Mathematical Methods MT2017: Problems 4

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1. Orthogonality

Suppose that the functions $\Psi_0(x)$, $\Psi_1(x)$, $\Psi_2(x)$, ... are orthogonal over the interval [a, b] with respect to the weight function w(x). Show that the $\Psi_n(x)$ are linearly independent.

2. Orthogonal, normalised eigenfunctions

The real functions $u_n(x)$ $(n = 1 \text{ to } \infty)$ 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

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

Show that

(i)

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

(ii)

$$\int_{a}^{b} [f(x)]^{2} dx = \sum_{n=1}^{\infty} a_{n}^{2}.$$
 (Q2.3)

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

$$\int_{a}^{b} (a_{1}u_{1}(x) + a_{2}u_{2}(x) + \cdots)(a_{1}u_{1}(x) + a_{2}u_{2}(x) + \cdots) dx$$

$$= \int_{a}^{b} [a_{1}^{2}[u_{1}(x)]^{2} + a_{2}^{2}[u_{2}(x)]^{2} + \cdots + 2a_{1}a_{2}u_{1}(x)u_{2}(x) + \cdots] dx.$$
(Q2.4)

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

3. Eigenvalues and eigenfunctions

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

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

with boundary conditions y(1) = y(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) $\frac{d}{dx} + x$ (b) $-i\frac{d}{dx} + x^2$ (c) $ix\frac{d}{dx}$ (d) $i\frac{d^3}{dx^3}$.

5. More Hermiticity

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

$$\int_{a}^{b} u^{\star}(x) \left[Av(x)\right] w(x) dx = \left[\int_{a}^{b} v^{\star}(x) \left[Au(x)\right] w(x) dx\right]^{\star} = \int_{a}^{b} \left[Au(x)\right]^{\star} v(x) w(x) dx.$$
(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

$$\int_{a}^{b} u^{\star}(x) \left[A^{\dagger} v(x) \right] w(x) dx = \int_{a}^{b} \left[A u(x) \right]^{\star} v(x) w(x) dx.$$
(Q5.2)

- (a) Let A be a non-Hermitian operator. Show that $A + A^{\dagger}$ and $i(A A^{\dagger})$ 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

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

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

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

Without assuming any results proved in lectures, show directly from equations (Q6.1) to (Q6.3) that

$$\int_{a}^{b} y_{n}(x)y_{m}(x)w(x)dx = 0$$
 (Q6.4)

when $n \neq m$.

7. Express the differential equation

$$xy'' + (k+1-x)y' = \lambda y,$$
 (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

$$H\psi(x) = E\psi(x), H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2.$$
(Q8.1)

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

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

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

Show that u(y) fulfils the ODE

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

- (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

$$a_{n+2} = a_n \frac{(2n+1-2\epsilon)}{(n+2)(n+1)}.$$
(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 $\epsilon = E/\hbar\omega$:

$$\epsilon_n = n + \frac{1}{2}, \quad n = 0, 1, 2, \dots$$
 (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*

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

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

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

9. Generating function

Hermite polynomials can be *defined* by the generating function

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

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

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

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

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

$$H'_{n}(x) = 2nH_{n-1}(x). (Q9.4)$$

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

$$H_n'' - 2xH_n' + 2nH_n = 0. (Q9.5)$$

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 **r** and the x-axis.

Derive an expression for the couple exerted on the quadrupole by a positive point charge Q at a position **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.