

# Exercise Session 1

## IESM Fall 2023-2024

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- Moodle page



The screenshot shows the top navigation bar of the EPFL Moodle system. On the left is a red vertical bar with a white right-pointing chevron. To its right is the EPFL logo in red, followed by a vertical line and the word MOODLE in red. On the far right of the bar are the language links FR and EN (with EN highlighted in red), and two small grey icons: a bell and a speech bubble. Below the navigation bar is a light grey horizontal line. Underneath this line is a white rectangular box containing the page title and breadcrumb trail.

> EPFL | MOODLE

FR | EN 🔔 💬

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## 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

 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  $\hat{V}(\mathbf{r})$  is multiplicative when applied to the real-space wavefunction.

```
# Check orthogonality
phi1phi2 = 0 # Replace with vector operation
print(f'<phi1|phi2> = {phi1phi2}')
```

- 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](https://noto.epfl.ch)



- On [noto.epfl.ch](https://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

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



Text cell

```
[1]: x = 1  
     y = 2
```

```
[ ]: print(x+y)
```



# Jupyter notebooks

- .ipynb files organized in cells
  - Markdown (text)
  - Code
- Run a code cell by pressing :arrow\_forward: (or Ctrl+Enter)



Text cell

```
[1]: x = 1  
     y = 2
```

```
[3]: print(x+y)
```

3

# Saving Jupyter notebooks as PDFs



- Run a code cell by pressing :arrow\_forward: (or Ctrl+Enter)



Text cell

# 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 representations and observables
- Chapter II Complement D<sub>II</sub> - A more detailed study of the  $\{|r\rangle\}$  and  $\{|p\rangle\}$  representations
- Chapter II Complement E<sub>II</sub> - 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](#)