# UNIVERSITY COLLEGE LONDON

University of London

## EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

*B.Sc.* *M.Sci.*

**Mathematics B6: Mathematical Methods In Chemistry**

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| COURSE CODE | : | **MATHB006** |
| UNIT VALUE | : | **0.50** |
| DATE | : | **09-MAY-05** |
| TIME | : | **14.30** |
| TIME ALLOWED | : | **2 Hours** |

05-C0910-3-30


**TURN OVER**

*All questions may be attempted but only marks obtained on the best* **five** *solutions will count.*
*The use of an electronic calculator is* **not** *permitted in this examination.*

1. If $y = \sum_{n=0}^{\infty} a_n x^n$ is a solution of the differential equation

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

where $b$ is a constant, find the recurrence relation relating $a_{n+2}$ and $a_n$. Write down the first three non-zero terms in each of the linearly independent series solutions of the differential equation.

Show that when $b = m$ ($m$ a positive integer) the differential equation has a polynomial solution. For the cases $m = 0, 1$ and $2$, verify that the resulting polynomial can be written in the form $y = C_m \cos m\theta$, where $x = \cos\theta$ and $C_m$ is a constant.

2. Show that $x = 0$ is a regular singular point of the Bessel equation of order one

$$x^2 y'' + xy' + \left(x^2 - 1\right) y = 0.$$

Assuming a solution of the form

$$y = \sum_{n=0}^{\infty} a_n x^{n+r},$$

show that the roots of the indicial equation differ by an integer. For the larger of these roots show that $a_1 = 0$ and find the recurrence relation satisfied by the coefficients $a_n$. Deduce that $a_{2n+1} = 0$ and

$$a_{2n} = \frac{(-1)^n a_0}{2^{2n}(n+1)!n!}, \quad n \geq 1.$$

Hence write down one series solution of the Bessel equation of order one.

3. (a) Laplace's equation in spherical polar coordinates for the case of axisymmetry is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right)=0.$$

If solutions for $u$ are sought in the separable form $u = T(\theta)R(r)$, show that $T(\theta) = f(\cos\theta)$, where $f(x)$ satisfies Legendre's equation

$$(1-x^2)f'' - 2xf' + kf = 0,$$

where $k$ is a constant.

(b) Let $k = n(n+1)$ where $n$ is a positive integer and let $P_n(x)$ be the corresponding polynomial solution of Legendre's equation. Write down the orthogonality relation for two Legendre polynomials of different order. If

$$Q(x) = a_m x^m + a_{m-1}x^{m-1} + \cdots + a_1 x + a_0,$$

where $m < n$ is a positive integer, show that

$$\int_{-1}^{1} Q(x)P_n(x)dx = 0.$$

Given the relation $nP_n(x) = xP_n'(x) - P_{n-1}'(x)$ show that

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

4. (a) Define a group. Prove that the inverse of each element in a group is unique.

(b) If $\gamma = e^{2\pi i/n}$, where $n$ is a positive integer, show that the numbers

$$1, \gamma, \gamma^2, \cdots, \gamma^{n-1}$$

form a cyclic group of order $n$.

(c) Let I,A,B,C be elements of a cyclic group $G$ of order 4. Write down the group multiplication table. Also write down the group multiplication table for a group of order 4 which is not isomorphic to $G$.

5. (a) Define a unitary matrix $U$. Show that the eigenvalues of a unitary matrix have modulus (i.e. absolute value) equal to 1.

   (b) Show that the set of $n \times n$ unitary matrices with determinant equal to 1 form a group under matrix multiplication. State carefully any properties of matrices you have used.

6. (a) Prove that the determinant of an orthogonal matrix is equal to $\pm 1$.

   (b) Write down the series expression (using summation notation) for $e^A$, where $A$ is an $n \times n$ matrix. If $B$ is also an $n \times n$ matrix, write down, without proof, the condition for the following to hold:

$$e^{A+B} = e^A e^B.$$

   (c) Let $C$ be a real square matrix. If $R = \exp(C - C^T)$ show that $R^T = \exp(C^T - C)$ and that $R$ is an orthogonal matrix.
   If $\lambda_i$ is an eigenvalue of $C - C^T$, show that $e^{\lambda_i}$ is an eigenvalue of $R$. Deduce that $\det(R) = +1$.

7. The motion of two linked particles with displacements $x_1$ and $x_2$ is governed by

$$\ddot{\mathbf{x}} = A\mathbf{x},$$

where $\mathbf{x}$ is a column vector with components $x_1$ and $x_2$ and

$$A = \begin{pmatrix} -5 & 4 \\ 4 & -5 \end{pmatrix}.$$

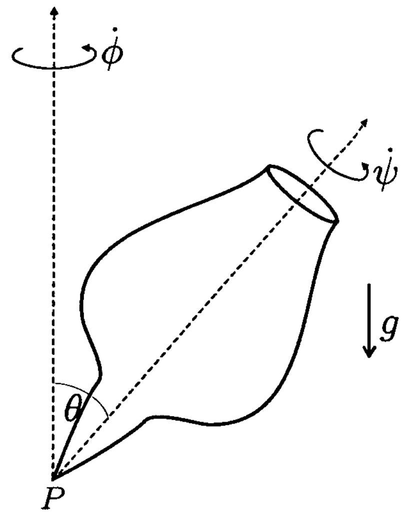
If the system is released from rest with $x_1 = 1$ and $x_2 = 2$ find $\mathbf{x}$ for all time.

By considering the eigenvalues of $A^{2n+1}$, find the general solution of the system of equations given by

$$\ddot{\mathbf{x}} = A^{2n+1}\mathbf{x},$$

where $n$ is a positive integer.

7. (a) Define the Lagrangian and Hamiltonian for a conservative system. Write down Lagrange's equations if the system has $n$ degrees of freedom.




(b) A symmetric top is pivoted at a point $P$ on its axis of symmetry at a distance $a$ from its centre of mass. The generalised coordinates (Euler angles) $\theta$, $\phi$ and $\psi$ are defined as the angle between the vertical and the symmetry axis, the measure of rotation of the symmetry axis about the vertical, and the measure of the rotation of the top about its symmetry axis respectively (see figure).
**You are given** that the total kinetic energy $T$ and potential energy $V$ of the system are

$$T(\phi, \psi, \theta) = \frac{1}{2}A\left(\dot{\phi}^2 \sin^2\theta + \dot{\theta}^2\right) + \frac{1}{2}C\left(\dot{\psi} + \dot{\phi}\cos\theta\right)^2,$$
$$V(\phi, \psi, \theta) = mga\cos\theta,$$

where $A$ and $C$ are known constants (moments of inertia) and a dot indicates a derivative with respect to time.
Use Lagrange's Equations to derive the following conservation laws,

$$\dot{\psi} + \dot{\phi}\cos\theta = N,$$
$$A\dot{\phi}\sin^2\theta + CN\cos\theta = M,$$
$$A\left(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta\right) + 2mga\cos\theta = 2E - CN^2,$$

where $N$, $M$ and $E$ are constants of the motion.
The top, initially spinning with angular velocity $\omega$ ($\dot{\psi} = \omega$) about its symmetry axis, is released from rest with its symmetry axis nearly vertical ($\theta \approx 0$ and $\dot{\phi} = 0$). The top is observed to move in such a way that the lowest position the symmetry axis reaches is the horizontal ($\theta = \pi/2$). Use the three conservation laws above to show that

$$\omega = \frac{\sqrt{2mgaA}}{C}.$$