Basics of higher mathematics for PhD students at the IPC PAS

Tomasz Skóra, Marcin Rubin

Two 90-minute-long classes per week, starting from the second half of October, ending before Christmas

Meeting details will be sent to the registered students; send an e-mail to tskora@ichf.edu.pl *or* mrubin@ichf.edu.pl *by October 11*

The course covers fundamental topics in mathematics (calculus, linear algebra, complex numbers, differential equations, Fourier transform) which are necessary to understand the basic physical chemistry courses. We focus on practical issues and exercises rather than redundant rigor and formalism. Each class is composed of a lecture part, practical part and take-home exercises. **ECTS points: 5**

1: Univariate calculus— concept of a *limit*, concept of a *derivative* and its interpretations (geometric, physical), derivatives of elementary functions, derivative of sum and product;

2: Univariate calculus— derivative of quotient, differentiation *chain rule*;

3: Univariate calculus — *Taylor* and *Maclaurin* series, function maxima, minima and inflection points;

4: Univariate calculus — concept of an *indefinite* and a *definite integral* and their interpretations (geometric, physical), fundamental relation between integral and derivative, integrals of elementary functions, integration *by substitution*;

5: Univariate calculus — integration *by parts*, integration using *partial fraction decomposition,* parity considerations;

6: Differential equations — concept of a differential equation, ways of classifying, boundary conditions, separable cases;

7: Differential equations — linear *homogeneous* and *inhomogeneous* differential equations, characteristic polynomials, integration factors, examples from physics and chemistry;

8: Complex numbers — concept of a *complex number*, *complex plane*, modulus, multiplication and division of complex numbers, complex *conjugates*, trigonometric and exponential form, powers;

9: Linear algebra — *vectors*, *dot* and *cross product*, projection operation, *orthogonality*, *linear independence*, norm, coordinate system, basis transformation;

10: Linear algebra — matrices, matrix addition and multiplication, matrix determinant, matrix inversion;

11: Linear algebra — matrix-vector multiplication, linear systems, *Cramer's rule*, rotation and projection matrices;

12: Linear algebra — *symmetric* and *hermitian* matrices, *orthogonal* and *unitary* transformations, *eigenvalues* and *eigenvectors*, Hilbert spaces;

13: Multivariate calculus — concept of a *partial derivative*, elements of *vector calculus*: *gradient*, *divergence*, *laplacian*;

14: Multivariate calculus — *Taylor* series in several variables, function maxima, minima, saddle points;

15: Multivariate calculus — *exact* and *inexact differentials*, triple product rule, *Maxwell relations*;

16: Multivariate calculus — multiple integrals, order of integration, gaussian integrals, *line integrals* and *path independence*;

17: Multivariate calculus — integrating multiple integrals *by substitution*, *Jacobi*an determinant, *polar* coordinate system, *spherical* coordinate system;

18: Differential equations — *partial differential equations*, separation of variables;

19: *Fourier series*, *Fourier transform*;

20: Questions, additional exercises or topics.

Literature

Donald A. McQuarrie *Mathematical Methods for Scientists & Engineers*
Peter Atkins, Julio de Paula *Atkins' Physical Chemistry*
Ramamurti Shankar *Principles of Quantum Mechanics (Chapter 1: Mathematical Introduction)*