NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER II EXAMINATION 2022-2023

MH1804 – MATHEMATICS FOR CHEMISTRY

Apr 2023 TIME ALLOWED: 2 HOURS

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR (4)** questions and comprises **FIVE (5)** pages.

2. Answer **ALL FOUR (4)** questions.

3. Each question is worth **25 marks**.

4. Answer each question beginning on a **FRESH** page of the answer book.

5. This is a closed-book examination.

Question 1

The Fresnel integrals, $S(x)$ and $C(x)$, are widely used in the description of near-field diffraction phenomena, encountered in the X-ray imaging of nanoscale objects. The integrals are defined as

$$S(x) = \int_0^x \sin(t^2)\, dt \tag{1}$$

and

$$C(x) = \int_0^x \cos(t^2)\, dt. \tag{2}$$

In this question, we will evaluate the power series expansions of these Fresnel integrals. Show all your work clearly; calculators are not required to solve this question.

a) Derive the power series expansion for $\sin x$. (8 marks)

b) Substitute $x = t^2$ into your answer from part (a) to obtain the power series expansion for $\sin(t^2)$. (3 marks)

c) Evaluate the integral given in Eq. 1 to obtain the power series expansion for $S(x)$. (6 marks)

d) Using the same approach for $S(x)$ or otherwise, derive the power series expansion for $C(x)$. (8 marks)

Question 2

The ammonia molecule, NH_3, has a trigonal pyramidal molecular shape. Its Cartesian coordinates are given below.

Atom	X / Å	Y / Å	Z / Å
N	0.000000	0.000000	0.096922
H	0.000000	0.969142	–0.226150
H	–0.839302	–0.484571	–0.226150
H	0.839302	–0.484571	–0.226150

a) Calculate the length of the N–H bond. (6 marks)

b) Calculate the H–N–H bond angle. (6 marks)

c) The overall dipole moment of NH_3 is 1.42 D. Calculate the dipole moment of an individual N–H bond. (6 marks)

d) In two-dimensional space, the rotation matrix that transforms the coordinates (x_1, y_1) to (x_2, y_2) is given by

$$\mathbf{R}(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix},$$

where

$$\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \mathbf{R}(\theta) \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}.$$

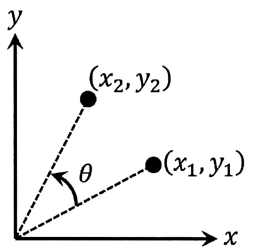

Fig. 1. Transformation of (x_1, y_1) to (x_2, y_2) by rotation about angle θ.

A sketch illustrating the angle θ and the coordinates (x_1, y_1) and (x_2, y_2) is given in Fig. 1. Show that the three H atoms in NH_3 are spaced 120° apart. (7 marks)

Question 3

Given the following kinetic scheme of a diverging reaction between species X, Y and Z:

$$\mathrm{Y} \xleftarrow{k_1} \mathrm{X} \xrightarrow{k_2} \mathrm{Z}$$

The solution of the rate equation can be expressed as

$$\mathbf{p}(t) = \exp(\mathbf{R}t) \times \mathbf{p}(0)$$

where $\mathbf{p}(t)$ is a column vector containing the time dependent concentrations (The top, middle and bottom elements of the vector should represent [X], [Y] and [Z] species respectively). Answer the following questions:

a) Write down the coupled rate equations and the matrix form of the rate equations with matrix **R** describing the rate kinetics of the three species. (3 marks)

b) Deduce the eigenvalues of **R**. (4 marks)

c) **R** can be diagonalized and expressed as $\mathbf{R} = \mathbf{M}\boldsymbol{\Lambda}\mathbf{M}^{-1}$ where $\boldsymbol{\Lambda}$ is the eigenvalue diagonal matrix and **M** is the eigenvector matrix, which has been partially solved for you below.

$$\mathbf{M} = \begin{pmatrix} M_{11} & 0 & 0 \\ M_{21} & 1 & 0 \\ M_{31} & 0 & 1 \end{pmatrix}$$

Determine the values of M_{11}, M_{21} and M_{31}. Determine $\mathbf{M}^{-1}$using the relation

$$\mathbf{M}^{-1} = \frac{1}{|\mathbf{M}|}\,\mathbf{C}^{T}$$

Where **C** is the cofactor matrix of **M**. (12 marks)

d) Derive the matrix $\exp(\mathbf{R}t)$ and write down the expression for [X], [Y] and [Z] in terms of the initial concentrations $[X]_0$, $[Y]_0$ and $[Z]_0$. (6 marks)

Question 4

Answer the following questions given that the Fourier transform (FT) of $f(t)$ is

$$\tilde{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) \exp(-i\omega t)\, dt$$

a) We have here a function

$$f(t) = \begin{cases} A \exp(+\gamma_1 t) & \text{for } t < 0 \\ A \exp(-\gamma_1 t) & \text{for } t \geq 0 \end{cases}.$$

Plot $f(t)$. Deduce and plot $\tilde{g}(\omega)$. (9 marks)

b) Deduce Δf and Δg, the full width half maxima of $f(t)$ and $\tilde{g}(\omega)$ respectively.

Show that $\Delta f \Delta g$ is a constant (8 marks)

c) Using the expression $\tilde{g}(\omega)$ given at the top of the question, prove that the FT of

$f(t)\exp(i\omega_0 t)$ is $\tilde{g}(\omega - \omega_0)$. (5 marks)

d) Use the proof in c) to deduce $\tilde{g}_1(\omega)$, the FT of

$$f_1(t) = \begin{cases} A \exp(+\gamma_1 t + i\omega_0 t) & \text{for } t < 0 \\ A \exp(-\gamma_1 t + i\omega_0 t) & \text{for } t \geq 0 \end{cases}$$

Plot $\tilde{g}_1(\omega)$. (3 marks)

End of Paper

MH1804 MATHEMATICS FOR CHEMISTRY

Please read the following instructions carefully:

1. **Please do not turn over the question paper until you are told to do so. Disciplinary action may be taken against you if you do so.**

2. You are not allowed to leave the examination hall unless accompanied by an invigilator. You may raise your hand if you need to communicate with the invigilator.

3. Please write your Matriculation Number on the front of the answer book.

4. Please indicate clearly in the answer book (at the appropriate place) if you are continuing the answer to a question elsewhere in the book.