Exercise Session 1

IESM Fall 2023-2024

Andrej Antalik, Simon Dürr, Sophia Johnson, Andrea Levy

October 2, 2023

- Moodle page

EPFL | MOODLE

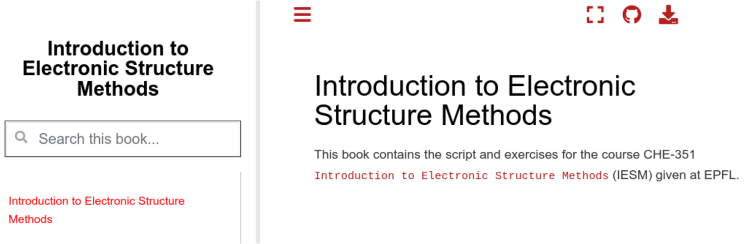
FR | EN

Introduction to electronic structure methods

Dashboard › Courses › Chimie, Génie Chimique (CGC) › CGC - Bachelor › CH-353

Exercise sessions

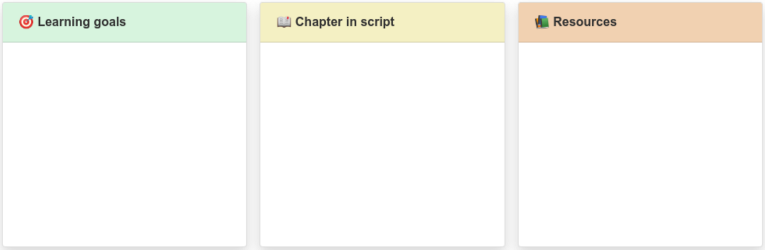
- Exercise website: **https://lcbc-epfl.github.io/iesm-public/**



Exercise structure

Introduction

- Learning goals
- Chapter in script
- Resources



Exercise structure

Theory section

- Relevant theory for the exercise
- Theoretical exercises

Practical exercises

- “Coding” exercises
- Interpretation of results

Exercise evaluation

- Examples:

Exercise 9

Give the commutator of the position and linear momentum operators in the position representation (consider one dimension only).

Bonus Exercise 10

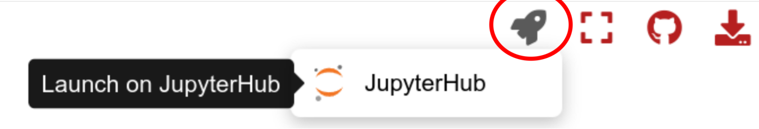
Show that the potential energy operator $\hat{\mathrm{V}}(\mathbf{r})$ is multiplicative when applied to the real-space wavefunction.

```python
# Check Orthogonality
ϕ1ϕ2 = 0 # Replace with vector operation
print(f'<ϕ1|ϕ2> = {ϕ1ϕ2}')
```

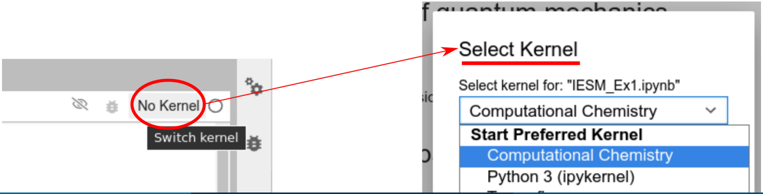
- Exercises contribute to 1/3 of final grade
- Submit report
  - `pdf` document answering the questions completely with relevant results
    - Handwritten portions ok (please verify legibility)
    - You can type responses in the noto notebook and save as a pdf
  - Due date is usually the next exercise session (check Moodle!)
  - Interviews during next exercise session
    - Test your understanding and discuss your doubts/questions
  - Detailed feedback via Moodle after the interview
    - No grade, but comments and detailed corrections

Computer environment

- We will use a virtual environment that you can directly launch from the exercise website
- Click the rocket button on the top right of the code files and choose JupyterHub to launch noto.epfl.ch

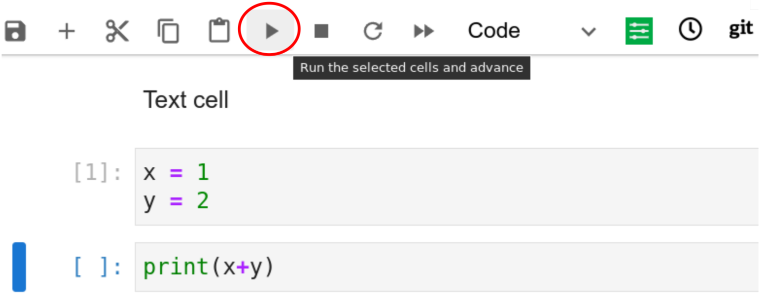


- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the `Computational Chemistry` kernel



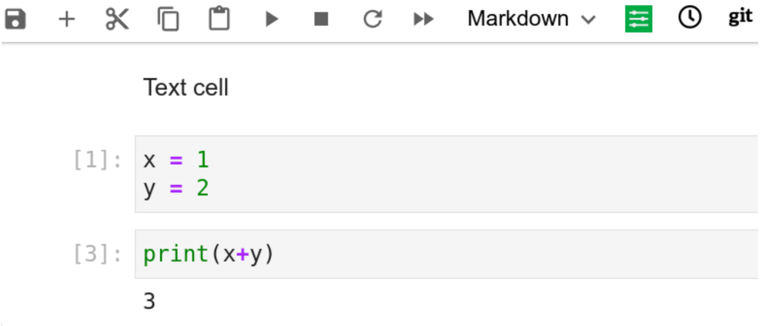
Jupyter notebooks

- `.iynb` files organized in cells
  - Markdown (text)
  - Code
- Run a code cell by pressing `Play` button (or `Ctrl`+`Enter`)

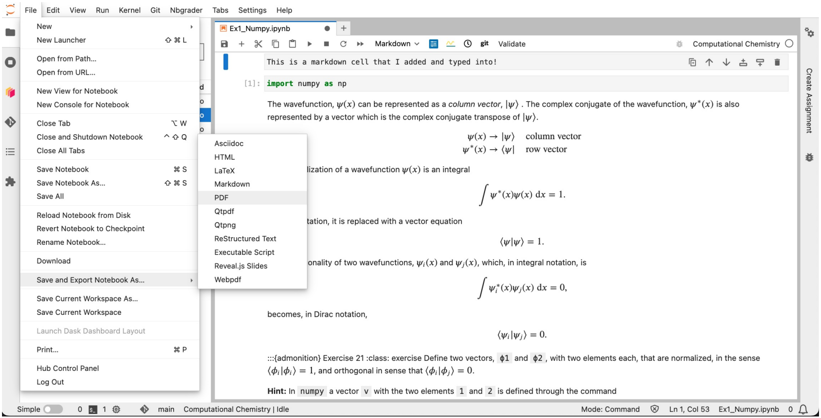


Jupyter notebooks

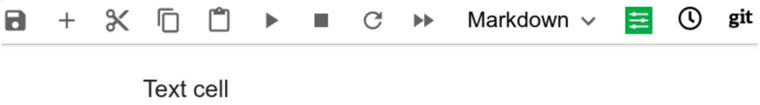
- `.iynb` files organized in cells
  - Markdown (text)
  - Code
- Run a code cell by pressing :arrow_forward: (or `Ctrl`+`Enter`)



Saving Jupyter notebooks as PDFs



- Run a code cell by pressing :arrow_forward: (or `Ctrl+Enter`)



Exercise 1 - Overview

Linear Algebra in Quantum Mechanics - Exercise page

- Linear Algebra in Quantum Mechanics
- Basic Concepts in Quantum Mechanics
- Working with vectors using Numpy

Learning goals

Review basic concept of linear algebra

Review basic notation of quantum mechanics

Chapter in script

Chapter 2 - Basic principles of Quantum Mechanics

Appendix A.1 - Vector space and scalar product

Resources

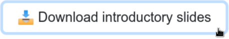
Cohen-Tannoudji, C., Diu, B., & Laloe, F. (1986). Quantum Mechanics, Volume 1.

- Chapter II B - State space, Dirac notation
- Chapter II C - Representations in the state space
- Chapter II D - Eigenvalue equations, observables
- Chapter II E - Two important examples of represantations and observables
- Chapter II Complement D_{II} - A more detailed study of the $\{|r\rangle\}$ and $\{|p\rangle\}$ representations
- Chapter II Complement E_{II} - Some general properties of two observables, Q and P, whose commutator is equal to $i\hbar$

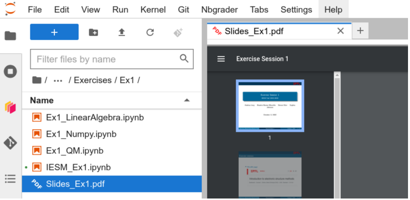
Exercise 1 - Tips

Tips!

- Start from Section 1.3 - Working with vectos using Numpy to get familiar with Noto environment and Jupyter Notebooks
- How to get the slides:
    - Download from the exercise page



    - Once you open Noto, in the exercise folder



    - Will be uploaded on the Moodle page