\mathrm{d}y_n}{\mathrm{d}x}\right]\Bigg|_{x=a} = \left[y_m p\frac{\mathrm{d}y_n}{\mathrm{d}x}\right]\Bigg|_{x=b}. \tag{Q6.3}$$

Without assuming any results proved in lectures, show by direct integration that

$$\int_a^b y_n(x)y_m(x)\, w(x)\mathrm{d}x = 0 \tag{Q6.4}$$

when $n \neq m$.

7. Express the differential equation

$$xy'' + (k + 1 - x)y' = \lambda y, \tag{Q7.1}$$

where k is a constant, as a Sturm–Liouville equation. What are the natural limits (a, b) to place on x to satisfy the Sturm–Liouville boundary conditions?

8. *Quantum harmonic oscillator*

Consider the time-independent Schrödinger equation for the quantum harmonic oscillator

$$\begin{aligned} H\psi(x) &= E\psi(x), \\ H &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2. \end{aligned} \tag{Q8.1}$$

(a) Using the substitutions $y = x\sqrt{\frac{m\omega}{\hbar}}$ and $\epsilon = E/\hbar\omega$ reduce the Schrödinger equation to

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2}\Psi(y) + (2\epsilon - y^2)\Psi(y) = 0. \tag{Q8.2}$$

(b) Consider the limit $y \to \infty$ and verify that in this limit

$$\Psi(y) \to Ay^k \mathrm{e}^{-y^2/2}. \tag{Q8.3}$$

Hint: you can neglect ϵ compared to y^2 in this limit.

(c) Separate off the exponential factor and define

$$\Psi(y) = u(y)\mathrm{e}^{-y^2/2}. \tag{Q8.4}$$

Show that $u(y)$ fulfils the ODE

$$u'' - 2yu' + (2\epsilon - 1)u = 0. \tag{Q8.5}$$

(d) Show that this differential equation can be converted to Sturm–Liouville form by multiplying both sides of the equation by e^{-y^2}. What is the weight function $w(y)$ of the Sturm–Liouville problem?

(e) Solve (Q8.5) by the ansatz

$$u(y) = \sum_{n=0}^{\infty} a_n y^n \tag{Q8.6}$$

by deriving a recurrence relation for the coefficients a_n. You should get

$$a_{n+2} = a_n \frac{(2n + 1 - 2\epsilon)}{(n + 2)(n + 1)}. \tag{Q8.7}$$

(f) We know from (b) that for $y \to \infty$ the function $u(y)$ must go to Ay^k. This means that the recurrence relation must *terminate*, i.e., we must have $a_n = 0$. This quantizes the allowed values of $\epsilon = E/\hbar\omega$:

$$\epsilon_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \ldots. \tag{Q8.8}$$

Find the polynomial solutions $H_n(x)$ corresponding to these values of ϵ for $n = 0$, 1, 2, 3. These polynomials are called *Hermite polynomials*.

(g) Show that your results for $n = 0$, 1, 2, 3 agree with *Rodrigues' formula*

$$H_n(x) = (-1)^n \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n}\mathrm{e}^{-x^2}. \tag{Q8.9}$$

(h) Show that the H_n can be normalized such that

$$\int_{-\infty}^{\infty} \mathrm{d}y\, \mathrm{e}^{-y^2} H_n(y) H_l(y) = \delta_{nl}\sqrt{\pi}2^n n!. \tag{Q8.10}$$

9. *Generating function*

Hermite polynomials can be *defined* by the generating function

$$G(x,t) = \mathrm{e}^{x^2}\mathrm{e}^{-(t-x)^2} = \mathrm{e}^{2tx-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}. \tag{Q9.1}$$

(a) Find $H_0(x)$, $H_1(x)$, $H_2(x)$ by expanding this generating function as a power law in t.
(b) By differentiating $G(x,t)$ with respect to t, show that

$$2(x-t)\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n(x)n\frac{t^{n-1}}{n!} \tag{Q9.2}$$

and hence that the $H_n(x)$ satisfy the recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x). \tag{Q9.3}$$

(c) By differentiating $G(x,t)$ with respect to x, show that

$$H_n'(x) = 2nH_{n-1}(x). \tag{Q9.4}$$

(d) Using the results from (b) and (c), show that the H_n defined in this way satisfy Hermite's differential equation

$$H_n'' - 2xH_n' + 2nH_n = 0. \tag{Q9.5}$$

10. *Legendre polynomials*

Position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are such that $r_2 \gg r_1$, where $r_1 = |\mathbf{r}_1|$ and $r_2 = |\mathbf{r}_2|$. Show that

$$\frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|} = \frac{1}{r_2}\left\{1 + \left(\frac{r_1}{r_2}\right)P_1(\cos\theta_{12}) + \left(\frac{r_1}{r_2}\right)^2 P_2(\cos\theta_{12}) + \cdots\right\}, \tag{Q10.1}$$

where θ_{12} is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$, and $P_1(\cos\theta) = \cos\theta$, $P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$.

An electric quadrupole is formed by charges Q and coordinates $(0, \pm a, 0)$ and charges $-Q$ at coordinates $(\pm a, 0, 0)$. Show that the potential V in the (x, y) plane at a distance r large compared to a is approximately

$$V = \frac{-3Qa^2\cos 2\theta}{4\pi\epsilon_0 r^3}, \tag{Q10.2}$$

where θ is the angle between $\mathbf{r}$ and the x-axis.

Derive an expression for the couple exerted on the quadrupole by a positive point charge Q at a position $\mathbf{r}$ in the (x, y) plane, where $r \gg a$.

Deduce the angles θ for which this couple is zero. If the charges of the quadrupole are rigidly connected and free to rotate about the z-axis, determine whether the equilibrium is stable or unstable in each case.