UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualifications:-

B.Sc. *M.Sci.*

Mathematics B6: Mathematical Methods In Chemistry

COURSE CODE	:	**MATHB006**
UNIT VALUE	:	**0.50**
DATE	:	**28-APR-06**
TIME	:	**14.30**
TIME ALLOWED	:	**2 Hours**

06-C0995-3-40

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. (a) Legendre's differential equation is

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

where α is a constant. By substituting the series $y = \sum_{n=0}^{\infty} a_n x^n$ into Legendre's equation derive the recurrence relation

$$a_{n+2} = \frac{(n-\alpha)(n+\alpha+1)}{(n+1)(n+2)} a_n,$$

for $n \geq 0$. Deduce that there are two linearly independent solutions, one even and one odd, to Legendre's equation (*there is no need to find exact formula for the coefficients in these series*). If $\alpha = m$ is a positive integer, show that one of these series solutions reduces to a polynomial of degree m.

(b) For the special case $\alpha = 1$, show that the general solution can be written as

$$y = c_1 x + c_2 \left[1 - \frac{x}{2}\ln\left(\frac{1+x}{1-x}\right)\right],$$

for $|x| < 1$ and c_1 and c_2 are constants.
[*Hint: You may assume that for* $|x| < 1$, $\ln(1+x) = x - x^2/2 + x^3/3 - \cdots$.]

2. (a) Write down the generating function relation for Legendre polynomials $P_n(x)$. Use the relation to show that $P_n(-x) = (-1)^n P_n(x)$ and $P_n(1) = 1$.

(b) Given that a function $f(x)$ can be expanded for $|x| < 1$ in terms of Legendre polynomials as

$$f(x) = \sum_{n=0}^{\infty} \alpha_n P_n(x),$$

use the Legendre polynomial orthogonality relation

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \begin{cases} 0, & m \neq n \\ \frac{2}{2n+1}, & m = n, \end{cases}$$

to derive an integral formula for the coefficients α_n. Find the first two non-zero terms in the Legendre polynomial expansion of $f(x) = e^x$.

3. Show that $x = 0$ is a regular singular point of the differential equation

$$4xy'' + 2y' - y = 0.$$

Assuming a solution of the form

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

find the indicial roots r. Show for the smaller of the two roots that

$$a_n = \frac{a_0}{(2n)!},$$

and hence find the corresponding series solution. Find also the series solution for the other indicial root. Write the general solution in terms of hyperbolic functions.

4. (a) Define a group. Show that the set of positive rational numbers a/b (a and b being non-zero integers) form a group under multiplication.

   (b) Let I,A,B,C be elements of a group G of order 4 with the property that each element multiplied by itself is the identity. 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. State which of these groups is cyclic, justifying your answer.

5. (a) Define an orthogonal matrix. Show that its determinant is ± 1.

   (b) Let $\mathbf{u}$ be a $n \times 1$ real matrix (i.e. a column vector). Show that the matrix

$$K = I - 2\frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}}$$

   is (i) symmetric and (ii) orthogonal. Show that $\mathbf{u}$ is an eigenvector of K with eigenvalue -1.
   If $\mathbf{u} = \mathbf{x} + |\mathbf{x}|\mathbf{v}$, where $|\mathbf{v}| = 1$, show that $K\mathbf{x} = -|\mathbf{x}|\mathbf{v}$, where $|\mathbf{x}| = \sqrt{\mathbf{x}^T\mathbf{x}}$ is the length of $\mathbf{x}$.

6. (a) State the Cayley-Hamilton theorem and verify it is true for the matrix

$$A = \begin{pmatrix} 3 & 4 \\ 1 & 2 \end{pmatrix}.$$

(b) Define (i) a Hermitian matrix A and (ii) a unitary matrix U. Write $\exp(iA)$ as an infinite series. Prove that $\exp(iA)$ is orthogonal, stating carefully any properties of matrices you have used.

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

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

If the system is released from rest with $x_1 = 3$ and $x_2 = 0$ find $\mathbf{x}$ for all time.

For the system of equations given by

$$\ddot{\mathbf{x}} = A^{-1}\mathbf{x},$$

write down the frequencies of the normal modes of vibration.