UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE	:	**PHAS2246**
ASSESSMENT PATTERN	:	**PHAS2246A**
MODULE NAME	:	**Mathematical Methods III**
DATE	:	**20-May-09**
TIME	:	**14:30**
TIME ALLOWED	:	**2 Hours 30 Minutes**

TURN OVER

All questions, including just parts of questions, may be attempted. Credit will be given for all correct work done.

For guidance: A student should aim to answer correctly the equivalent of five questions in the time available.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

1. (a) Define what is meant by a "conservative vector field". If the curl of a field $\underline{F}$ vanishes, then what can one say about the field $\underline{F}$ being conservative or not? [3 marks]

The vector fields $\underline{F}_1(x, y, z)$ and $\underline{F}_2(x, y, z)$ are defined, in Cartesian coordinates, by:

$$\begin{aligned} \underline{F}_1(x,y,z) &= (2xy - z^5)\hat{\underline{e}}_x + x^2\hat{\underline{e}}_y - (5xz^4 + 1)\hat{\underline{e}}_z \,, \\ \underline{F}_2(x,y,z) &= (2xy - z^5)\hat{\underline{e}}_x + x^2\hat{\underline{e}}_y + (5xz^4 + 1)\hat{\underline{e}}_z \,. \end{aligned}$$

Is either of these vector fields conservative? Show which one of these field is conservative. For this field determine (up to an additive constant) the scalar potential from which such a field arises. [6 marks]

(b) Stokes' theorem states that the line integral of a vector field $\underline{G}$ along a closed loop C is equal to the flux of the curl $\underline{\nabla} \times \underline{G}$ through the surface enclosed by C:

$$\oint_C \underline{G} \cdot \mathrm{d}\underline{r} = \int_C (\underline{\nabla} \times \underline{G}) \cdot \mathrm{d}\underline{S} \,,$$

where $\mathrm{d}\underline{S}$ points towards the region of space from where an observer would see the loop integral as anti-clockwise.

Consider the vector field $\underline{G}(x, y, z)$ given, in Cartesian coordinates, by:

$$\underline{G}(x,y,z) = 2y\hat{\underline{e}}_x - 3x\hat{\underline{e}}_y + z^2\hat{\underline{e}}_z \,.$$

Find the curl $\underline{\nabla} \times \underline{G}$. Evaluate the line integral $\oint \underline{G}(x, y, z) \cdot \mathrm{d}\underline{r}$ around the square lying in the xy plane ($z = 0$) and bounded by the lines $x = 3$, $x = 5$, $y = 1$ and $y = 3$, either directly or by applying Stokes' theorem (take the line integral anti-clockwise as seen from the positive z semi-space). [5 marks]

(c) By virtue of the divergence theorem, the outward flux of a vector field $\underline{G}$ through any closed surface S is equal to the volume integral of its divergence $\underline{\nabla} \cdot \underline{G}$ over the volume V enclosed by the surface:

$$\int_S \underline{G} \cdot \mathrm{d}\underline{S} = \int_V \underline{\nabla} \cdot \underline{G} \, \mathrm{d}V \,,$$

where $\mathrm{d}\underline{S}$ points outward from the closed surface.

Consider the scalar field in Cartesian coordinates:

$$H(x,y,z) = x^3 + xy^2 - z \,.$$

Express H in cylindrical polar coordinates ρ, θ and z (where $\rho^2 = x^2 + y^2$ and $\theta = \arctan(y/x)$). Given the expression for the Laplacian in cylindrical polar coordinates

$$\nabla^2 f = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial f}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2},$$

determine $\nabla^2 H(\rho, \theta, z)$.

Either directly or by applying the divergence theorem, evaluate the outgoing flux of the gradient $\underline{\nabla} H$, given by

$$\int \underline{\nabla} H \cdot \mathrm{d}\underline{S},$$

over the total surface of a cylinder of radius R and height h with its base lying on the $z = 0$ plane and centred at the origin. [6 marks]

2. Consider the following second-order linear differential equation

$$x\frac{d^2y}{dx^2} + (2 - x)\frac{dy}{dx} + by = 0, \qquad (1)$$

where b is a constant. By writing equation (1) in the form $y'' + p(x)y' + q(x)y = 0$, or otherwise, determine where this equation is singular. [2 marks]

Solutions of equation (1) can be written in the form:

$$y = \sum_{n=0}^{\infty} a_n x^{n+k}, \qquad a_0 \neq 0.$$

Show that $k = 0$ or $k = -1$. [4 marks]

Derive the recurrence relation

$$a_{n+1} = \frac{n + k - b}{(n + k + 1)(n + k + 2)} a_n.$$ [5 marks]

Demonstrate that the series solutions converge for all values of x. [2 marks]

In the special case of $b = m$, a positive integer, show that the series with $k = 0$ terminates at $n = m$ to yield a polynomial solution. [3 marks]

Obtain this solution for the case of $b = m = 2$ and demonstrate that it satisfies the differential equation (1). [4 marks]

3. If a matrix $\underline{H}$ is described as Hermitian, what property does it have? Prove that the eigenvalues of a Hermitian matrix are real. What property must the associated eigenvectors have? **[7 marks]**

The matrix $\underline{A}$ is given by

$$\underline{A} = \begin{pmatrix} 5 & -5 & 1 \\ -5 & 11 & -5 \\ 1 & -5 & 5 \end{pmatrix} .$$

Is $\underline{A}$ Hermitian? What is its trace? **[2 marks]**

Verify that $\lambda_1 = 16$ is an eigenvalue of $\underline{A}$ and that its associated eigenvector can be written as $\underline{v}_1 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$.

Show that $\lambda_2 = 4$ is also an eigenvalue and obtain the third eigenvalue, λ_3. Find the *normalised* eigenvectors corresponding to eigenvalues λ_2 and λ_3. **[11 marks]**

4. A particle of mass $m = 1$ is moving on a plane. Its position is represented, in Cartesian coordinates, by the two-dimensional vector $\underline{r} =$

The particle is subject to a conservative force field $\underline{F}(\underline{r})$, with potential energy $U(\underline{r})$

$$U(\underline{r}) = \frac{2-\sqrt{2}}{\quad} {}_2 \quad \frac{1-\sqrt{2}}{\quad} {}_2 \quad \frac{1}{\quad}(\qquad)^2$$

Write down the general relation between the force $\underline{F}(\underline{r})$ and the potential energy $U(\underline{r})$ $\underline{F}(\underline{r})$ acting on the particle. **[3 marks]**

Find the work done against the force $\underline{F}(\underline{r})$ when the particle moves from the point $(0, 0$ **[2 marks]**

Write down the particle's equation of motion and show that it can be written as

$$\ddot{\underline{r}} = \underline{A}\,\underline{r}$$

where $\underline{A}$ is the 2×2 real matrix **[4 marks]**

$$\underline{A} = \begin{pmatrix} -2 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix} .$$

Find the eigenvalues and eigenvectors of $\underline{A}$. **[5 marks]**

Use these eigenvalues and eigenvectors to obtain two uncoupled differential equations describing the motion. Solve these equations for the initial conditions $x =$ $y = \frac{dy}{dt} = 0$
y. **[6 marks]**

5. In atomic units the Schrödinger equation for the hydrogen atom can be written as

$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right)\psi = E\psi$$

where, in spherical polar coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,.$$

By writing

$$\psi = R(r)\Theta(\theta)\Phi(\phi)$$

show that $\Phi(\phi)$ must satisfy the equation

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi\,.$$

[4 marks]

What are the solutions of this equation? Explain why m, the constant of separation, must take integer values. [3 marks]

Hence show that $R(r)$ must satisfy the radial equation

$$\frac{1}{2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + Rr + ERr^2 = \lambda R\,,$$

where λ is another constant of separation. Obtain the corresponding equation for $\Theta(\theta)$. [6 marks]

For the special case of $\lambda = 0$, show that the radial equation can be written as

$$\frac{1}{2}\frac{d^2U}{dr^2} + \left[\frac{1}{r} + E\right]U = 0$$

where $U(r) = rR(r)$. Show that for large values of r [3 marks]

$$U(r) = A\exp(\alpha r) + B\exp(-\alpha r)$$

where $\alpha = (-2E)^{\frac{1}{2}}$. How can this solution be simplified for bound states of the hydrogen atom? [4 marks]

6. (a) Any continuous function $f(x)$ in $-1 \le x \le 1$ can be expanded in terms of Legendre polynomials as

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x) \quad \text{for} \quad -1 \le x \le +1 \, .$$

Given the orthogonality relation

$$\int_{-1}^{+1} P_m(x) P_n(x) \, \mathrm{d}x = \delta_{mn} \frac{2}{2n+1} \, ,$$

derive a formula for the coefficients a_n. **[5 marks]**

Given the first two Legendre polynomials

$$P_0(x) = 1 \, , \quad P_1(x) = x \, ,$$

find the first two coefficients a_0 and a_1 of the expansion of the function $\alpha \, \mathrm{e}^{\alpha |x|}$, where α is real. **[5 marks]**

(b) The electrostatic potential of a charge Q located on the z axis at the point $(0, 0, d)$ (in Cartesian coordinates; note that d can be either positive or negative), reads, in spherical polar coordinates:

$$V(r, \theta, \qquad \begin{matrix} Q \\ 4\pi\varepsilon_0 r \end{matrix} \; {}^{\infty}_{l=0} \left(\begin{matrix} d \\ r \end{matrix} \right)^{l}$$

Add now a second charge $-Q$ on the z axis at point $(0, 0, -d)$. Write down an expression for the total potential V_T created by the charges Q and $-Q$ in spherical polar coordinates. **[4 marks]**

Consider a charge q very far from the origin ($d \ll r$). By approximating the total potential V_T due to charges Q and $-Q$ to the first non-zero term of the expansion in Legendre polynomials, and using the expression of the gradient in spherical polars (given below), find the electrostatic force acting on the charge q in this case. **[6 marks]**

The gradient operator in spherical polar coordinates is

$$\underline{\nabla} = \underline{\hat{e}}_r \frac{\partial}{\partial r} + \underline{\hat{e}}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \underline{\hat{e}}_\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi} \, .$$

7. (a) Let $f(x)$ be a function of period π defined by

$$f(x) = \sin(x) \quad \text{for} \quad -\frac{\pi}{2} < x < +\frac{\pi}{2} \, .$$

Is $f(x)$ an even or odd function?

Show that the Fourier expansion of $f(x)$ can be written as

$$f(x) = \sum_{n=1}^{\infty} b_n \sin(2nx)$$

where the coefficients b_n are given by **[4 marks]**

$$b_n = \frac{2}{\pi} \int_{-\pi/2}^{\pi/2} \sin(2nx) \sin(x) \, \mathrm{d}x \, .$$

Determine the coefficients b_n and hence show that **[5 marks]**

$$f(x) = \frac{1}{\pi} \sum_{n=1}^{\infty} (-1)^n \frac{8n}{1-4n^2} \sin(2nx) \, .$$

Parseval's identity for a function $f(x)$ with general period $2L$ reads

$$\frac{1}{2L} \int_{-L}^{+L} [f(x)]^2 \, \mathrm{d}x = (a_0/2)^2 + \frac{1}{2} \sum_{n=1}^{\infty} (a_n^2 + b_n^2) \, .$$

Apply Parseval's identity to prove **[3 marks]**

$$\sum_{n=1}^{\infty} \frac{n^2}{(1-4n^2)^2} = \frac{\pi^2}{64} \, .$$

(b) The function $g(x)$ is defined by

$$\begin{aligned} g(x) &= \sin(x) \quad \text{for} \quad -l < x < +l \, , \\ g(x) &= 0 \quad \text{for} \quad |x| \geq l \, , \end{aligned}$$

where l is real and positive. The Fourier transform $\tilde{g}(k)$ of $g(x)$ is defined as

$$\tilde{g}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-ikx} g(x) \, \mathrm{d}x \, .$$

Give the general way to obtain the original function $g(x)$ from its Fourier transform $\tilde{g}(k)$ (*i.e.*, to obtain the inverse Fourier transform of $\tilde{g}(k)$). **[3 marks]**

Prove that, in the limit $l \longrightarrow +\infty$, one has **[5 marks]**

$$\lim_{l \to \infty} \tilde{g}(k) = i \sqrt{\frac{\pi}{2}} \, [\delta(k+1) - \delta(k-1)] \, ,$$

where δ stands for the Dirac delta function.

END OF PAPER