Problem sheet - MT tutorial 3

Self-assessed questions

Q1. Expansion of a function in terms of an orthonormal set

The real functions $u_n(x) (n = 1 \text{ to } \infty)$ are an orthogonal, normalized, set on the interval (a, b). The function $f(x)$ is expressed as a linear combination of the $u_n(x)$'s via

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

Show

(i)

$$a_n = \int_a^b u_n(x) f(x) dx;$$

(ii)

$$\int_a^b [f(x)]^2 dx = \sum_{n=1}^{\infty} a_n^2.$$

[Hint for this part: the left hand side is, when written out in long-hand notation,

$$\int_b^a (a_1u_1(x) + a_2u_2(x) + ...)(a_1u_1(x) + a_2u_2(x) + ...)dx = \int_a^b \{a_1^2[u_1(x)]^2 + a_2^2[u_2(x)]^2 + ...$$

$$+2a_1a_2u_1(x)u_2(x) + ...\}dx.$$

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?]

[MM Q3.2]

Q2. Operator matrix elements

Let Q be an operator. Under what circumstances is the complex number $\langle a|Q|b\rangle$ equal to the complex number $(\langle b|Q|a\rangle)^*$ for any state $|a\rangle$ and $|b\rangle$?

[JB QM Q1.9]

Q3. Common orthogonal sets of functions

You will need certain integrals repeatedly over the next few weeks. They are given here; make sure that you can do them and then keep this piece of paper handy.

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{a}{2}, & \text{if } n = m; \\ 0, & \text{otherwise.} \end{cases}$$

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) = \begin{cases} \frac{2an}{\pi(n^2-m^2)}, & \text{if } n + m \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases}$$

[JMR QM MT Q3.1]

Q4. Determining when continuous operators are hermitian

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.

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

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

[MM Q3.3]

Q5. Bayes probability

Analyse the following using Bayes' Theorem: Mrs. Trellis (from North Wales) has 2 children, born 3 years apart. One of them is a boy. What is the probability that Mrs. Trellis has a daughter?

[SB PS Q5]

Main questions

Q1. Polarisation identities

Let V be a (complex) inner product vector space with inner product $\langle\cdot,\cdot\rangle$ and associated norm $\|\cdot\|$ defined in the usual way as $\| \mathbf{v} \| = \sqrt{\langle \mathbf{v}, \mathbf{v}\rangle}$.

(a) Show that

$$\langle \mathbf{v}, \mathbf{w}\rangle = \frac{1}{4}\left(\| \mathbf{v}+\mathbf{w} \|^2 - \| \mathbf{v}-\mathbf{w} \|^2 - i\| \mathbf{v}+i\mathbf{w} \|^2 + i\| \mathbf{v}-i\mathbf{w} \|^2\right) , \qquad (1)$$

for all $\mathbf{v}, \mathbf{w} \in V$. (This identity, also called polarisation identity, implies that the scalar product is completely determined by its associated norm.)

(b) Find the polarisation identity if V is a real inner product space.

(c) Let $T : V \to V$ be a linear operator on the complex inner product space V. Show that the following generalisation of the polarisation identity holds:

$$\begin{aligned}\langle \mathbf{v}, T\mathbf{w}\rangle &= \frac{1}{4}\left(\langle \mathbf{v}+\mathbf{w}, T(\mathbf{v}+\mathbf{w})\rangle - \langle \mathbf{v}-\mathbf{w}, T(\mathbf{v}-\mathbf{w})\rangle\right.\\ &\quad \left. -i\langle \mathbf{v}+i\mathbf{w}, T(\mathbf{v}+i\mathbf{w})\rangle + i\langle \mathbf{v}-i\mathbf{w}, T(\mathbf{v}-i\mathbf{w})\rangle\right) . \end{aligned} \qquad (2)$$

(d) Suppose $T : V \to V$ is a linear operator on a complex inner product space V with $\langle \mathbf{v}, T\mathbf{v}\rangle = 0$ for all $\mathbf{v} \in V$. Use the result from part c) to show that $T = 0$.

(e) Show that the linear operator $T : V \to V$ is hermitian if and only if $\langle \mathbf{v}, T\mathbf{v}\rangle \in \mathbb{R}$ for all $\mathbf{v} \in V$. (Hint: Apply the statement of part (d) to $T - T^\dagger$.)

[AL MM Q1.2]

Q2. The normed vector space ℓ^p and the parallelogram identity

(a) Let V be an inner product vector space with inner product $\langle\cdot,\cdot\rangle$ and associated norm $\|\cdot\|$. Show that the associated norm satisfies the parallelogram identity

$$\| \mathbf{v}+\mathbf{w} \|^2 + \| \mathbf{v}-\mathbf{w} \|^2 = 2\left(\| \mathbf{v} \|^2 + \| \mathbf{w} \|^2\right) , \qquad (3)$$

for all $\mathbf{v}, \mathbf{w} \in V$.

(b) Consider the normed vector space ℓ^p of sequences $(x_i)_{i=1}^{\infty}$, where $x_i \in \mathbb{C}$, with $(\sum_{i=1}^{\infty} |x_i|^p)^{1/p}$ finite. Show that, for $1 < p < \infty$, the expression

$$\| (x_i) \| := \left(\sum_{i=1}^{\infty} |x_i|^p\right)^{1/p} \qquad (4)$$

defines a norm on ℓ^p.

(c) For the normed space ℓ^p consider the vectors $\mathbf{v} = (1, 0, 0, \ldots)$ and $\mathbf{w} = (0, 1, 0, 0, \ldots)$ together with the parallelogram identity from part (a) to show that the above norm on ℓ^p is not associated to an inner product for $p \neq 2$.

[AL MM Q1.3]

Q3. Quadratic forms

(i) Show that the quadratic form $4x^2 + 2y^2 + 2z^2 - 2xy + 2yz - 2zx$ can be written as $\vec{x}^T V \vec{x}$ where V is a symmetric matrix. Find the eigenvalues of V. Explain why, by rotating the axes, the quadratic form may be reduced to the simple expression $\lambda x'^2 + \mu y'^2 + \nu z'^2$; what are λ, μ, ν.?

(ii) The components of the current density vector $\vec{j}$ in a conductor are proportional to the components of the applied electric field $\vec{E}$ in simple (isotropic) cases: $\vec{j} = \sigma \vec{E}$. In crystals, however, the relation may be more complicated, though still linear, namely of the form $j_i = \sum_{j=1}^{3} \sigma_{ij} E_j$, where σ_{ij} form the entries in a real symmetric 3×3 matrix, and i runs from 1 to 3.

In a particular case, the quantities σ_{ij} are given (in certain units) by $\begin{pmatrix} 4 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & 2 \end{pmatrix}$.

Explain why by a rotation of the axes, the relation between $\vec{j}$ and $\vec{E}$ can be reduced to $j'_1 = \tilde{\sigma}_1 E'_1, j'_2 = \tilde{\sigma}_2 E'_2, j'_3 = \tilde{\sigma}_3 E'_3$ and find $\tilde{\sigma}_1, \tilde{\sigma}_2$ and $\tilde{\sigma}_3$.

[MM Q2.12]

Q4. Diagonalisation and normal modes

Three particles of masses m, M, m, lying in a straight line in this order, are connected by massless springs of constant k and execute small oscillations along the line of the springs. Let x_i be the displacement of the particle i from its equilibrium position. Show that the equations of motion are

$$\sum_{j=1}^{3} (T_{ij}\ddot{x}_j + V_{ij}x_j) = 0, \quad \text{for } i = 1, 2, 3$$

where the matrices T and V are

$$T = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix} \qquad V = k \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}.$$

By considering solutions of the form $x_i = a_i e^{i\omega t}$ show that the a_i satisfy

$$\begin{pmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0.$$

Hence deduce the allowed values of ω and describe qualitatively the type of motion associated with each allowed value.

If the CO_2 molecule can be considered as linear, with each oxygen atom connected to the carbon atom by a spring with constant 1000Nm^{-1}, calculate the frequencies of the natural vibrations of this molecule. Which mode could be excited by infra-red radiation?

[MM Q2.13]

Q5. Continuous hermitian operators

Recall that an operator $\hat{H}$ is hermitian if

$$\int dx\ v^*(x)\ \hat{H}\ u(x) = \left[\int dx\ u^*(x)\ \hat{H}\ v(x)\right]^* = \int dx\ u(x)\ (\hat{H}\ v(x))^*\ .$$

The action of the hermitian conjugate of an operator A is defined as

$$\int dx\ u^*(x) A^\dagger\ v(x) = \int dx\ (Au(x))^* v(x).$$

(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.

[MM Q3.4]

Q6. Stationary states of a particle in a box

Consider the particle in the infinitely deep square well potential ($V = 0$ for $0 < x < a$, $V = \infty$ for $x \leq 0, x \geq a$).

(i) Show that the allowed energy values are $E_n = \hbar^2 n^2 \pi^2 / 2ma^2$ for $n = 1, 2, \ldots$ and that the associated normalised eigenfunctions are

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{14}$$

Why is there no state with $E = 0$? What does it mean to say that the ϕ_n are orthogonal?

(ii) Show qualitatively by means of a sketch that the eigenfunctions $\phi_1(x)$ and $\phi_2(x)$ are orthogonal.

(iii) For a particle with energy E_1, calculate the quantum-mechanical expectation value of x, denoted by $\langle x \rangle$.

(iv) Without working out any integrals, show that $\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - a^2/4$. Hence find $\langle (x - \langle x \rangle)^2 \rangle$ using the result

$$\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}. \tag{15}$$

(v) A classical analogue of this problem is that of a particle bouncing back and forth between two perfectly elastic walls, with uniform velocity between bounces. Calculate the classical averages values $\langle x \rangle_c$ and $\langle (x - \langle x \rangle_c)^2 \rangle_c$, and show that for high values of n the quantum and classical results tend to each other.

[JMR QM MT Q3.2]

Q7. Dynamics of a particle in a box

Suppose the state is described at time $t = 0$ by the wavefunction

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}} (\phi_1(x) + \phi_2(x))$$

i) Show that ψ is correctly normalized.

ii) Show that this is not an energy eigenfunction. What are the possible results of a measurement of the energy of the particle, what are the corresponding amplitudes, and what are the corresponding probabilities? What do you expect the expectation value of the energy to be?

iii) Repeat (ii) but with the wavefunction

$$\psi'(x, t = 0) = \frac{1}{\sqrt{2}} \left(\phi_1(x) + e^{i\theta}\phi_2(x)\right)$$

iv) Reverting to ψ, explain why at subsequent times the wavefunction is given by

$$\psi(x, t) = \frac{1}{\sqrt{2}} \left(\phi_1(x)e^{-iE_1t/\hbar} + \phi_2(x)e^{-iE_2t/\hbar}\right)$$

Does the outcome of a measurement of the energy of the particle depend on when the measurement is made?

v) Show that

$$|\psi(x, t)|^2 = \frac{1}{a}\left\{\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos\omega t\right\}$$

where $\omega = (E_2 - E_1)/\hbar = 3E_1/\hbar$. Make rough sketches of $|\psi|^2$ for $t = 0$, $t = h/12E_1$, $t = h/6E_1$, $t = h/4E_1$. Does the outcome of a measurement of the position of the particle depend on when the measurement is made?

vi) Given that

$$\int_0^a x \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right) dx = -\frac{8a^2}{9\pi^2},$$

show that a particle with this wavefunction has $\langle x\rangle = a/2$ - $(16a/9\pi^2)\cos\omega t$. Discuss the connection between this result and the sketches of $|\psi|^2$.

vii) What is the value of ω for an electron confined to a distance comparable to the size of an atom (say 10^{-10} m)? What is the wavelength of radiation having this (circular) frequency?

[JMR QM MT Q3.3]

Q8. Determining signal above background [SB PS Q6]

Suppose you are looking for evidence of a rare particle produced following a cosmic ray interaction in your detector. The particle decays in the characteristic exponential fashion with a mean lifetime of τ, and you aim to look for a signal produced by the by-products of this process. However, there is also a constant level of background interactions due to the decays of radioactive isotopes in your detector that can mimic the signal, so you plan to look for an excess of events above this background within a given time period following the cosmic ray event. What is the optimal time window duration to choose so as to maximise the sensitivity of your search?