

Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year	AY2025-2026
Semester/Trimester/Others (specify approx. Start/End date)	Semester 2
Course Author * Faculty proposing/revising the course	Loh Zhi Heng, Tan Howe Siang
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Course Title	Mathematics for Chemistry
Course Code	CM1804
Academic Units	2
Contact Hours	26
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	MH1802
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This course aims to:

ensure students acquire the mathematical skills and analytical capability to read higher level core physical chemistry courses which cover topics such as quantum chemistry, spectroscopy, kinetics, and thermodynamics

equip students with adequate mathematical reading skills so that they can read and understand related mathematical content in the basic and popular scientific and engineering literature

equip students with mathematical communication skills so that they can effectively and rigorously present their mathematical ideas to mathematicians, scientists and engineers.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	use the appropriate coordinates when solving problems with the corresponding symmetry and perform coordinate transformations
ILO 2	transform functions between Cartesian and polar or spherical coordinate systems
ILO 3	apply change of variables to simplify multiple integrals and partial differential equations
ILO 4	visualize the shapes of atomic orbitals given their mathematical functions
ILO 5	manipulate complex numbers using Euler's formula and de Moivre's theorem to solve related problems
ILO 6	express functions in terms of a power series
ILO 7	apply power series to obtain meaningful approximate solutions to problems in chemistry
ILO 8	perform vector multiplications to solve related problems
ILO 9	apply the concept of basis sets and use it for the expansion of functions
ILO 10	perform transformation of basis vectors
ILO 11	demonstrate understanding of the concepts and properties of matrices through solving problems
ILO 12	perform simple matrix operations
ILO 13	determine eigenvectors and eigenvalues of a given matrix and use them to solve related problems
ILO 14	apply the above-mentioned concepts to solve problems in chemistry (such as rate kinetics, optics, and applied quantum mechanics problems)
ILO 15	recognize the use of Fourier Transforms and be able apply it whenever appropriate
ILO 16	apply FT to understand molecular spectroscopy: Fourier Transform Infrared (FTIR) and Nuclear Magnetic Resonance (NMR) Spectroscopy

Course Content

Cartesian and Spherical Coordinates (CSC)

Polar and spherical coordinates; Change of variables in double and triple integrals; Jacobians.

Complex numbers (CN)

Polar representation of complex number; de Moivre's theorem; Euler's formula.

Summation, Series and Expansion of Functions (SSE)

Maclaurin and Taylor series; Applications to chemical problems.

Vectors (V)

Vector multiplications; Basis Sets; Transformation of basis vectors.

Linear Algebra and Matrices (LAM)

Determinants; Matrix operations; Matrix diagonalization; Eigenvector and eigenvalue; Coupled rate equations; Applications to other selected topics in quantum mechanics and optics.

Fourier Transform (FT)

Fourier Transform Equations; Fourier Transform Infrared Spectroscopy; Free Induction Decay in NMR spectroscopy.

Reading and References (if applicable)

Applying Maths in the Chemical & Biomolecular Sciences. An example based approach, Godfrey Beddard. Oxford University Press, 1st edition (2009), ISBN-13: 978-0199230914.

Mathematical Methods for Physics and Engineering: A Comprehensive Guide, K. F. Riley, M. P. Hobson, S. J. Bence. Cambridge University Press, 3rd edition (2006), ISBN: 0521861535.

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Change of coordinates in integration; Jacobian; Cartesian vs. polar & spherical coordinates	1, 2			
2	Change of variables for two- and three-dimensional integrals	1, 3			
3	Change of variables in partial differential equations; atomic orbitals as solutions to Schrödinger's equation; mathematical expressions for atomic orbitals	1, 3, 4			
4	Mathematical operations with complex numbers; the complex conjugate, different representations of complex numbers; De Moivre's theorem	5			

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
5	Convergence of power series; Maclaurin series; Taylor series	6, 7			
6	Mathematical operations of vectors; scalar and vector products	8			
7	Basis vectors; transformation of basis	9, 10			
8	Matrices	11, 12			
9	Eigenvectors and eigenvalues	13			
10	Applications of matrices in chemistry	14			
11	Fourier transform	15			
12	Fourier transform	15			
13	Applications to Chemistry and Spectroscopy	16			

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Derivation of formulas and demonstrating problem solving (Lecture and Tutorial)	Train students to be independent learners who are able to derive ideas/concepts from first principles and take ownership of their own learning. Help students understand the motivation behind mathematical theorems, definitions and formulas. Develop the train of thought in problem solving and presentation skills in presenting mathematical solutions.
Problem solving (Lecture)	Develop competence in solving chemical problems using mathematical skills.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Class Participation()	All	Competence	5		Individual	Analytic	Multistructural
2	Continuous Assessment (CA): Others(Homework)	All	Competence	11		Individual	Analytic	Multistructural
3	Continuous Assessment (CA): Test/Quiz(Midterm 1)	All	Competence	12		Individual	Analytic	Multistructural
4	Continuous Assessment (CA): Test/Quiz(Midterm 2)	All	Competence	12		Individual	Analytic	Multistructural
5	Summative Assessment (EXAM): Final exam()	All	Competence	60		Individual	Analytic	Relational

Description of Assessment Components (if applicable)

Formative Feedback

[Components 1, 2] Formative feedback will be given through discussion during lectures. Interactive, computer-based hints will also accompany the online homework assignments.

[Component 3, 4] Feedback is also given after each midterm on the common mistakes and level of difficulty of the problems.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Problem Solving	Basic
Critical Thinking	Basic

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

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Policy (Absenteeism)

Absence Due to Medical or Other Reasons

If you are sick and unable to attend your class (particularly the mid-terms), you have to:

Send an email to the instructor regarding the absence and request for a replacement class.

Submit the original Medical Certificate* to administrator.

Attend the assigned replacement class (subject to availability).

*The medical certificate mentioned above should be issued in Singapore by a medical practitioner registered with the Singapore Medical Association.

Policy (Others, if applicable)

Diversity and Inclusion Policy

Integrating a diverse set of experiences is important for a more comprehensive understanding of science. It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences, and that honours your identities; including ethnicity, gender, socioeconomic status, sexual orientation, religion or ability.

To help accomplish this:

- If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety

disorder or social phobia;

- If you feel like your performance in the class is being impacted by your experiences outside of class;
- If something was said in class (by anyone, including the instructor) that made you feel uncomfortable;

Please drop an email to our CCEB-Student Team at CCEB-StudentOffice@ntu.edu.sg about how we can help facilitate your learning experience.

As a participant in course discussions, you should also strive to honour the diversity of your classmates. You can do this by: using preferred pronouns and names; being respectful of others opinions and actively making sure all voices are being heard; and refraining from the use of derogatory or demeaning speech or actions.

All members of the class are expected to adhere to the NTU anti-harassment policy. if you witness something that goes against this or have any other concerns, please speak to your instructors or a faculty member.

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Last Updated By: Natasha Bhatia (Dr)