UR / NDSU
Department of Physics and Astronomy
Department of Chemistry and Biochemistry

Instructor:	Braden M. Weight	**Office:**	Braden's Zoom
E-mail:	bweight@ur.rochester.edu		(Zoom ID: 5807617640)
Phone:	701.202.0603	**Off. Hrs:**	By Request

Course Description

Introductory course aimed at the investigation of realistic math and physics problems useful in modern day research with simple computer science skills (Python V3.5+). Throughout this course, the students are expected to acquire skills toward proper and readable code development as well as to accomplish weekly projects ranging from simple tasks to complex simulations of real physics problems that require knowledge of calculus, classical mechanics, quantum mechanics, and others. By the end of the course, students will have hand-developed codes to rigorously solve one-particle quantum mechanics problems (*e.g.*, discrete variable representation) and perform Born-Oppenheimer quantum dynamics simulations (*e.g.* split operator), using skills developed throughout the course, such as the Runge-Kutta propagation scheme and Numerov-Cooley shooting method as well as numerical root-finding (*e.g.*, Newton-Raphson and secant methods) and diagonalization techniques (*e.g.*, Krylov sub-space, Lanczos, etc.).

Key Learning Outcomes

- ❏ Intermediate understanding of the Python3 language
- ❏ Intermediate understanding of introductory one-particle quantum mechanics
- ❏ Intermediate understanding of introductory techniques for solving a variety of problems with root finding, optimization, and eigenvalue techniques
- ❏ Intermediate understanding of generating publication-quality figures

Grading Scheme

There will be no grades for this learning experience.

Hopes of the Instructor

- ☞ Students should demonstrate interest in learning.
- ☞ No work will be officially examined unless requested on a case-by-case basis.
- ☞ The student holds responsibility to ask questions to the instructor.

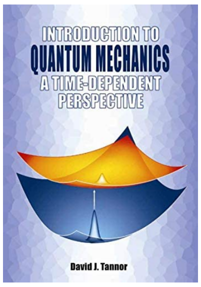
Prerequisites

- ☞ A solid grasp of algebraic manipulation
- ☞ Some introduction to calculus topics (*e.g.*, differentiation and integration)
- ☞ Some introduction to linear algebra (*e.g.*, vector/matrix algebra)

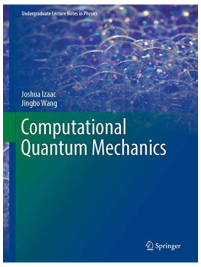
Textbooks and Course Materials

Online Resources: Lecture notes, Python3 example codes, useful websites, and peer-reviewed articles will be provided to students throughout the course.

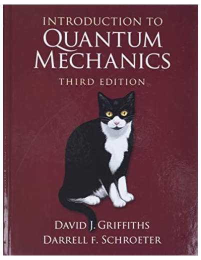
textbook: There is no required textbook for this course. However, the following is a list of textbooks that are strongly recommended for this course, in order of decreasing importance:



Title: Introduction to Quantum Mechanics: A Time-Dependent Perspective
Author: David J. Tannor
Publisher: University Science Books, 2006
ISBN-13: 978-1891389238
Available at: Amazon



Title: Computational Quantum Mechanics (Undergraduate Lecture Notes in Physics)
Author: Joshua Izaac and Jingbo Wang
Publisher: Springer, 2018
ISBN-13: 978-3319999296
Available at: Amazon



Title: Introduction to Quantum Mechanics (Any Edition)
Author: David J. Griffiths and Darrell F. Schroeter
Publisher: Cambridge University Press, 2018
ISBN-13: 978-1107189638
Available at: Amazon

Required Software and Tools

- **Operating system:** Windows OS, Linux/etc. OS, or MAC OS
- **Remote Access to a Cluster:**
  Windows users: WinSCP and a terminal application (e.g., Putty, MobaXTerm, or SolarPutty)
  MAC OS: Need to install some file transfer proxy. Integrated system terminal is good enough.
- **Python3**:
  Suggestion: Miniconda or Anaconda environment with Python V3.5 or higher
  Minimum requirements for environment: Numpy, Scipy, Matplotlib

Course Policies

- **Questions to the instructor are required.**
  Minimum Requirement: One question per session from each student.
- **Student-student correlations and collaborations are encouraged.**
  Without collaboration, the projects may be difficult.
- **Be careful of your time.**
  Less than 3-4 hours per week should be devoted, including lecture/group time.

Tentative Course Content

Chapter	**Topics** & **Homework**
1 (Comp. Sci.)	Course outline discussion, & python environment check. Make a plot of your favorite 1D (Line and Scatter) and 2D (Contour and Heatmap) functions using Numpy and Matplotlib
2 (Comp. Sci.)	**Computer Science !** Code styling (*e.g.*, spaces between operators) and readability (*e.g.*, **COMMENTS** and definitions/functions). Data structures (*e.g.*, integers, floats, strings, booleans, arrays, tuples, dictionaries, and lists). Useful operations (*e.g.*, for-loops, while-loops, breaks, continuations, cases, if-statements). How many ways can we count to 100 and store the data ?
3 (Math)	Numerical integration and differentiation of analytic 1D and 2D functions. Introduction to root-finding algorithms. Plot functions, their integrals, and their derivatives. Find the roots of the functions and their derivatives using the bisection, Newton-Raphson, and secant methods.
4 (Math)	Fourier analysis (e.g., Fourier series and transformations) Examining functions in real and reciprocal spaces. Finding resonant frequencies of complicated functions. Solving differential equations with fourier transforms.
5 (Physics)	Time-propagation. Initial value problems. Euler, Velocity-verlet, and Runge-Kutta propagation schemes. Bouncing ball/gravity Brownian motion and Langevin Dynamics (if time permits)

6 (Math)	Linear algebra (*e.g.* eigenvalue problems, dot products, matrix multiplication, etc.) General tensor manipulation: "numpy.einsum" tool. Note: Entire chapter uses bra-ket $\langle a\|b\rangle$ notation ! If time permits, Krylov and Lanczos diagonalization techniques by hand and with SciPy.
7 (Physics)	The time-independent Schrödinger equation (TISE) in one dimension. Boundary values. Shooting and Numerov-Cooley methods. Direct diagonalization with finite-difference and spectra functions (*e.g.*, discrete value representation). Infinite square well, double square well, harmonic oscillator, and double-well potentials.
8 (Physics)	The time-independent Schrödinger equation (TISE) in higher dimensions. 1D, 2D, and 3D infinite square well and 1D, 2D, and 3D quantum harmonic oscillator
9 (Physics)	The time-dependent Schrödinger equation (TDSE) for a single electronic state (*i.e.*, Born-Oppenheimer dynamics). Wavepackets and initial distributions. Unitary evolution operator, Euler, and split-operator methods. Time-dependence of electronic-only Hilbert spaces. 1D free space/vacuum, 1D infinite square well and 1D quantum harmonic oscillator (Bonus: Crank-Nicholson)
10 (Physics)	Central potentials and the hydrogen atom. Numerov-Cooley and direct diagonalization of the radial equation.
11 (Physics)	Mixed quantum-classical Ehrenfest Dynamics Tully and morse model systems.
12 (Physics)	Class-chosen Topics. Examples: (I) Polaritons, (II) Classical Monte Carlo, (III) Quantum Monte Carlo, ...

NOTE: The above outline may be modified depending on class progress. Open discussion with the instructor is encouraged if the pace of the course is not advantageous to all members of the group.